# Quantum Mechanics without Observers

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# Contents

"... to skeptics, heretics and naïve realists everywhere.
Keep doubting; let others keep the faith."

David Wick in: *The Infamous Boundary* [1]

"I have never been able to discover any well-founded reasons as to why there exists so high a degree of confidence in the .....current form of quantum theory."

David Bohm in: *Wholeness and the Implicate Order* [2]

"Many physicists pay lip service to the Copenhagen interpretation, and in particular to the notion that quantum mechanics is about observation or results of measurement. But hardly anybody truly believes this any more - and it is hard for me to believe that anyone really ever did."

Sheldon Goldstein in: *Physics Today* [3]

# 1 Synopsis

The present article is aimed at removing most of the obstacles in understanding the quantum mechanics of massive particles. We advance the opinion that the probabilistic character of quantum mechanics does not originate from uncertainties caused by the process of measurement or observation, but rather reflects objectively existing vacuum fluctuations whose action on massive particles is calibrated by Planck's constant and effects an irregular motion of each particle in addition to its Newtonian motion. It appears to be likely that these energy fluctuations are just a manifestation of dark energy. Hence, we fundamentally disagree with the standpoint taken in the so-called Copenhagen interpretation of quantum mechanics as expressed, for example, by Heisenberg. (Two statements illustrating this standpoint are given below.)
As in the theory of diffusion the behavior of a single particle will be described by an ensemble of identically prepared but statistically independent one-particle systems. Energy conservation despite the occurrence of a Brownian-type additional motion is achieved by subdividing the ensemble into two equally large sub-ensembles for each of which one obtains an equation of motion that has the form of a Navier-Stokes- or "anti"-Navier-Stokes-type equation, respectively, the latter involving an anti-Brownian motion enhancing process. By averaging over the total ensemble one obtains a new equation of motion which describes classical motion modified by reversible scattering processes which appear as conservative diffusion. This equation of motion can be converted into the time-dependent Schrödinger equation. Stimulated by de Broglie's particle/wave concept [4] Schrödinger [5] set up this equation invoking certain analogies, but actually he could not derive it from Newtonian mechanics by allowing for an additional mechanism. To-

day the prevailing opinion continues to insist on its non-derivability. We clarify the problem of the uniqueness of the wave function and the quantization of orbital momentum. The concept allows the inclusion of electromagnetic fields and can be extended to interacting N-particle systems. Spontaneous light emission proves to be treatable without requiring electromagnetic field quantization. We analyze the problem of how an experimental setup can consistently be decomposed into the quantum system under study and the residual quantum system "apparatus". The irregular extra motion of the particle under study allows a decomposition of the associated ensemble into two subensembles the members of which perform, respectively, a right-handed or left-handed irregular circular motion about a given axis which becomes physically relevant in the presence of a magnetic field. We demonstrate that this orientation-decomposed "Zitterbewegung" behaves - in accordance with Schrödinger's original idea - as a spin-type angular momentum which appears in addition to a possible orbital angular moment of the particle. We derive the non-relativistic time-dependent Pauli equation and propose a theory of the Stern-Gerlach experiment. The Dirac equation proves to be derivable by drawing on similar arguments used in obtaining the Pauli equation.
Based on the concept of our derivation one is led to conclude that every conceivable situation of a physical system is exhaustively described by the respective solution to the time-dependent Schrödinger equation, and that there can be no independent measurement problem. As for this point we side with J. Bell [6] who argues that the attempt to base the interpretation of quantum mechanics on some notion of "measurement" has raised more problems than it has solved. As we shall outline in Section 25 "measurements" relate outcomes, e. g. detector readings, to characteristic properties of a quantum system by using solutions to the Schrödinger (or Pauli) equation as primordial information. Without this equation and its solutions "measurements", i. e. in general, detector or "pointer" readings, constitute a set of worthless data. This is in keeping with Einstein's view which he stated in a conservation with Heisenberg in 1926 [7]: "From a principal point of view it is completely wrong to build a theory solely on observable quantities. Because in reality it is just the other way around: It is the theory which decides what can be observed." [1]

The fact that our approach yields essentially the entire framework of quantum mechanics proves that a foundation of quantum mechanics without involving observers or "measurers" is possible as opposed to fundamental statements of Heisenberg:
....the idea of an objective real world whose smallest parts exist in the same

[1] "Aber vom prinzipiellen Standpunkt aus ist es ganz falsch, eine Theorie nur auf beobachtbare Größen gründen zu wollen. Denn es ist ja in Wirklichkeit umgekehrt. Die Theorie entscheidet darüber, was man beobachten kann.."

sense as stones and trees exist, independently whether or not we observe them.....is impossible"[8] and
"We can no longer speak of the behavior of the particle independently of the process of observation" [9].

## 2 Origin of quantum mechanical randomness

We interpret the fact that microscopic particles move and behave differently from macroscopic objects as reflecting the active role of the vacuum providing the space for energy fluctuations. The latter will henceforth be referred to as vacuum fluctuations. The consequences of their existence have already been discussed quite some time ago, s. e. g. Bess [10], Puthoff [11], [12], Boyer [13], Calogero [14], Carati and Calgani [15]. From this point of view it appears to be likely that vacuum fluctuations originate in the dark energy frequently discussed by cosmologists in the recent past.
Present day quantum mechanics is strongly shaped by historical contingencies in its development, and it has become almost impossible to tell fiction from facts. Crucial constituents as, for example, the Schrödinger equation fall essentially out of the blue and associating Hermitian operators with "observables" is regarded as "scientific guessing". Statements on "the measurement of positions at different times" and "there is no momentum of a particle in advance of its measurement" are typical of this school of thought (s. e. g. Streater [16]), yet they are definitely void of meaning. What kind of experimental setup should allow a perfectly accurate position measurement at a perfectly accurate time point? And how does the setup look like that allows the measurement of a particle's momentum in the spirit of orthodox quantum mechanics; i. e. with zero dispersion? It is totally impossible to perform non-fictional measurements on quantities that would conform to their quantum mechanical definition, e. g. measuring commuting observables like energy and angular momentum at the same time. The "observables" around which a substantial portion of quantum mechanical literature revolves are in reality non-observables. Further, there is simply no evidence of a causal interrelation between the probabilistic character of quantum mechanics and indeterminacies introduced by "the observer".
By contrast, there is every reason to believe that vacuum fluctuations are real and constitute an objective property of nature. Zero point motion of particles constitutes the most obvious evidence of their existence. It is this zero point motion which, for example, keeps liquid $^4$He "molten" down to the very lowest temperatures and explains this extraordinary material property.
One could view vacuum fluctuations as caused by an exchange of energy between the mechanical system in question and the embedding vacuum that serves as an energy reservoir in terms of virtual particles: if that reservoir

reduces its content of virtual particles, the energy of the system under study increases so that the energy of the entire system comprising this "vacuum reservoir" is conserved. Considerations of Calogero [14] point in a similar direction. In that sense quantum mechanical systems may be viewed as open systems like classical point mass systems in contact with a heat bath. This analogy will become particularly visible in our treatment. We shall use the terms "point mass" and "point charge" with the reservation that the actual size of the particles in question might well be finite of the order $10^{-13}$ cm, but very small compared to atomic diameters of the order $10^{-8}$ cm. Occasionally "point mass" will stand for the center of gravity of an atom or some composite system. Even molecules that contain several hunderts of atoms display well defined interference patterns after diffraction at lattices of standing optical waves [17]

In the following we shall focus on the description of the subsystem "point mass in real-space" which is open to an active vacuum and whose energy is therefore conserved only on average.
An implication of this concept is that charged point masses, despite their irregular motion, do not emit or absorb radiation on the average. In stationary situations a charged point mass will exchange photons with the vacuum in a way that does not change its average energy and momentum.

*Radiation only occurs when the particle's probability density of being at its various positions in space, or the associated current density becomes time-dependent.*

This is analogous to a system kept by non-heat conducting fibers in a vacuum chamber whose walls serve as a heat bath. In a stationary state situation the system exchanges constantly photons with the heat bath without changing its average energy. However, if its temperature is, for example, higher than that of the wall, the system starts radiating, that is, there is now a net flow of photons leaving the system.

If one disregards the details of the energy transfer between the two systems, vacuum fluctuations appear as an irregular temporary departure of the particle in question from its energy conserving trajectory in that it changes its energy by an average amount $\Delta E$ for an average time interval $\Delta t$ so that

$$\Delta E\,\Delta\, t = f\,\hbar \quad \text{where} \quad f \text{ ranges from } \approx \frac{1}{2} \quad \text{to } \approx 2\,. \tag{1}$$

Here $h = 2\,\pi\hbar$ denotes Planck's constant. It is this departure from classical energy conservation which explains, as already alluded to, why a harmonic oscillator in its state of lowest energy is irregularly driven out of the position where it would be classically at rest. Furthermore, it explains the stability of a hydrogen atom in its groundstate (which applies quite generally to all atoms and their compounds), the zero-point motion of atoms in molecules

and solids and the "tunneling" of particles through a potential wall which actually amounts to overcoming that wall.
Zero-point motion is commonly associated with Heisenberg's uncertainty relation which, however, merely shifts the problem of understanding a non-classical phenomenon to understanding the origin of a non-classical relation. Moreover, it amounts to keeping a blind eye on the fact that one is dealing here with a groundstate phenomenon which is certainly not observer-induced. Only if the contrary would apply, one would be justified in referring to the uncertainty relation.
The uncertainty range of the factor $f$ in Eq.(1) might look suspicious. But this uncertainty disappears once the Schrödinger equation has been derived.

A Boltzmann distribution over the energy levels of some system is completely independent of the details and the kind of the energy exchange between the heat bath and the system. The distribution contains -apart from the temperature - only one universal parameter, viz. Boltzmann's constant. Similarly, a system's stationary zero-temperature states that emerge from exchanging energy with the vacuum do not depend on the details of this exchange and on the kind of particles involved, but only depend on another universal constant, viz. Planck's constant.
The envisaged derivation implies that particle trajectories persist under the influence of the stochastic vacuum forces. Their existence becomes particularly obvious with tracks of $\alpha$-particles in a track chamber, but also with the trajectories of electrons in a field electron microscope. Their property of forming straight lines from the field-emission tip (assumed semi-spherical) to the monitoring screen is actually presupposed in calculating the magnification of the microscope. Conversely, purely quantum mechanical behavior occurs at lowest energies when the trajectories do no longer possess a classical reference in the limit $\hbar \to 0$. Trajectories still persist in that case, but the respective particle now performs a purely irregular motion.
The existence of particle trajectories is denied by the Copenhagen school of thought because "things that cannot be observed do not exist". Supporter of this view have to live with the conflict that a complex-valued wavefunction or its associated state vector, which constitutes the center of quantum mechanics, cannot be observed as well. By contrast, we believe that the validity of assumptions can only be scrutinized by checking the consistency of the resulting theory against experimentally accessible quantities and laws. We are here accord with Ballentine who states in his seminal article [18]:

*"...quantum theory is not inconsistent with the supposition that a particle has at any instant both a definite position and a definite momentum, although there is a widespread folklore to the contrary."*

One might compare the properties of this "active vacuum" with a realistic model, viz. superfluid $^4$He which is known to consist of $^4$He-atoms that are

not completely close-packed and move irregularly due to zero-point motion. Hence, if one would inject a particle into the fluid, it would hit various atoms on its way and be scattered off its trajectory along which it would move if the $^4$He-atoms were absent. However, if its average velocity remains below the critical velocity it cannot lose linear momentum to the fluid on average. This defines superfluidity. If one were to place a two-slit diaphragm across the direction of its motion it can, of course, continue its motion only by moving through one of the slits, but its trajectory evolves differently depending on whether or not the other slit is open.
In the Section 3 we analyze some fundamental phenomena which are a direct consequence of vacuum fluctuations, each reflecting a key feature of quantum mechanics.

In Section 4 we briefly discuss the construction of ensemble averages of quantities that appear in the Navier-Stokes equation given in Section 5. We regard this equation as a mathematical object that derives entirely from classical concepts. Details of its derivation, which goes essentially back to Gebelein [19], will be relegated to the Appendix, Section 39. We discuss the construction of a "Brownian" and an "anti-Brownian" sub-ensemble. The motional behavior of the latter is governed by an "anti-Navier-Stokes" equation. We explain why a system of statistically independent particles moves according to the arithmetic mean of these two equations when their motion is governed by classical mechanics plus "conservative" stochastic forces. On forming this arithmetic mean we arrive at an equation that can be converted into the time-dependent Schrödinger equation. We demonstrate that Wallstrom's objection [20] against the legitimacy of this conversion and his arguments in favor of the standard approach to the quantization of orbital momentum are based on a misunderstanding and ignores fundamental considerations of Pauli [21] and Born and Jordan [22] in the early days of "conventional" quantum mechanics. In Section 15 we show how the derivation of the time-dependent Schrödinger equation can be extended to comprise electromagnetic fields. The derivation can be extended further to interacting many-particle systems. A considerable portion of our elaboration is devoted to the phenomenon of particle spin and the associated equations of motion, i. e. the Pauli- and the Dirac-equation.

## 3 Fundamental phenomena of quantum mechanics

As already alluded to above, there are several fundamental phenomena whose existence is directly connected with vacuum fluctuations:

- Stability of atoms
- Zero-point motion of harmonic oscillators
- Heisenberg's uncertainty relation

- Tunneling, e. g. from a pointed metal cathode
- Occurrence of the de Broglie-wavelength
- Spreading width of a particle's trajectory
- Interference at a double-slit diaphragm
- Short-range forces mediated by massive messenger particles

**1. Stability of atoms**

Rutherford's model of the hydrogen atom offered a plausible explanation of his scattering experiments, but it remained unclear why the hydrogen electron does not constantly loose energy by light emission and eventually stops at the atomic nucleus. Bohr's model did not resolve this fundamental problem but rather removed it by postulating the non-radiative stability of electronic orbitals whose angular momenta were integer multiples of Planck's reduced constant $\hbar = \frac{h}{2\pi}$. Schrödinger [5] could later demonstrate that these states of stability correspond to eigenfunctions of his partial differential equation. But again, it remained enigmatic what an electron in the lowest eigenstate (which does not possess angular momentum) prevents from being swallowed by the nucleus or being as close as possible to it. In extending Schrödinger's theory to many-electron atoms, it became clear that the solutions to this $N$-electron equation wouldn't either give a hint of the mechanism behind atomic stability. As this fundamental question of stability is not raised any more in present-day quantum mechanics, there seems to be a tacit agreement that one should no longer look for an answer.
As already indicated, one of the central messages of the present exposition will be that vacuum fluctuations are responsible for the stability of atoms and thus explain also the existence of atomic and condensed matter in the universe. We confine ourselves to the hydrogen atom and give a rough estimate of its linear dimension which results from those fluctuations. The considerations apply similarly to any other atom of the Periodic Table.
We assume that the electron is kicked off its position near the nucleus by receiving $n$ successive and **equal** portions of kinetic energy $\Delta E_{kin}$ so that it moves up the nuclear Coulomb potential in small time-steps $\Delta t_\nu$ toward the atomic periphery. These time-steps are implicitly defined through

$$\Delta E_{kin}\,\Delta t_\nu = \int_{t_\nu}^{t_\nu+\Delta t_\nu} \frac{m_0}{2}\,\dot{r}^2(t)\,dt\;; \quad m_0 = \text{mass of electron}\,.$$

Here $\dot{r}(t)$ denotes the radial velocity of the electron in a spherical coordinate system centered at the atomic nucleus.
We thus have for the total action $\Delta E\,\frac{\Delta t}{2}$ that has been transferred to the

electron within a time interval $\frac{\Delta t}{2}$

$$\Delta E_{kin}\,\tfrac{\Delta t}{2} = \sum_{\nu=1}^{n} \Delta E_{kin}\,\Delta t_\nu = \int_0^{\frac{\Delta t}{2}} \frac{m_0}{2}\,\dot{r}^2(t)\,dt\,.$$

At the end of this time span the electron has used up its last portion of kinetic energy and comes to a stop at a distance $R$ from the nucleus. One could just as well say that the electron possessed during the time intervall $\frac{\Delta t}{2}$ the average kinetic energy

$$\Delta E_{kin} = \tfrac{1}{\frac{\Delta t}{2}} \int_0^{\frac{\Delta t}{2}} \frac{m_0}{2}\,\dot{r}^2(t)\,dt\,. \tag{2}$$

While moving upwards in the nuclear potential this average energy, provided by the vacuum, is finally used up when the electron reaches the distance $R$ from the nucleus. In the ensuing equally large time interval the electron falls back toward the nucleus where it delivers the gained kinetic energy back to the vacuum. Hence, the duration of the full fluctuation process is $\Delta t$.
When the electron comes to a stop at $r = R$, its kinetic energy at a smaller distance $r < R$ from the nucleus is given by

$$\frac{m_0}{2}\,\dot{r}^2 = \frac{e^2}{4\pi\epsilon_0 r} - \frac{e^2}{4\pi\epsilon_0 R} \tag{3}$$

$e$ = elementary charge ; $\epsilon_0$ = permittivity of the vacuum .

This can be rewritten

$$\dot{r} = \frac{1}{\beta}\sqrt{\frac{1}{r} - \frac{1}{R}}$$

or alternatively

$$\frac{dt}{dr} = \beta R^{\frac{1}{2}} \frac{r^{\frac{1}{2}}}{\sqrt{R-r}} \tag{4}$$

where

$$\beta = \frac{1}{e}\sqrt{2\pi m_0\,\epsilon_0}\,. \tag{5}$$

Insertion of Eq.(3) into Eq.(2) yields

$$\Delta E_{kin}\,\tfrac{\Delta t}{2} = \frac{e^2}{4\pi\epsilon_0} \int_0^R \left(\frac{1}{r} - \frac{1}{R}\right) \frac{dt}{dr}\,dr\,.$$

Here the lower integration limit has approximately been equated to $r = 0$. If one now uses Eq.(4) and evaluates the integral one obtains

$$\Delta E_{kin}\,\Delta t = \frac{e^2}{4\pi\epsilon_0}\pi\,\beta\sqrt{R}\,. \tag{6}$$

According to Eq.(1) the left-hand side is equal to $f\hbar$. Hence, inserting this and $\beta$ from Eq.(5) into Eq.(6) and solving for $R$ one obtains

$$R = \frac{\hbar^2}{m_0\, e^2}\, 4\pi\, \epsilon_0 \tag{7}$$

where we have set $f = 2.2$ as one of the $f$-values which are considered admissable. This "stop-value" of $R$ is the Bohr radius which represents quite generally a fundamental length in atomic, molecular and solid state physics.

**2. Zero-point oscillations and localization energy**

The preceding considerations apply similarly to a harmonic oscillator whose potential energy in a spherical coordinate system is given by

$$V(r) = \frac{m_0}{2}\, \omega^2\, r^2$$

where $m_0$ is the oscillating point mass and $\omega$ stands for the angular frequency. One starts again from Eq.(2) and obeserves

$$\frac{m_0}{2}\, \dot{r}^2 = \frac{m_0}{2}\, \omega^2 \left(R^2 - r^2\right)$$

where $R$ denotes the point at which the mass comes to a stop and reverses its motion. All parts of the previous line of thought carry over and one obtains

$$R = \sqrt{\frac{\hbar}{m_0\, \omega}}\,. \tag{8}$$

Here we have set $f = \frac{\pi}{4} = 0.78$ which is at the lower limit of the admissable range. The classical energy of a harmonic oscillator for an oscillation amplitude $R$ is given by

$$\Delta E = \frac{m_0}{2}\, \omega^2 R^2\,.$$

Insertion of $R$ from Eq.(8) yields the well known expression for the zero-point energy

$$\Delta E = \frac{\hbar\omega}{2}\,. \tag{9}$$

The average potential energy is one third of this energy

$$\overline{V} = \frac{m_0}{2}\, \omega^2\, \overline{\Delta r^2} = \frac{1}{3}\frac{\hbar\omega}{2}\,; \qquad \overline{r^2} = \frac{1}{R}\int_0^R r^2\, dr\,. \tag{10}$$

One can define an effective diameter of the oscillator by setting

$$d_0 = \sqrt{3\overline{\Delta r^2}} = \sqrt{\frac{\hbar}{m_0\, \omega}}\,. \tag{11}$$

By employing Eq.(9) this relation can be recast

$$\Delta E = \frac{\hbar^2}{2m_0}\,\frac{1}{d_0^2}\,.$$

This expression is occasionally referred to as "localisation energy". It obviously increases as $d_0$ decreases.
Eq.(11) illustrates an interesting feature of oscillating atoms as constituents of some matter. Consider, for example, liquid Ne: the atoms keep a certain average distance at a given temperature $T$. This distance shrinks as one lowers the temperature, and the atoms form eventually a solid lattice where they end up merely performing a zero-point motion about a (more or less) regular array of rest positions at $T = 0$. However, the latter situation is only possible if the width $d_0$ of their zero-point motion is considerably smaller than the distance between neighboring rest positions. Liquids of all rare gases meet this requirement except for liquid He. Since the atomic mass of He is smallest, the width is largest. It turns out that a stable lattice cannot be formed any more. Liquid He melts in its own zero-point motion so to speak. Nevertheless, it can be solidified by applying pressure which reduces the interatomic distance and thereby narrows the potential well in which the atoms oscillate. The oscillation frequency $\omega$ in this narrower potential well is higher than before, and hence, because of Eq.(11), $d_0$ decreases thereby making a stable lattice now possible.
The existence of zero-point motion of atoms in molecules has first been demonstrated by Mullikan[23] in 1924.
A more spectacular experiment was carried out by Clusius[24] in 1942. He adsorbed light hydrogen molecules on a solid surface where they do not desintegrate and where they are thus bound by a weaker (negative) adsorption potential in which they can perform (almost harmonic) oscillations. The associated zero-point energy $\Delta E$ is by the amount $\frac{\hbar\omega}{2}$ above the lowest point $V_0$ of the adsorption potential. The absolute value of the latter would be the sublimation energy of the hydrogen in the absence of zero-point motion. Due to its presence one measures a smaller amount $|V_0 + \Delta E|$ instead. If one replaces the light hydrogen with heavy hydrogen, the adsorption potential remains unaffected because it is only controlled by the interaction between the hydrogen- and the substrate-electrons. However, because of the greater mass of heavy hydrogen and because of

$$\omega = \sqrt{\frac{\kappa}{m_0}}\,; \qquad \kappa = \text{effective spring constant}$$

$\Delta E$ becomes smaller, and the sublimation energy goes up. Clusius obtained two sublimation energies 184 cal/mol and 274 cal/mol for light and heavy hydrogen, respectively. This large difference is entirely due to the presence of zero-point motion.

### 3. Heisenberg's uncertainty relation

One of the most popular effects caused by vacuum fluctuations is the seeemingly fundamental interconnection between the dispersion $\overline{\Delta x_i^2}$ of a particle's position $\boldsymbol{r} = (x_1, x_2, x_3)$ and the dispersion $\overline{\Delta p_i^2}$ of its linear momentum $\boldsymbol{p} = (p_1, p_2, p_3)$. Again, the harmonic oscillator is particularly well suited to demonstrate this interrelation. We limit ourselves to the one-dimensional case. The mean square displacement $\overline{\Delta x^2}$ which is caused by vacuum fluctuations is linked to the average kinetic energy through

$$\overline{E_{kin}} = \frac{\overline{\Delta p^2}}{2m_0} = \frac{1}{2}\,\frac{\hbar\omega}{2}\,; \qquad \Delta p \stackrel{def}{=} p\,.$$

Solving for $\overline{\Delta p^2}$ one obtains

$$\overline{\Delta p^2} = \frac{\hbar}{2}\, m_0\, \omega\,.$$

From Eq.(10) one gets

$$\overline{\Delta x^2} = \frac{\hbar}{2}\,\frac{1}{m_0\omega}\,.$$

Hence we have

$$\overline{\Delta p^2}\,\overline{\Delta x^2} = \frac{\hbar^2}{4}\,,$$

or cast differently

$$\Delta p\,\Delta x = \frac{\hbar}{2} \tag{12}$$

$$\text{where} \quad \Delta x \stackrel{def}{=} \sqrt{\overline{\Delta x^2}}\,; \quad \Delta p \stackrel{def}{=} \sqrt{\overline{\Delta p^2}}\,.$$

Eq.(12) constitutes a special case of Heisenberg's [25] famous uncertainty relation which he put forward in 1927. Since its inception it has gained the recognition of a corner stone of quantum mechanics in particular in connection with the "process of measurement". It falls essentially out of the blue as many other important items of quantum mechanics, and it seems that the idea it might have it roots in vacuum fluctuations has never dawned on the opinion leaders in this field.

### 4. Tunnelling

To explain another quantum mechanical phenomenon which doesn't have a classical counterpart we refer to the following figure. It depicts a situation where a particle moves parallel to the $x$-axis in the potential of a harmonic oscillator and is, in addition, exposed to an external force field $F(x)$ . The potential associated with the latter is given by $-F\,x$ and appears in the figure superposed with the parabolic potential of the oscillator. The superposition lowers the parabola slightly and shifts the vertex to the right.

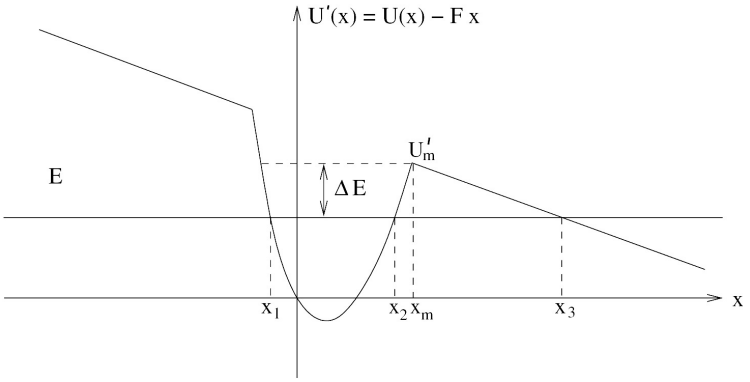


Figure 1: Harmonic oscillator in a uniform electric field

The energy of the particle is indicated by a horizontal line.The points $x_1$ and $x_2$ mark turning points where the particle reverses its classical motion. Classically, the point $x_3$ cannot be reached. However, under the influence of vacuum fluctuations it can overcome the potential barrier at the high point $U'_m$ if its energy is temporarily lifted by the amount $\Delta E = U'_m - E = \hbar/\Delta t$. (Here we have set $f = 1$.) Hence we have:

$$\Delta t = \frac{\hbar}{U'_m - E}\,. \tag{13}$$

Within this time span the particle must finally return to point $x_2$ or reach the point $x_3$ where - in either case - the extra energy must be returned to the vacuum. Only the second option is of interest for the envisaged explanation of the tunnelling phenomenon. The particle's acceleration is right of $x_m$. i. e. within the range of the uniform force field, given by $F/m_0$. Hence, the particle takes $\Delta t'$ seconds to cover the distance $x_3 - x_m$ where $\Delta t'$ results from

$$x_3 - x_m = \frac{F}{2m_0}\,(\Delta t^{'})^2\,. \tag{14}$$

If that time is shorter than the fluctuation time $\Delta t$

$$\Delta t^{'} \leq \Delta t$$

the particle can, nevertheless, reach the region right of $x_3$, and hence one can cast Eq.(14) as

$$x_3 - x_m \leq \frac{F}{2M_0}\,\left(\frac{\hbar}{\Delta E}\right)^2\,, \tag{15}$$

where Eq.(13) has been used. As one notices from Fig.1 the external force can be expressed

$$F = \frac{\Delta E}{x_3 - x_m}\,.$$

If one eliminates $x_3 - x_m$ from Eq.(15) by using this relation one obtains

$$\frac{\sqrt{2m_0}}{F\,\hbar}\,\phi^{3/2} \leq 1\,. \tag{16}$$

The quantity $\phi = U'_m - E$ represents the workfunction, i. e. the minimum energy required to extract an electron from its potential well. Expression (16) combines the various constituents exactly the same way as they appear in the Fowler-Nordheim equation [26] which describes the electron emission from a cold cathode under the influence of an external electric field.
If one inserts $\hbar = 6.5822 \cdot 10^{-16}\,eVs$ and $\phi \approx 5\,eV$ into Eq.(13) one obtains an extremely short tunnelling time of $\approx 10^{-16}s$.
The expression $\sqrt{2m_0}\,\phi^{3/2}/(\hbar\,F)$ becomes equal to unity for an electric field strength $\hat{E} \approx 5 \cdot 10^8\,V\,cm^{-1}$ and for $\phi = 4.6\,eV$ which is the workfunction of tungsten, one of the favorite metals for cathodes. These are the working conditions for "field emission" which stands for electron tunneling from sharply pointed metal tips. In a typical field electron microscope - which attracted much attention about 60 years ago before it was superseded by the field ion microscope - the tungsten tip was etched down to a semisphere with a radius $R$ of about $0.5 \cdot 10^{-5}cm$. Under these conditions the electric field at the tip is given by $V/R$ where $V$ denotes the Voltage between the tip and some anode within the evacuated apparatus. According to Eq.(16) the tip yields field emission when $V \approx 2.5\,kV$, largely in agreement with the experiment.
From our discussion it is obvious that tunnelling actually means overcoming a potential barrier which is only possible with the aid of energy fluctuations. If one adheres to the classical perception of an "inert vacuum" one is forced to assume that the particle can reach the point $x_3$ only when it digs itself a horizontal tunnel from $x_2$ and $x_3$. It is this idea which explains the actually unphysical term "tunnelling".

**5. Occurrence of a "de Broglie-wavelength"**

As we shall see later when our concept of energy fluctuation has been cast into a more precise form, these fluctuations give rise to a **non**-undulatory probability of the particle's appearance in space when it is bound in some potential at lowest energy. This situation is referred to as "groundstate". The first two cases discussed above represent examples of it. By contrast, excited states display an undulatory probability distribution. Conventional quantum mechanics considers this property as a proof of "particle/wave-duality". In our approach, which deals exclusively with point-like particles, the undulatory behavior of their motion emerges naturally from vacuum fluctuations.
In classical mechanics a bound particle is at rest at the point of lowest potential energy. If one allows energy fluctuations $\Delta E$ to occur as a result of which the particle leaves its position of lowest energy, $\Delta E$ can only be

positive. However, if one considers a particle that moves classically already at a velocity $\bar{v}$ and possesses, therefore, a kinetic energy $\frac{m_0}{2}\,\bar{v}^2$ at the outset, it can temporarily transfer this energy to the vacuum. That means that for a duration time $\Delta t$ of this fluctuation the exchanged energy $\Delta E$ is negative. In a subsequent time interval of the same length $\Delta t$ the original energy $\frac{m_0}{2}\,\bar{v}^2$ is not only restored but also increased by $\frac{m_0\,\bar{v}^2}{\pi}$ of fluctuative energy. Here $\pi$ appears in place of 2 after one has averaged over an assumed sinusoidal time-dependence. All quantities that come into play are displayed in Fig.2 where the factor $f$ in Eq.(1) has been set $f = 1$.
The little algebra shown in the figure may be summarized as follows:

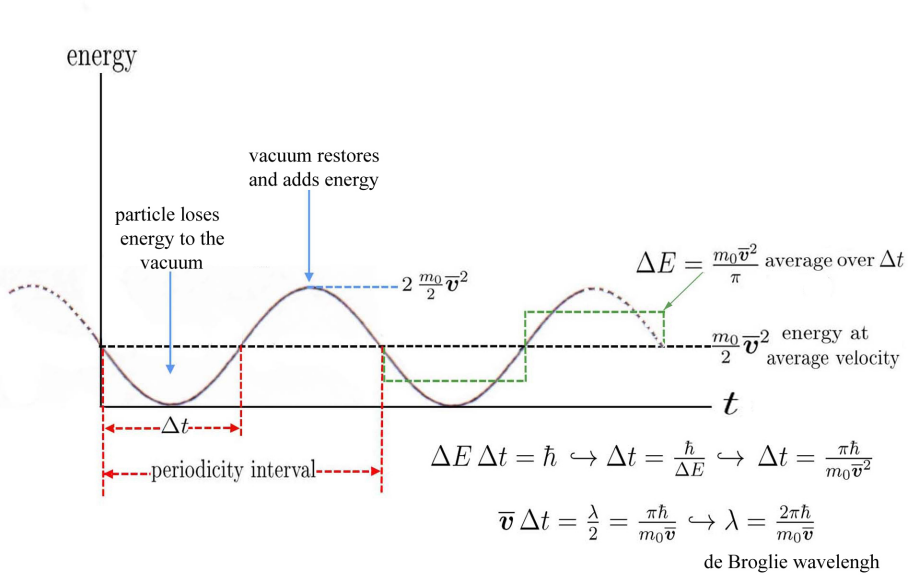


Figure 2: Connection between energy fluctuation $\Delta E$ and de Broglie wavelength $\lambda$

After the particle has slowed down it must pick up speed again to establish the original state. Thus, $\lambda \stackrel{def}{=} 2\bar{v}\Delta t$ presents an interval of periodicity in real-space, where the velocity of the particle drops and increases again. For that interval of periodicity one obtains

$$\lambda = \frac{2\pi\,\hbar}{m_0\bar{v}}\,. \tag{17}$$

This constitutes de Broglie's famous result of 1924 for the "wavelength of a matter wave" [4] which he obtained by "educated guessing" from Einstein's article on "light quanta" [27] of 1905.
If a particle moves freely, there are no specific points in space that would offer themselves as a marking for the beginning and the end of a spatial

oscillation period. However, when the particle moves, for example, in a harmonic oscillator potential or in a potential well, the classical turning points represent special points of this kind. In this case the sections of larger (or smaller) kinetic energy density for the forward and backward motion coincide, and thus the waviness of its energy density along the direction of its motion becomes visible. According to Eq.(17) there are longer periodicity intervals (wavelengths) where $\bar{v}$ is small, viz. toward the turning points, and shorter intervals around the potential minimum where $\bar{v}$ is large. Beyond the turning points where classical motion is not possible any more, the kinetic energy density drops smoothly similar to its behavior in the groundstate of the particle. This behavior is illustrated in Fig.3 which refers to a particle that oscillates along the $x$-direction in a harmonic oscillator potential. Clearly, given the energy of the particle, stationary states can only occur if

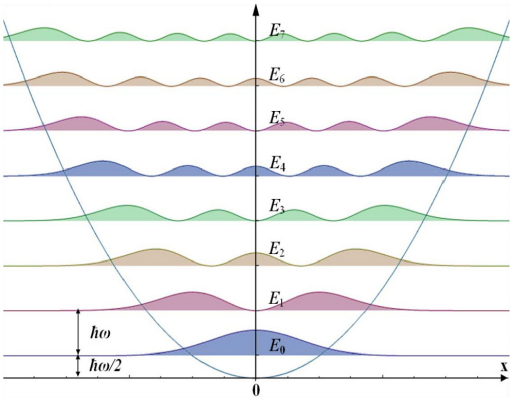


Figure 3: Stationary states of a harmonic oscillator

an integer multiple of fluctuation intervals can develop between the classical turning points. The respective energies have been denoted $E_0$ to $E_7$ in the above figure.
In the following we imagine the $x$-axis subdivided into sufficiently small equal portions $\Delta x$. As the particle moves back and forth along the $x$-direction in a varying potential, its velocity - averaged over a fluctuation interval - changes as $\bar{v}(x)$, which means, it spends different "residence times" $\Delta t(x) = \frac{\Delta x}{\bar{v}(x)}$ per oscillation period $T$ in those intervals. The quantity $\frac{\Delta t(x)}{T}$ may therefore be interpreted as a probability of the particle being in the respective interval $\Delta x$. The figure below refers to a stationary state that would correspond to $E_{11}$ in the numbering of Fig.3. We have depicted the associated oscillatory probability density (in grey) that results from the fluctuating energy exchange with the vacuum compared to the probability distribution in case the particle moves classically at the same energy. The classical turning

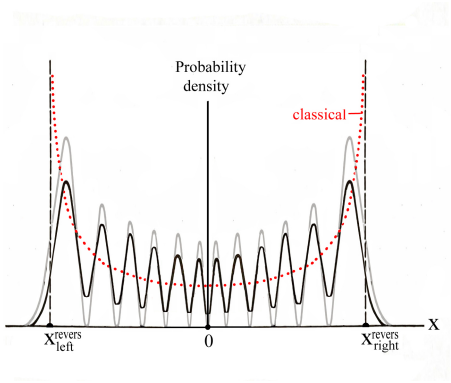


Figure 4: Classical (.....) vs. oscillatory probability density of a particle in the potential of a harmonic oscillator

points are marked by vertical broken lines. The solid oscillatory curve refers to a thought experiment where it has been assumed that the magnitude of $\hbar$ is reduced, but the lengths of the oscillations and $\bar{v}(x)$ have been kept fixed. From the equations employed in Fig.2 we have

$$\bar{v}\Delta t = \frac{\lambda}{2} \hookrightarrow \Delta t \,\text{fixed}\,.$$

It follows then from $\Delta E \Delta t = \hbar$ that $\Delta E$ shrinks as $\hbar$ is continuously lowered. That means that the portions of energy exchanged with the vacuum become smaller and smaller so that the oscillatory solid curve in Fig.4 gradually approaches the classical curve.

**6. Spreading width of a particle's trajectory**

If a free particle traverses the vacuum with a momentum $\mathbf{p}$ its energy $\mathbf{p}^2/2\,m_0$ undergoes temporary changes $\Delta E = (2\,\mathbf{p}\cdot\Delta\mathbf{p} + \Delta\mathbf{p}^2)/2\,m_0$ that cause changes of its momentum in all directions. Those with components perpendicular to $\mathbf{p}$ lead to shifts $\Delta\mathbf{r}_\perp$ sideways to its previous trajectory. After $\Delta t$ seconds the original momentum (and energy) is restored so that one can regard the whole process as a phenomenon of reversible scattering, which, however, leads to a shift $\Delta\mathbf{r}_\perp$. Since the subsequent shifts can have both signs, only their square remains non-zero on averaging over sufficiently many reversible scattering processes of this kind. The average can be obtained by invoking $\Delta E\,\Delta t \approx \hbar/2$ and setting $\Delta E = \Delta\mathbf{p}_\perp^2/2\,m_0 = \frac{1}{2}m_0(\Delta\mathbf{v}_\perp)^2$ which yields $\hbar\,\Delta t/2 \approx \frac{1}{2}m_0(\Delta\mathbf{v}_\perp\,\Delta t)^2$. We observe that $\Delta\mathbf{v}_\perp\,\Delta t = \Delta\mathbf{r}_\perp$, and hence

$$\overline{\Delta\mathbf{r}_\perp^2} \approx \frac{\hbar}{m_0}\,\Delta t\,. \tag{18}$$

To keep the notation simple we have used the overline only in the last line to indicate averaging. The above equation has the form of Einstein's law

on the mean square displacement of a particle that performs a Brownian motion. This is not a coincidence and will prove to be of crucial importance in the derivation of the Schrödinger equation.
One may now define a cone which is rotational symmetric around the particle's classical trajectory and has a cross section of $\sqrt{\frac{4\hbar t}{m_0}}$ in diameter when the particle has moved for $t$ seconds. It comprises essentially all irregular portions of the perturbed trajectory and its cross section widens in time as the particle moves further. If the particle is very fast or heavy or both, and if the length of its trajectory as a free particle is limited for practical reasons, the diameter of this cone remains small everywhere and can well prove undetectable in practice. It is often sufficient that the particle is fast. The traces of $\alpha$-particle trajectories in a track chamber constitute a well known example. If an $\alpha$-particle is emitted from some radioactive nucleus it possesses a kinetic energy of $\approx 5$ MeV. After it has covered a distance of 10 cm the apparent width of its trajectory has only grown to $\approx 1{\cdot}10^{-6}$ cm. In the case of a macroscopic particle, a steel ball, for example, which drops in a vacuum chamber, it appears to be clear at first sight that there will be no aberration from its classical trajectory. However, on a microscopic scale the trajectory of its center of gravity is irregular as well, but the diameter of the cone remains tiny everywhere because $m_0$ is large. All these examples sum up to the conclusion: The laws of quantum mechanics remain valid in the world of macroscopic physics, contrary to a widely held conviction.

**7. Interference behind a double-slit diaphragm**

Given the fact that vacuum fluctuations are real and cause an irregular motion of particles, how can one understand the phenomenon of what seems to be an "interference of matter waves"? The latter relates to a hardcore experiment of quantum mechanics, i. e. to a setup that consists essentially of a cathode which emits electrons toward a two-slit diaphragm and a detector plane behind it where the electrons are monitored. The overall impression is that one observes in the distribution of the electrons hitting the monitor a Fraunhofer-type interference pattern. Feynman regarded this apparently inexplicable phenomenon as the key problem of quantum mechanics. To demonstrate that one is dealing here with a single-particle phenomenon, one lowers the particle current in the experiment to the extent that there is only one particle at a time in the experimental setup. Once the particle has been detected in the monitor plane by some channel of an extremely fine-meshed channeltron, for example, the next particle starts from the cathode, and so on. It is instructive to use a plotting paper with a quadratic line network as a one-to-one map of the array of the channels. Every time a channel detects a particle, the respective square in the line-network is blackened. The following figure shows the result one obtains after 11, 200, 6000, 40.000 and 140.000 particles have passed the setup and hit the channeltron. The pattern has been inverted from white to black so that the detected par-

ticles appear as white spots. (The mentioned number of particles refer to the panels a, b, c, d and e in the figure.) If one closes one of the slits, the

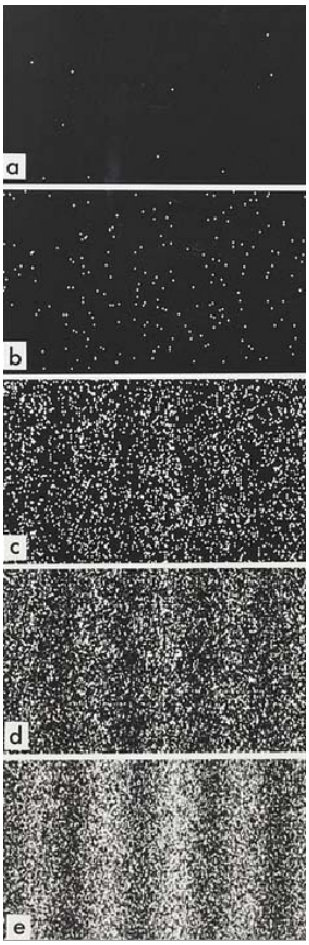


Figure 5: Effective interference pattern

typical diffraction pattern disappears.

To make the message of the above diffraction experiment even more dramatic, one could, in principle, use 140.000 identical setups distributed over 140.000 different laboratories of the world. If each laboratory would obtain only one spot on its associated plotting paper - after the setup has been switched on - and if one would afterwards collect the 140.000 different plotting papers and project them on top of each other, the result would look like panel e in the above figure.

Our entire exposition rests crucially on the assumption that each particle moves along a trajectory which - though being irregular - is elongate without loops. Hence, each particle can only move through one of the slits. How can

it feel whether or not the other slit is open? The following figure depicts some details that refer to this question. As for the electrons coming from

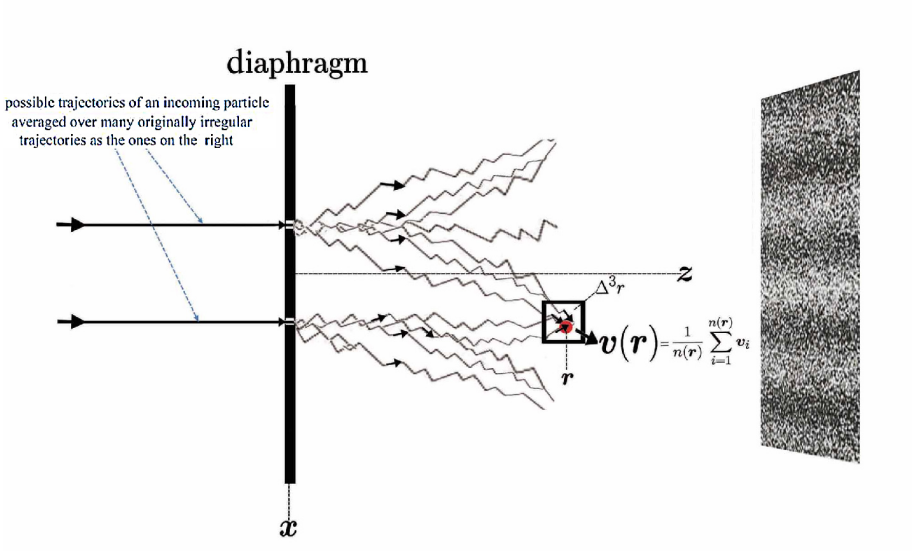


Figure 6: Origin of interference

the left the situation has been simplified in the following figure. The two straight trajectories running toward their respective slit are obtained from averaging over a very large ensemble of identical setups in each of which only one electron is emitted from the cathode. One imagines the wiggly trajectory of each electron plotted along its way from the cathode to the monitor. These trajactories are thought to be projected on top of each other to form an average $\boldsymbol{v}(\boldsymbol{r})$ of their velocities $\boldsymbol{v}_i(\boldsymbol{r})\,; i = 1, 2, ...$ and the density $\rho(\boldsymbol{r})$ of their position at each point $\boldsymbol{r}$. This averaging yields a set of parallel trajectories, and the ones that are shown represent just two which hit the respective slit in the middle. The occurrence of the other parallel trajectories will not modify the conclusions drawn from the behavior of the two particular ones.

No averaging has been performed on the right-hand side of the diaphragm. However, we show only twelf irregular trajectories from twelf separate equivalent setups picked at random. It appears to be an enduring problem in understanding quantum mechanics that it deals with statements on $\rho(\boldsymbol{r})$ and $\boldsymbol{v}(\boldsymbol{r})$ referring to **one** particle in a specifically chosen setup, but these two quantities are determined by averaging over the respective positions and velocities of a infinitely large number of particles in **separate** equivalent setups. This will be explained in more detail in Section 4. The construction of these setups is guided by the idea that each of the particles in its setup-referenced coordinate system would move exactly along the same trajectory if the embedding vacuum were inactive. Hence, when the activity of the

latter is turned on, the trajectories, which are now all different, display the range of possibilities as to how Newtonian trajectories can be deformed by reconstructive stochastic forces. Since $\boldsymbol{v}(\boldsymbol{r})$ is the weighted sum of the velocities $\boldsymbol{v}_i(\boldsymbol{r})$ within an elemental volume $\Delta^3 r$ about $\boldsymbol{r}$, this velocity changes, of course, when one closes one of the slits. Often one relies on ergodicity and envisions the set of separate systems as equivalent to one system where the trajectory evolves for some limited time and the whole process is repeated then periodically. If one wants to know for some position $\boldsymbol{r}$ the average velocity $\boldsymbol{v}(\boldsymbol{r})$ which the particle possesses in repeated experiments, one has to form the weighted sum of the individual velocities in subsequent processes as indicated in the above figure. Although in one of the experiments (processes) only one of the trajectories is realized, the velocity $\boldsymbol{v}(\boldsymbol{r})$ at $\boldsymbol{r}$ depends on the other trajectories that are realized at another time. The salient point here is: The associated Schrödinger equation for the setup under study only yields the wavefunction $\psi(\boldsymbol{r}) = |\psi(\boldsymbol{r})|\, e^{i\,\varphi(\boldsymbol{r})}$ where $\frac{\hbar}{m_0}\nabla\varphi(\boldsymbol{r}) = \boldsymbol{v}(\boldsymbol{r})$. (For an explanation see Section 6.) In other words: the quantum mechanics of the experiment **does not provide** information on any of the individual trajectories that are actually occurring in reality.

**8. Short-range forces mediated by massive messenger particles**

This topic is an almost classical example of the fundamental Eq.(1) governing vacuum fluctuations. However, Eq.(1) is rarely adressed as such, i. e. as a rule of great generality in microphysics.

The strong internuclear forces are believed to be mediated by pions which possess a rest energy $m_0c^2$ of $\approx$ 135 MeV. By allowing sufficiently large energy fluctuatuations $\Delta E$ to occur these pions can spontaneously pop up from the vacuum and live for some time while they are moving. We imagine they move at a speed $0.6\,c$ whereby their energy increaes up to $\approx$ 169 MeV. Hence their lifetime is according to Eq.(1)

$$\Delta t = \frac{2\hbar}{169\ \text{MeV}} \approx 8 \cdot 10^{-24} s$$

where we have set $f = 2$. Because of their speed of $0.6\,c$ they cover within this time span a distance of $1.4{\cdot}10^{-13}$ cm which is about the experimental value of the range of internuclear forces.

We have chosen a speed of $0.6\,c$ because a larger speed would increase the effective energy of the pion and thereby lower $\Delta t$ and subsequently lower the covered distance.

# 4 Defining ensembles and averages

As in the theory of diffusion we start with considering a point-like particle that is driven by an external conservative force $\boldsymbol{F}(\boldsymbol{r})$ and moves in an envi-

ronment where it is exposed to additional stochastic forces. To gain access to quantities that are commonly discussed within this framework we construct a sufficiently large set of $N$ identical systems (an ensemble of systems) under the supposition that there is no correlation between the stochastic forces of different systems. As a fundamental consequence, one is led then, as in the theory of diffusion, to a form of quantum mechanics that merely describes ensemble behavior. But this, again, is in accord with Ballentine's view [18]: *"..in general, quantum theory predicts nothing which is relevant to a single measurement (excluding strict conservation laws like those of charge, energy or momentum)."*
To fully understand this approach, one should always have a clear picture of the two key items defined in the following. In asking for the relative frequency with which a particle appears in an elementary volume $\Delta^3\boldsymbol{r}$ about a point $\boldsymbol{r}$ one imagines that the **same** elementary volume $\Delta^3\boldsymbol{r}$ is marked in all the $N$ systems of the ensemble each of which contains only **one** particle. "Identical systems" in that context means that they are in every respect identical except that the stochastic forces in them are independent so that a stochastic force at a point $\boldsymbol{r}$ is not identical with the stochastic force in any of the other systems at the same point. How could one check that these stochastic forces are independent but physically equivalent? If one counts $n$ particles in those $N$ elementary volumes about $\boldsymbol{r}$ and forms $\frac{n(\boldsymbol{r})}{N}$, this relative number must be independent of $N$ if the latter is large enough. If one speaks of "the number of particles in $\Delta^3\boldsymbol{r}$" it always implies an imagined projection of those $N$ elementary volumes into one.

After these preliminaries we define as set out above: The relative freqency with which the particle appears at the time $t$ in an elementary volume $\Delta^3\boldsymbol{r}$ about the point $\boldsymbol{r}$ is given by

$$\frac{n(\boldsymbol{r},t)}{N} = \rho(\boldsymbol{r},t)\,\Delta^3\boldsymbol{r} \tag{19}$$

where $n(\boldsymbol{r},t)$ is the number of particles in $\Delta^3\boldsymbol{r}$, and $\rho(\boldsymbol{r},t)$ denotes the probability density. We, furthermore, introduce $N_{\boldsymbol{r}}$ for the number of elementary volumes into which the total volume $\mathcal{V}$ is thought to be subdivided. Since the sum over all elementary cells yields $N$ particles we have

$$\sum_{\boldsymbol{r}}^{N_{\boldsymbol{r}}} \frac{n(\boldsymbol{r},t)}{N} = 1 \quad \text{that is} \quad \int_{\mathcal{V}} \rho(\boldsymbol{r},t)\,d^3\boldsymbol{r} = 1\,. \tag{20}$$

We refrain here from discussing the proper limiting case $N \to \infty$ and relating relative frequencies to probabilities, as this matter has extensively been analyzed elsewhere (s. e. g. Streater [16]). We assume that there will always be a smooth function $\rho(\boldsymbol{r},t)$ for any finite $N$ that provides a least mean square fit to the actually histogram-type function $\frac{n(\boldsymbol{r}_j,t)}{N}$ in real-space where

$j$ numbers the cubes into which the normalization volume $\mathcal{V}$ is thought to be subdivided, and $\boldsymbol{r}_j$ denotes the centroid of the particle positions in the respective cube.

The relative frequency $\frac{n(\boldsymbol{r},t)}{N}$ which we shall express below as the mod squared of some wave function $\psi(\boldsymbol{r},t)$, refers - when multiplied by $\Delta^3 r$ - to the subset of identically prepared systems where the particle appears at $\boldsymbol{r}$ and nowhere else simultaneously, otherwise the term "particle" would be meaningless. We think that the commonly used phraseology "probability of **finding** the particle at $\boldsymbol{r}$" is inappropriate because it suggests that one would have placed a detector at $\boldsymbol{r}$ monitoring the occurrence of that particle. However, a detector would - apart from causing various uncontrollable perturbations - terminate the motion of the particle on impact, and hence there would be a shadow area behind the detector where $\frac{n(\boldsymbol{r},t)}{N} \approx 0$, different from the original unperturbed situation. Wherever in the following the quantity $\frac{n(\boldsymbol{r},t)}{N}\,\Delta^3 r$ or $\rho(\boldsymbol{r},t)\,\Delta^3 r$ will appear it is clearly to be understood as the probability of the particle **being** in $\Delta^3 r$ about $\boldsymbol{r}$.

We temporarily number the particles in $\Delta^3\boldsymbol{r}$ at time $t$ by an index $i$:

$$i = 1, 2 \ldots n(\boldsymbol{r},t)\,.$$

The particles move, in general, at different velocities $\boldsymbol{v}_i(t)$. We define the ensemble average of the latter as

$$\boldsymbol{v}(\boldsymbol{r},t) = \frac{1}{n(\boldsymbol{r},t)} \sum_{i=1}^{n(\boldsymbol{r},t)} \boldsymbol{v}_i(t)\,. \tag{21}$$

As is familiar from the theory of diffusion, the individual velocities $\boldsymbol{v}_i(t)$ in $\Delta^3\boldsymbol{r}$ will in general be quite different from $\boldsymbol{v}(\boldsymbol{r},t)$ which we shall come back to later in Section 11. By contrast, in Bohm's version of quantum mechanics [28] the true particle trajectories are, for no obvious reason, regarded as the flowlines of the velocity field $\boldsymbol{v}(\boldsymbol{r},t)$. This is one of the points where our approach differs fundamentally from Bohm's and reflects a concomitant feature of our definition of $\boldsymbol{v}(\boldsymbol{r},t)$:
In performing the average according to Eq.(21) one sums over velocities $\boldsymbol{v}_i(t)$ of different trajectories that run through sometimes very different regions of the available space of the one-particle system. Hence, they are influenced by the classical field $\boldsymbol{F}(\boldsymbol{r})$ in those regions. This carries over to the ensemble average $\boldsymbol{v}(\boldsymbol{r},t)$. That means: if one places a two-slit diaphragm somewhere away from $\boldsymbol{r}$ and closes one of the slits, a continuous subset of trajectories is blocked out, and hence $\boldsymbol{v}(\boldsymbol{r},t)$ changes. That kind of non-local sensitivity explains why the flowlines of the field $\boldsymbol{v}(\boldsymbol{r},t)$ are affected by portions of the space which may be far away. The unfamiliar feature of non-locality will be illustrated by a particularly surprising example in Section 10.

As a general property of the stochastic forces that act on the respective particle in each system, we require them to ensure ergodicity in the following sense:
If the system is not explicitly time-dependent, that is, when it is in a bound stationary state and if one would follow the particle on its trajectory within the range it is bound to, one would see it successively occur in all the cubes $\Delta^3 r$ over which - in the ensemble average - all particles of the ensemble are distributed at a certain instant $t$. Thus, instead of forming the ensemble average according to Eq.(19) it can for a single particle just as well be defined as

$$\lim_{T\to\infty} \frac{\overline{\Delta t}(\boldsymbol{r})}{T} = \rho(\boldsymbol{r})\,\Delta^3 r \tag{22}$$

where $\overline{\Delta t}(\boldsymbol{r})$ denotes the overall time which the particle has spent occurring repeatedly in $\Delta^3 r$ about $\boldsymbol{r}$ within the total time span $T$.
The velocity $\boldsymbol{v}(\boldsymbol{r})$ can be defined analogously

$$\boldsymbol{v}(\boldsymbol{r}) = \frac{1}{\hat{n}(\boldsymbol{r})} \sum_{i=1}^{\hat{n}(\boldsymbol{r})} \boldsymbol{v}(t_i) \tag{23}$$

where $\hat{n}(\boldsymbol{r}) = \rho(\boldsymbol{r})\,\Delta^3 r$ is the number of times the particle has occurred in $\Delta^3 r$ about $\boldsymbol{r}$, and $t_i$ denotes some point within the time span the particle has spent there the $i^{th}$ time. In realistic cases in which the system under study undergoes transitions between quasi-stationary states, one has to allow $T$ to be finite, and quasi-stationarity can only be ensured if the changes are sufficiently slow on a time scale of unit length $T$. Practical experience shows, that this applies to the majority of cases. However, in Section 24 we shall give an example where $T$ must be expected to be far too long to justify a classification of the states in a photo emission transition as quasi-stationary. Yet, the bulk of this article will deal with ensemble averages.

# 5 Navier-Stokes equations

If a particle of mass $m_0$ moves in an environment of kinematic viscosity $\nu$ the resulting ensemble average of its velocity $\boldsymbol{v}(\boldsymbol{r},t)$ is just the sum of the so-called "convective velocity" $\boldsymbol{v}_c(\boldsymbol{r},t)$ and a "diffusive velocity" $\boldsymbol{u}(\boldsymbol{r},t)$ driven by the stochastic forces of the embedding medium:

$$\boldsymbol{v}(\boldsymbol{r},t) = \boldsymbol{v}_c(\boldsymbol{r},t) + \boldsymbol{u}(\boldsymbol{r},t) \tag{24}$$

Employing the Smoluchowski equation (s. Section 39) for the probability density $\rho(\boldsymbol{r},t)$, similarly for the probability current density $\boldsymbol{j}_c(\boldsymbol{r},t) =$

$\rho(\boldsymbol{r},t)\,\boldsymbol{v}_c(\boldsymbol{r},t)$ and invoking Einstein's law [29] for the mean square displacement we obtain a Navier-Stokes-type equation of the form

$$\frac{\partial}{\partial t}\,(\boldsymbol{v}-\boldsymbol{u}) + [(\boldsymbol{v}+\boldsymbol{u})\cdot\nabla(\boldsymbol{v}-\boldsymbol{u})] - \nu\,\Delta(\boldsymbol{v}-\boldsymbol{u}) = \frac{1}{m_0}\,\boldsymbol{F}(\boldsymbol{r})\,. \tag{25}$$

with $\boldsymbol{F}(\boldsymbol{r}) = -\nabla V(\boldsymbol{r})$ denoting the external conservative force acting on the particle. The "osmotic" or "diffusive" velocity $\boldsymbol{u}(\boldsymbol{r},t)$ is defined by

$$\boldsymbol{u}(\boldsymbol{r},t) = -\nu\,\frac{\nabla\rho(\boldsymbol{r},t)}{\rho(\boldsymbol{r},t)}\,, \tag{26}$$

or equivalently in terms of the diffusive current density $\boldsymbol{j}_D$

$$\boldsymbol{j}_D(\boldsymbol{r},t) = -\nu\,\nabla\rho(\boldsymbol{r},t) \quad \text{"Fick's law"} \tag{27}$$

where

$$\boldsymbol{j}_D(\boldsymbol{r},t) = \rho(\boldsymbol{r},t)\,\boldsymbol{u}(\boldsymbol{r},t)\,. \tag{28}$$

In the special case when $\boldsymbol{v}_c \equiv 0$ the equation of continuity reduces to

$$\frac{\partial}{\partial t}\,\rho + \nabla\cdot\rho\,\boldsymbol{u} = 0\,, \tag{29}$$

which on insertion of $\boldsymbol{u}(\boldsymbol{r},t)$ from Eq.(26) attains the form of the diffusion equation

$$\frac{\partial}{\partial t}\,\rho = \nu\,\Delta\rho\,. \tag{30}$$

On the other hand, when $\nu = 0$ one has $\boldsymbol{u}(\boldsymbol{r},t) \equiv 0$, and hence all particles move now along smooth trajectories $\boldsymbol{r}(t)$ so that the various velocities $\boldsymbol{v}_i(t)$ under the sum in Eq.(21) become equal: $\boldsymbol{v}_i(t) = \boldsymbol{v}(\boldsymbol{r}(t))$. Thus

$$\frac{\partial}{\partial x_k}\,\boldsymbol{v}(\boldsymbol{r}(t)) \equiv 0 \quad (k=1,2,3) \quad \to \boldsymbol{v}\cdot\nabla\,\boldsymbol{v} \equiv 0\,,$$

and consequently Eq.(25) reduces to Newton's second law.

The set of equations (25) to (27) will be derived in Section 39.
Eq.(26) may be rewritten

$$\boldsymbol{u}(\boldsymbol{r},t) = -\nu\frac{\nabla\rho(\boldsymbol{r},t)}{\rho(\boldsymbol{r},t)} = -\nu\,\nabla\,\ln[\rho(\boldsymbol{r},t)/\rho_0] \tag{31}$$

where $\rho_0$ denotes a constant density that has merely been inserted for dimensional reasons. As $\boldsymbol{u}(\boldsymbol{r},t)$ can be expressed as a gradient of a function, we have

$$\nabla\times\boldsymbol{u}(\boldsymbol{r},t) = 0\,, \tag{32}$$

and hence

$$(\boldsymbol{u}\cdot\nabla)\boldsymbol{u} = \nabla\,\frac{\boldsymbol{u}^2}{2}\,. \tag{33}$$

If we, further, make use of the identity

$$\nabla\times(\nabla\times\boldsymbol{a}) = \nabla(\nabla\cdot\boldsymbol{a}) - \Delta\boldsymbol{a} \tag{34}$$

and observe Eq.(32) we obtain $\Delta\boldsymbol{u}(\boldsymbol{r},t) = \nabla(\nabla\cdot\boldsymbol{u}(\boldsymbol{r},t))$. Thus, Eq.(25) in conjunction with Eq.(26) may be cast as

$$m_0\frac{d}{dt}\boldsymbol{v}(\boldsymbol{r},t) = \boldsymbol{F}(\boldsymbol{r}) - \nabla V_{stoch}(\boldsymbol{r},t) + \vec{\Omega}(\boldsymbol{r},t)\,, \tag{35}$$

where $V_{stoch}(\boldsymbol{r},t)$ and $\vec{\Omega}(\boldsymbol{r},t)$ are abbreviations which stand for

$$V_{stoch} = \nu^2\,\left[\frac{1}{2}\left(\frac{\nabla\rho}{\rho}\right)^2 - \frac{\nabla^2\rho}{\rho}\right]\,, \tag{36}$$

and

$$\vec{\Omega} = \frac{\partial\boldsymbol{u}}{\partial t} + (\boldsymbol{v}\cdot\nabla)\,\boldsymbol{u} - (\boldsymbol{u}\cdot\nabla)\,\boldsymbol{v} + \nu\,\Delta\,\boldsymbol{v}\,.$$

In deriving (36) we have observed that $\frac{1}{\nu}\,\nabla\boldsymbol{u} = -\frac{\Delta\rho}{\rho} + (\frac{\nabla\rho}{\rho})^2$. Furthermore, we have introduced $\frac{d\boldsymbol{v}}{dt}$ as the "convective (or hydrodynamic) acceleration" which in the present context merely represents an abbreviation

$$\frac{d\boldsymbol{v}(\boldsymbol{r},t)}{dt} = \frac{\partial\,\boldsymbol{v}}{\partial t} + \boldsymbol{v}\cdot\nabla\boldsymbol{v}\,. \tag{37}$$

The "stochastic potential" $V_{stoch}(\boldsymbol{r},t)$ depends on $\nu^2$ whereas $\vec{\Omega}(\boldsymbol{r},t)$ is proportional to $\nu$.
The latter constant is associated with the occurrence of the stochastic forces which - in the absence of an external force $\boldsymbol{F}(\boldsymbol{r})$ - would slow down the particle within a characteristic time $\tau$.
Since the physical vacuum does not represent an embedding medium whose stochastic forces can cause a particle to slow down completely, we modify the character of the stochastic forces by assuming that they change periodically after a time lapse of $\approx\,\tau$ sec from down-slowing "Brownian" to motion enhancing "anti-Brownian" and vice versa. The "anti-Brownian" forces act as if the kinematic viscosity would have a negative sign. Hence, the corresponding equation of motion has the form

$$m_0\frac{d}{dt}\boldsymbol{v}(\boldsymbol{r},t) = \boldsymbol{F}(\boldsymbol{r}) - \nabla V_{stoch}(\boldsymbol{r},t) - \vec{\Omega}(\boldsymbol{r},t)\,. \tag{38}$$

In Section 16 we give an example of an embedding medium that acts on a test particle by alternating Brownian/anti-Brownian forces.

If we now additionally assume that the temporal changes that occur with all quantities in Eqs.(35) and (38) are slow on a scale of unit length $\tau$ - which is the standard requirement also in diffusion theory - the motion of the ensemble will be governed by the arithmetic mean of these equations, that is by

$$m_0 \frac{d}{dt} \boldsymbol{v}(\boldsymbol{r}, t) = \boldsymbol{F}(\boldsymbol{r}) - \nabla V_{stoch}(\boldsymbol{r}, t)\,. \tag{39}$$

A more detailed definition of the stochastic forces that ensure "conservative diffusion" will be given in Section 13. Wavelike solutions to Eq.(39) show now friction-less behavior.
One might suspect that our subdivision into a Brownian "B"-ensemble and an anti-Brownian "A"-ensemble is unnecessarily clumsy and could be avoided at the outset by assuming vacuum forces that neither possess down-slowing components nor counterparts that effect motion enhancement, but rather consist of random (Gaussian) forces whose components form a normal distribution. However, from Einstein's theory of Brownian motion the kinematic viscosity (or "diffusion constant") emerges as

$$\nu = \frac{k_B\, T\, \tau}{m_0} \quad (\text{Einstein: } \overline{\Delta x_i\, \Delta x_j} = 2\, \delta_{ij}\, \nu\, \Delta t\,; \quad i, j = 1, 2, 3\,) \tag{40}$$

where $m_0$ is the mass of the particle under study, $\Delta x_i\,, \Delta x_j$ are displacements of its position and $T$ is the effective temperature of the embedding medium. This temperature enters into the derivation as the width of the distribution of the random (Gaussian) forces that act on the particle apart from the **directional** down-slowing force. Because of the latter there is a down-slowing motion that we have already alluded to. The associated time constant is denoted by $\tau$. Equating the down-slowing forces to zero amounts to $\tau \to \infty$ which would yield infinite kinematic viscosity. Hence, there is no alternative to our approach.
Obviously, the physical dimension of the numerator of the above fraction in Eq.(40) is that of an action, i.e. energy$\times$time. As $\nu$ appears via $V_{stoch}(\boldsymbol{r}, t)$ in Eq.(39) which is constructed to describe dissipationless motion in a "stochastic vacuum" whose effect on a particle can only be associated with a new constant of nature, one is justified in equating $k_B\, T\, \tau$ with $\frac{1}{2}\,\hbar$ where $h = 2\pi\,\hbar$ is Planck's constant. Of course, instead of $1/2$ there could be any other dimensionless prefactor in front of $\hbar$, but it turns out that the numerical results of all quantum mechanical calculations that follow from Eq.(39) are only consistent with the above choice. *Clearly, that choice can only be made once and for all.*
Having thus calibrated the "vacuum-$\nu$"we rewrite Eq.(39) in the form

$$m_0 \frac{d}{dt} \boldsymbol{v}(\boldsymbol{r}, t) = \boldsymbol{F}(\boldsymbol{r}) - \nabla V_{QP}(\boldsymbol{r}, t)\,, \tag{41}$$

where we have substituted the subscript "$QP$" for"$stoch$"

$$V_{QP} = \tfrac{\hbar^2}{4\,m_0}\,\left[\frac{1}{2}\left(\frac{\nabla\rho}{\rho}\right)^2 - \frac{\nabla^2\rho}{\rho}\right] \text{ "quantum potential" }, \tag{42}$$

or even shorter

$$V_{QP} = \frac{\hbar^2}{2\,m_0}\,\frac{\nabla^2 R}{R}\,, \tag{43}$$

where we have set

$$\frac{\hbar}{2m_0} = \nu = \frac{k_B\,T\,\tau}{m_0} \quad \text{and} \quad \rho = R^2\,. \tag{44}$$

The "quantum potential" has first been introduced by de Broglie [30] and later been taken up again by David Bohm [28]. Obviously Eq.(41) may be viewed as a modification of Newton's second law. If not stated differently, we shall assume $\boldsymbol{F}(\boldsymbol{r})$ to be conservative:

$$\boldsymbol{F}(\boldsymbol{r}) = -\nabla V(\boldsymbol{r})\,. \tag{45}$$

The assumption made above, viz. that all changes of the ensemble properties have to be sufficiently slow on a time scale of unit length $\tau$ may raise questions about the validity of such a constraint. Eqs.(41) and (42) will prove equivalent to the time-dependent Schrödinger equation whose validity is unquestioned at the non-relativistic level. Hence, $\tau$ is obviously sufficiently small within the experimentally tested range of the Schrödinger equation. Conversely, as one may conclude then from Eq.(44) the "effective temperature" of the vacuum must be very high compared to those temperatures commonly considered in applied thermodynamics and astrophysics.

Fundamentally different from our approach Bohm [28] derives Eqs.(41) and (42) by choosing the opposite direction starting from the time-dependent Schrödinger equation which he just considers given. Hence, he does not offer any new insight into what makes the motion of a microscopic particle different from Newtonian mechanics. In the context of Bohm's mechanics Eq.(41) is frequently cast such that it resembles the Hamilton-Jacobi equation. To this end one sets

$$\boldsymbol{v}(\boldsymbol{r},t) = \frac{1}{m_0}\,\nabla S(\boldsymbol{r},t)\,.$$

This implies that $\boldsymbol{v}(\boldsymbol{r},t)$ is irrotational, which is at best plausible, but remains unproven.
Eq.(41) in conjunction with (42) then attains the form

$$\frac{1}{m_0}\,\nabla\left[\frac{\partial S}{\partial t} + \frac{(\nabla S)^2}{2\,m_0} + V(\boldsymbol{r}) - \frac{\hbar^2}{2\,m_0}\,\frac{\Delta R}{R}\right] = 0\,.$$

This is equivalent to

$$\frac{\partial S}{\partial t} + \frac{(\nabla S)^2}{2\,m_0} + V(\boldsymbol{r}) - \frac{\hbar^2}{2\,m_0}\,\frac{\Delta R}{R} = 0\,,$$

and becomes identical with the Hamilton-Jacobi equation in the limit $\hbar \to 0$. However, the connection to classical mechanics is far more evident from Eq.(41), which reduces to Newton's second law

$$\boldsymbol{F} = m_0\,\frac{d}{dt}\boldsymbol{v}$$

as $\hbar$ tends to zero. In addition, Eq.(41) lends itself to a thought-experiment that is particularly illustrative of the quantum character of particle motion. One starts with setting $\hbar = 0$ and assumes that all particles of the ensemble commence their motion under identical initial conditions. Their positions and trajectories will coincide then at any later time. One now lets $\hbar$ take on a finite value. As a consequence of the now occurring stochastic forces whose action on some particle is statistically independent from that on any other particle, the particle positions start diverging and form a cloud about the formerly common position along the trajectory. The particles of the ensemble now reach positions that are not accessible under energy conservation. It is hence obvious that the vacuum provides an embedding medium of a "universal noise" consisting of energy fluctuations which cause shifts of the individual particle trajectories such that the classical momentum and the energy are conserved on the average. This is reflected in the expectation value of the "vacuum force" $\boldsymbol{F}_{QP} = -\nabla V_{QP}(\boldsymbol{r}, t)$ which equals zero:

$$\int \rho(\boldsymbol{r}, t)\,\boldsymbol{F}_{QP}(\boldsymbol{r}, t)\,d^3r = 0\,. \tag{46}$$

We shift the proof of this equation to Section 14. Eq.(46) may be interpreted in the sense that the particles undergo only reversible scatterings. Figuratively speaking, the vacuum keeps track of the energy balance and remembers at later positions of a particle departures from its classical momentum and energy that occurred at previous positions. The undulatory properties of the **probability density** reside in this memory effect which gives rise to an unfamiliar non-locality. Hence, from our point of view it is illegitimate to correlate these properties with a **wave-like character of the particle**. We definitely side with Nevill Mott (1964) who argues:

*"Students should not be taught to doubt that electrons, protons and the like are particles....The waves cannot be observed in any way than by observing particles."*

# 6 The time-independent Schrödinger equation

As a first application we discuss the stationary state of a particle that is bound to a potential without symmetry elements. Hence, the real-space dependence of the potential does not display any distinct direction. That means, when a particle of the ensemble appears with a velocity $\boldsymbol{v}_i(t)$ in the elementary volume $\Delta^3 r$ about $\boldsymbol{r}$ there will always be another particle in that volume with approximately the opposite velocity, so that

$$\boldsymbol{v}(\boldsymbol{r},t) = \frac{1}{n(\boldsymbol{r},t)} \sum_i^{n(\boldsymbol{r},t)} \boldsymbol{v}_i(t) \equiv 0\,. \tag{47}$$

Hence, if one recalls (45) Eq.(41) reduces to

$$\nabla \left( \frac{\hbar^2}{4\,m_0} \left[ -\frac{1}{\rho}\nabla^2\rho + \frac{1}{2}\left(\frac{\nabla\rho}{\rho}\right)^2 \right] + V(\boldsymbol{r}) \right) = 0\,.$$

This is equivalent to:

$$\frac{\hbar^2}{4\,m_0} \left[ -\frac{1}{\rho}\nabla^2\rho + \frac{1}{2}\left(\frac{\nabla\rho}{\rho}\right)^2 \right] + V(\boldsymbol{r}) = E\,, \tag{48}$$

where $E$ denotes a constant. Eq.(48) represents a **non-linear** partial differential equation in $\rho(\boldsymbol{r})$.
On replacing $\rho(\boldsymbol{r})$ by a function $\psi(\boldsymbol{r})$ defined through

$$\rho(\boldsymbol{r}) = \psi^2(\boldsymbol{r}) \tag{49}$$

one obtains because of

$$\nabla\rho = 2\,\psi\,\nabla\psi\;; \quad \frac{1}{2}\left(\frac{\nabla\rho}{\rho}\right)^2 = 2\left(\frac{\nabla\psi}{\psi}\right)^2$$

and

$$\nabla^2\rho = 2\,\psi\,\nabla^2\psi + 2\,(\nabla\psi)^2$$
$$-\frac{1}{\rho}\,\nabla^2\rho = -2\,\frac{\nabla^2\psi}{\psi} - 2\left(\frac{\nabla\psi}{\psi}\right)^2$$

a **linear** differential equation

$$\frac{\hbar^2}{2\,m_0}\left[-\frac{1}{\psi}\nabla^2\psi\right] + V(\boldsymbol{r}) = E \quad \text{that is}$$
$$-\frac{\hbar^2}{2\,m_0}\,\nabla^2\psi + V(\boldsymbol{r})\,\psi = E\,\psi \tag{50}$$

which constitutes the time-independent Schrödinger equation.

# 7 Including currents

For the familiar problem of a particle in a box Eq.(50) reduces in the one-dimensional case to

$$\left[\frac{d^2}{dx^2} + k^2\right] \psi(x) = 0 \tag{51}$$

where we have set

$$k^2 = \tfrac{2m_0}{\hbar^2}\, E\,; \quad E = \tfrac{m_0}{2}\, v^2$$

and

$$V(x) = \begin{cases} 0 & \text{for } 0 \le x \le a \\ \infty & \text{else} \end{cases}$$

The solutions

$$\psi(x) = \tfrac{1}{\sqrt{a/2}}\, \sin k_n x \;\text{ where } k_n = \frac{\pi}{a}\, n\,; \;\; n = 1, 2, 3.. \tag{52}$$

may be recast as

$$\psi(x) = \tfrac{1}{\sqrt{2}}\, [\psi_+(x) + \psi_-(x)]$$

where

$$\psi_\pm(x) = \tfrac{1}{\sqrt{a}}\, e^{\pm\, i\varphi(x)}\,; \quad \varphi(x) = k_n x + \tfrac{\pi}{2}\,.$$

In the spirit of our approach the two independent solutions to the differential equation (51), $\psi_\pm(x)$, refer to the particle moving with a velocity $v_n = \frac{\hbar\, k_n}{m_0}$ either to the right or (after reflection at $x = a$) to the left where it is reflected again at $x = 0$.
We are thus led to surmise that we have in the general case of a freely moving particle

$$\psi(\boldsymbol{r}) = |\psi(\boldsymbol{r})|\, e^{i\varphi(\boldsymbol{r})} \quad \text{and} \quad \boldsymbol{v}(\boldsymbol{r}) = \frac{\hbar}{m_0}\, \nabla\varphi(\boldsymbol{r})\,. \tag{53}$$

The validity of this conjecture will be shown in Section 8.
In a stationary state of the one-particle system in which $\frac{\partial}{\partial t}\boldsymbol{v} = 0$ but $\boldsymbol{v}(\boldsymbol{r}) \neq 0$ we have according to Eq.(37) $\frac{d}{dt}\boldsymbol{v} = \boldsymbol{v}\cdot\nabla\boldsymbol{v} = \frac{1}{2}\nabla\boldsymbol{v}^2$ where we have exploited in advance that, according to Eq.(53), $\boldsymbol{v}(\boldsymbol{r})$ is irrotational. Hence, in the presence of a stationary current Eq.(48) contains the kinetic energy $\frac{m_0}{2}\,\boldsymbol{v}^2$ as an additional term, that is

$$\tfrac{\hbar^2}{4\, m_0}\left[-\frac{1}{\rho}\nabla^2\rho + \frac{1}{2}\left(\frac{\nabla\rho}{\rho}\right)^2\right] + V(\boldsymbol{r}) + \frac{m_0}{2}\,\boldsymbol{v}^2 = E\,. \tag{54}$$

If one now makes use of Eq.(53) instead of Eq.(49)

$$\rho(\boldsymbol{r}) = |\psi(\boldsymbol{r})|^2 = \left(\psi(\boldsymbol{r})\, e^{-i\varphi(\boldsymbol{r})}\right)^2 \tag{55}$$

and substitutes $\frac{\hbar}{m_0}\,\nabla\varphi(\boldsymbol{r})$ for $\boldsymbol{v}(\boldsymbol{r})$ the bracketed term in Eq.(54) becomes

$$\frac{\hbar^2}{4\,m_0}\left[-\frac{1}{\rho}\nabla^2\rho+\frac{1}{2}\left(\frac{\nabla\rho}{\rho}\right)^2\right]=-\frac{\hbar^2}{2\,m_0}\,\frac{1}{\psi}\nabla^2\psi+\underbrace{\frac{\hbar^2}{2m_0}\,(\nabla\varphi)^2}_{=\frac{m_0}{2}\,\boldsymbol{v}^2}$$
$$+\underbrace{i\left[\frac{\hbar^2}{2\,m_0}\,\nabla^2\varphi+\frac{\hbar^2}{2\,m_0}\,\left(2\,\nabla\varphi\cdot\frac{\nabla\psi}{\psi}\right)\right]}_{=\frac{i\hbar}{2}\left[\nabla\cdot\boldsymbol{v}+2\boldsymbol{v}\cdot\frac{\nabla\psi}{\psi}\right]}.$$

Invoking the equation of continuity in the form

$$\nabla\cdot\boldsymbol{j}=\nabla\cdot\rho\,\boldsymbol{v}=\rho\,\nabla\cdot\boldsymbol{v}+\boldsymbol{v}\cdot\nabla\rho=0$$

it can readily be shown that the term $i[...]$ on the right-hand side equals $-m_0\,\boldsymbol{v}^2$. Hence we have from Eq.(54)

$$-\frac{\hbar^2}{2\,m_0}\,\frac{1}{\psi}\nabla^2\psi+V(\boldsymbol{r})=E\,,$$

that is

$$-\frac{\hbar^2}{2\,m_0}\,\nabla^2\psi+V(\boldsymbol{r})\,\psi=E\,\psi \tag{56}$$

as before without a current.
It should be noticed that $\varphi$ may well be time-dependent even when $\nabla\varphi$ is not, that is, we have in general

$$\varphi(\boldsymbol{r},t)=\varphi_0(\boldsymbol{r})+f(t)$$

where $f(t)$ is a real-valued function. In this case the wave function $\psi(\boldsymbol{r},t)$ attains the form

$$\psi(\boldsymbol{r},t)=\hat{\psi}(\boldsymbol{r})\,e^{i\,f(t)}\quad\text{where}\quad\hat{\psi}(\boldsymbol{r})=|\hat{\psi}(\boldsymbol{r})|\,e^{i\,\varphi_0(\boldsymbol{r})} \tag{57}$$

and hence, its time-derivative may be cast as

$$i\hbar\,\frac{\partial}{\partial t}\psi(\boldsymbol{r},t)=-\hbar\,\dot{f}\,\psi(\boldsymbol{r},t)\,. \tag{58}$$

Since $f(t)$ is primarily unspecified and $-\hbar\dot{f}$ possesses the dimension of an energy the latter may justifiably be equated with the energy $E$ which is the only energy-related constant characterizing the wave function of the system:

$$-\hbar\,\dot{f}=E\,;\quad\text{that is}\quad if(t)=-\frac{i}{\hbar}E\,t\,. \tag{59}$$

As a result, we have from Eq.(57)

$$\psi(\boldsymbol{r},t) = \hat{\psi}(\boldsymbol{r})\, e^{-\frac{i}{\hbar}E\,t} \tag{60}$$

for a wave function in a stationary state. Furthermore, we have from Eqs.(56), (58) and (59)

$$-\frac{\hbar^2}{2\,m_0}\,\nabla^2\psi(\boldsymbol{r},t) + V(\boldsymbol{r})\,\psi(\boldsymbol{r},t) = i\hbar\,\frac{\partial}{\partial t}\psi(\boldsymbol{r},t) \tag{61}$$

which constitutes the time-dependent Schrödinger equation. Its validity is here still restricted to stationary systems, but it will be shown in Section 11 that it retains this form also for non-stationary systems. However, in order to achieve this consistency, one has to introduce the negative sign in Eq.(59) which seems to lack reason and can actually not be justified without reference to Section 11.

## 8 The velocity potential and phase uniqueness

We rewrite Eq.(41) in the form

$$\frac{d}{dt}\boldsymbol{v}(\boldsymbol{r},t) = -\nabla P(\boldsymbol{r},t) \tag{62}$$

where

$$P(\boldsymbol{r},t) = \frac{1}{m_0}\left[V(\boldsymbol{r}) + V_{PQ}(\boldsymbol{r},t)\right],$$

and we have made use of Eq.(37) defining the "hydrodynamic" or convective acceleration

$$\frac{d}{d\,t}\boldsymbol{v}(\boldsymbol{r},t) = \frac{\partial}{\partial\,t}\boldsymbol{v} + (\boldsymbol{v}\cdot\nabla)\,\boldsymbol{v}\,.$$

In hydrodynamics Eq.(62) corresponds to the Euler equation of perfect (frictionless) fluids and constitutes the starting point of Helmholtz's theory of vortices. Thomson's more elaborate analysis on vortices [33] builds on Helmholtz's considerations. We confine ourselves here to reporting only the general ideas as far as they directly concern the present theory.
If we set $\vec{\omega} = \nabla\times\boldsymbol{v}$ for the curl of the ensemble average of the particle velocity, we have from Eq.(34)

$$(\boldsymbol{v}\cdot\nabla)\,\boldsymbol{v} = \nabla\frac{\boldsymbol{v}^2}{2} - \boldsymbol{v}\times\vec{\omega}\,.$$

We now form the curl of Eq.(62) and use this expression together with Eq.(37). The result may be cast as

$$\frac{\partial}{\partial t}\,\vec{\omega}(\boldsymbol{r},t) - \nabla\times\left[\boldsymbol{v}(\boldsymbol{r},t)\times\vec{\omega}(\boldsymbol{r},t)\right] = 0\,, \tag{63}$$

where we have used $\nabla \times \nabla P = 0 \quad$ and $\quad \nabla \times \nabla \boldsymbol{v}^2 = 0$. One recognizes from Eq.(63) that $\frac{\partial}{\partial t}\,\vec{\omega}(\boldsymbol{r},t)|_{t=0}$ becomes zero for some chosen time, which we here equate to zero for convenience, if $\vec{\omega}(\boldsymbol{r},t)|_{t=0} = 0$ at that time. Forming the time derivative of Eq.(63) and setting again $t = 0$ we see that the second time derivative of $\vec{\omega}(\boldsymbol{r},t)$ vanishes as well. This can be carried further to any higher order of the time derivative. Hence, the system stays irrotational if it is irrotational at $t = 0$. We now consider an ensemble of free particles ($\boldsymbol{F}(\boldsymbol{r}) \equiv 0$) when $\hbar = 0$. They may start their motion at $t = 0$ at the same point in real-space and with the same momentum $\boldsymbol{p}_0 = m_0\,\boldsymbol{v}_0$. If one allows $\hbar$ to attain its natural value, the particle positions diverge and form a point cloud. Outside this cloud there are no particles and therefore $\boldsymbol{v}(\boldsymbol{r},t) \equiv 0$. Since the ensemble does not exchange momentum with the vacuum on the average and consequently no angular momentum, we have everywhere within the space of normalization

$$\nabla \times \boldsymbol{v}(\boldsymbol{r},t) = \vec{\omega}(\boldsymbol{r},t) \equiv 0 \quad \forall\, \boldsymbol{r}, t\,. \tag{64}$$

If one now turns on some (physically realistic) potential $V(\boldsymbol{r})$, weighting it with a smooth switch function from zero to one, starting at $t = t_0$, the velocity distribution $\boldsymbol{v}(\boldsymbol{r},t)$ for $t > t_0$ will now change differently, of course, but because of Eqs.(63) and (64) for $t = t_0$, we have as before $\vec{\omega}(\boldsymbol{r},t_0) \equiv 0$ and $\frac{\partial}{\partial t}\,\vec{\omega}(\boldsymbol{r},t)|_{t=t_0} \equiv 0$ which again applies to any higher order time-derivative at $t = t_0$. We thus arrive at the conclusion that an ensemble whose equation of motion is given by Eq.(62) is irrotational. In other words, $\boldsymbol{v}(\boldsymbol{r},t)$ possesses a potential $\varphi(\boldsymbol{r},t)$ which we express in the form

$$\boldsymbol{v}(\boldsymbol{r},t) = \frac{\hbar}{m_0}\,\nabla\varphi(\boldsymbol{r},t)\,. \tag{65}$$

Because of the prefactor $\hbar/m_0$ the function $\varphi(\boldsymbol{r},t)$ becomes dimensionless. Eq.(65) may equivalently be cast as

$$\varphi(\boldsymbol{r}) = \frac{m_0}{\hbar}\int_{\boldsymbol{r}_0}^{\boldsymbol{r}} \boldsymbol{v}(\boldsymbol{r}')\cdot d\boldsymbol{r}' \tag{66}$$

where we have omitted the time-dependence in confining ourselves to a stationary state situation. As in the theory of perfect fluids there may be singular vortex lines which occur if $V(\boldsymbol{r})$ possesses axial or spherical symmetry. A vortex line then defines an axis of quantization. The latter may be regarded as the boundary line of a semi-plane. Even in the presence of a vortex line, can $\varphi(\boldsymbol{r})$ be defined such that it remains unique if one only stipulates that the starting point of the line integral in Eq.(66), $\boldsymbol{r}_0$, lies on one side of this semi-plane and that the path along which the integral is performed never crosses that semi-plane. The point $\boldsymbol{r}_0$ may be chosen at will. In general, $\varphi(\boldsymbol{r})$ will now be discontinuous at the semi-plane. The ensuing section deals with this particular problem.

# 9 Quantization of angular momentum

The primary objective of this section is to disprove Wallstrom's notable objection [20] against Madelung's conviction, also held by other theorists of this school of thought, that Newton's modified second law (41) is equivalent to the time-dependent Schrödinger equation which we shall derive below. In so doing we have to exploit the uniqueness of the velocity potential shown in the preceding section. By contrast, in standard quantum mechanics the time-dependent Schrödinger equation is regarded as given. It is customarily converted into the equation of continuity

$$\dot{\rho} + \nabla \cdot [\tfrac{\hbar}{2i\,m_0}\{\psi^* \nabla\,\psi - \psi\,\nabla\,\psi^*\}] = 0$$

to show that the bracketed expression has to be interpreted as the current density $\boldsymbol{j}(\boldsymbol{r},t)$. This conclusion is only legitimate if $\boldsymbol{j}(\boldsymbol{r},t)$ has been proven to be irrotational which, however, is only tacitly presupposed. Inserting

$$\psi(\boldsymbol{r},t) = |\psi(\boldsymbol{r},t)|\, e^{i\varphi(\boldsymbol{r},\,t)} \tag{67}$$

into the bracketed expression yields

$$\boldsymbol{j}(\boldsymbol{r},t) = |\psi(\boldsymbol{r},t)|^2 \underbrace{\frac{\hbar}{m_0}\,\nabla\varphi(\boldsymbol{r},t)}_{=\boldsymbol{v}(\boldsymbol{r},t)}\,,$$

as a consequence of which one obtains Eq.(65). If one is dealing with a stationary state whose velocity field contains a vortex line, e. g. an excited state of a hydrogen electron possessing an orbital momentum, we have

$$\oint \boldsymbol{v}(\boldsymbol{r}) \cdot d\boldsymbol{r} \neq 0 \tag{68}$$

for any path encircling the vortex line (=quantization axis). On inserting here $\boldsymbol{v} = \frac{\hbar}{m_0}\,\nabla\varphi$ one obtains

$$\int_{\boldsymbol{r}_0}^{\boldsymbol{r}} \nabla\varphi(\boldsymbol{r}) \cdot d\boldsymbol{r} = \varphi(\boldsymbol{r}) - \varphi(\boldsymbol{r}_0) \neq 0 \tag{69}$$

where $\boldsymbol{r}$ and $\boldsymbol{r}_0$ are two points facing each other across the semi-plane, introduced in Section 8, at an infinitesimal distance. Thus, in general the phase of the wave function, and consequently the wave function itself, will be discontinuous at the semi-plane as opposed to $\rho(\boldsymbol{r})$ and $\boldsymbol{j}(\boldsymbol{r})$ which may be presupposed to be smooth functions everywhere.
Clearly, as follows from Eq.(67), $\psi(\boldsymbol{r})$ remains continuous at the semi-plane if

$$\varphi(\boldsymbol{r}) - \varphi(\boldsymbol{r}_0) = 2m\,\pi \quad \text{where} \quad m = \text{integer}\,. \tag{70}$$

But there is no immediately obvious reason why one should require $\psi(\boldsymbol{r})$ to be continuous because only $\rho(\boldsymbol{r})$ and $\boldsymbol{j}(\boldsymbol{r})$ can be regarded as reflecting physical properties of the system. We are hence led to conclude that without an additional argument **neither** our derivation **nor** standard quantum mechanics yields a justification of the proven relation

$$m_0 \oint \boldsymbol{v}(\boldsymbol{r}) \cdot d\boldsymbol{r} = 2m\pi\,\hbar = m\,h \quad \text{where } m = \text{integer} \tag{71}$$

which comprises Eqs.(65), (68) to (70). This has already been pointed out more than 75 years ago by Pauli [21] and Born and Jordan [22]. As opposed to these considerations Wallstrom states in his paper [20]: *"To the best of my knowledge, this condition* (Eq.(71)) *has not yet found any convincing explanation* **outside the context of the Schrödinger equation***"*.
This is definitely incorrect: within that context the assumption of continuity (Eq.(70)) has to be justified by an additional argument as well.

What else necessitates then the continuity of $\psi(\boldsymbol{r})$ everywhere?

To keep the formalism as simple as possible we confine the considerations to a two-dimensional one-particle system in which the potential $V(\boldsymbol{r})$ is cylindrically symmetric. For this case the time-independent Schrödinger equation (50) attains the form

$$\left(-\frac{\hbar^2}{2\,m_0}\left[\frac{\partial^2}{\partial r^2}+\frac{1}{r}\frac{\partial}{\partial r}+\frac{1}{r^2}\frac{\partial^2}{\partial\varphi^2}\right]+V(r)\right)\phi(r,\varphi)=E\,\phi(r,\varphi)\,.$$

If one introduces

$$\phi(r,\varphi)=R(r)\,e^{i\,\hat{\varphi}(\varphi)} \quad \text{where} \quad \hat{\varphi}(\varphi)=k\,\varphi\,;\; k\in\Re\,,$$

the Schrödinger equation becomes

$$\left[\frac{d^2}{dr^2}+\frac{1}{r}\frac{d}{dr}-\frac{k^2}{r^2}+\varepsilon-v(r)\right]R(r)=0 \quad \text{where} \quad \varepsilon-v(r)=\tfrac{2\,m_0}{\hbar^2}[E-V(r)]\,. \tag{72}$$

For any choice of $k$ and for an appropriate value of $\varepsilon$ one can always find a normalizable solution to this differential equation which is regular at $r=0$ and vanishes exponentially for $r\to\infty$, provided that $V(r)$ is not ill-behaved and allows bound states. In this case one can always think of performing a numerical integration of this differential equation to obtain a bound state $R(r)$. If $R(r)$ satisfies Eq.(72), then $\phi(r,\varphi)$ satisfies the Schrödinger equation everywhere even if $k$ is **non-integer**. True, $\phi(r,\varphi)$ is discontinuous within the interval $0<\varphi\leq 2\pi$ for $\varphi=0$ since

$$e^{i\,k\,2\pi}\neq 1\,,$$

however $|\phi(r,\varphi)|^2$ and

$$\boldsymbol{v}(r,\varphi) = \tfrac{\hbar}{m_0}\,\tfrac{1}{r}\,\tfrac{\partial}{\partial\varphi}\,\tilde{\varphi}(\varphi)\,\boldsymbol{e}_\varphi = \tfrac{\hbar}{m_0}\,\tfrac{k}{r}\,\boldsymbol{e}_\varphi$$

remain smooth functions everywhere, and the associated angular momentum is

$$\frac{1}{2\pi}\oint m_0\,\boldsymbol{v}(r,\varphi)\cdot\boldsymbol{d}r = \frac{\hbar}{2\pi}\int_0^{2\pi}\frac{k}{r}\,r\,d\varphi = k\,\hbar\,.$$

We now consider two functions $R_{k_1}$ and $R_{k_2}$ which solve Eq.(72) for two non-integer values $k_1$ and $k_2$, respectively. We choose an appropriate normalization

$$2\pi\int_0^\infty R_{k_1}^2(r)\,r\,dr = 1 \qquad 2\pi\int_0^\infty R_{k_2}^2(r)\,r\,dr = 1$$

and cast their energy eigenvalues $\varepsilon_{k_1}, \varepsilon_{k_2}$, obtained from numerical integration, for example, as

$$\varepsilon_{k_1} = \hbar\,\omega_{k_1} \quad \text{und} \quad \varepsilon_{k_2} = \hbar\,\omega_{k_2}\,.$$

As already alluded to in Section 7 the time-dependent Schrödinger equation which we are going to derive in Section 11 , has the form

$$\left(-\frac{\hbar^2}{2\,m_0}\,\left[\frac{\partial^2}{\partial r^2}+\frac{1}{r}\frac{\partial}{\partial r}+\frac{1}{r^2}\frac{\partial^2}{\partial\varphi^2}\right]+V(r)\right)\phi(r,\varphi,t) = i\,\hbar\,\frac{\partial}{\partial t}\,\phi(r,\varphi,t)\,.$$

Since it constitutes a linear partial differential equation it will be satisfied also by a linear combination of the two functions

$$\begin{aligned}\phi(\boldsymbol{r},t) = \tfrac{1}{\sqrt{2\pi}}[&c_{k_1}\,R_{k_1}(r)\,e^{i(\,k_1\,\varphi-\omega_{k_1}\,t)}\\ &+c_{k_2}\,R_{k_2}(r)\,e^{i(\,k_2\,\varphi-\omega_{k_2}\,t)}]\,.\end{aligned}$$

Without loss of generality the two coefficients $c_{k_1}, c_{k_2}$ may be chosen as real-valued. We now form the expression for the norm of $\phi(\boldsymbol{r},t)$

$$\begin{aligned}\int\underbrace{|\phi(\boldsymbol{r},t)|^2}_{=\rho(\boldsymbol{r},t)}\,d^2r \stackrel{!}{=} 1 = c_{k_1}^2 + c_{k_2}^2 + c_{k_1}\,c_{k_2}\,I_{k_1\,k_2}\times\\ \frac{1}{2\pi}\left[\int_0^{2\pi}e^{i(k_2-k_1)\varphi}\,d\varphi\;\;e^{i(\omega_{k_1}-\omega_{k_2})\,t}+c.c.\right]\,.\end{aligned}$$

Here $I_{k_1\,k_2}$ denotes

$$I_{k_1\,k_2} = \int_0^\infty R_{k_1}(r)\,R_{k_2}(r)\,r\,dr\,.$$

If $k_2 - k_1$ is non-integer, $I_{k_1\,k_2}$ does not vanish, and the norm of $\phi(\boldsymbol{r},t)$ becomes time-dependent which is inadmissible, of course. Hence $k_2 - k_1$ has to be integer. Since the groundstate of the system, associated with $\varepsilon_{k_1}$, for example, is definitely associated with zero current, i. e. $k_1 = 0$, it follows immediately that $k_2$ must be integer for any state with angular momentum ($k_2 \neq 0$).

# 10 An instructive objection, quantum beats and a possible which-way detection

An apparently serious objection against a stochastic foundation of quantum mechanics along the lines of the preceding sections goes back to Mielnik and Tengstrand [31]. The authors refer to an experimental setup as sketched in Figure 7 where the test particle enters from a distant source on the left-hand side and is kept within a tube that extends up to a screen on the right. The tube contains an impermeable partition that completely seals off the upper part (A) from the lower part (B). It possesses a limited, but macroscopic length of, say, 10 cm. The authors argue that according to conventional quantum mechanics the incoming wave would split up into an upper and totally independent lower portion. Yet both portions retain their capability of interfering with each other when they merge again within the area C and beyond. However, if the wave portions are replaced by the set of irregular trajectories which stochastic quantum mechanics claims to be an equivalent of, it seems to be very unlikely that stochastic-force controlled trajectories can preserve information over so long a distance as well as waves. This criticism amounts to perceiving the preceding derivation of the Schrödinger equation from Eq.(41) as ill-founded or even erroneous. It is just the solution to the Schrödinger equation for the particular setup around which the present authors' consideration revolve. On the other hand, it is easy to verify the validity of the derivation. There is simply no step where one may be in doubt. But one has to keep in mind that the solutions $\psi(\boldsymbol{r}) = |\psi(\boldsymbol{r})|\, e^{i\varphi(\boldsymbol{r})}$ to the Schrödinger equation provide only information on ensemble properties and not on a particular trajectory that is a member of the ensemble under study. For example, the velocity $\boldsymbol{v}(\boldsymbol{r}) = \frac{\hbar}{m_0}\nabla\varphi(\boldsymbol{r})$ at some point in the area marked C represents such an average over all trajectories of the ensemble running through that point. This ensemble defines the probability

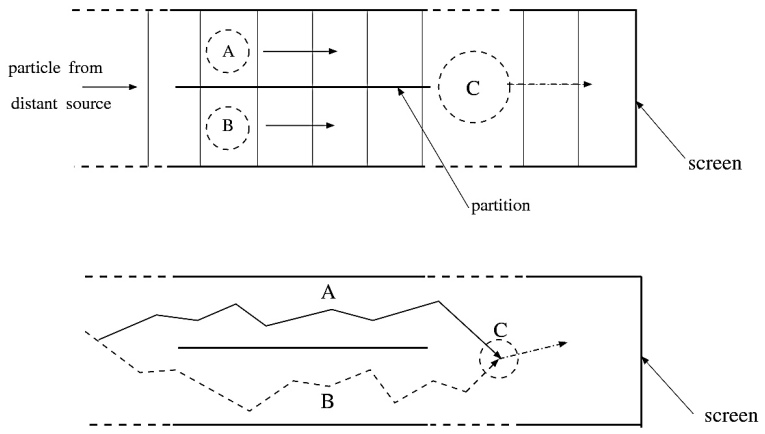


Figure 7: Interference of trajectories

in which direction a particular particle that has arrived at C, e. g. along the "A"-trajectory, will move further. (S. Figure **??**, lower panel.) This is analogous to considerations we shall discuss in the context of the Smoluchowski equation (Section 39). The properties of the ensemble are just an image of the property of the vacuum fluctuations to ensure the absence of dissipation. This manifests itself in the fact that $\boldsymbol{v}(\boldsymbol{r})$ is irrotational as in ideal fluids. An individual particle that has moved along the "A"-trajectory and arrives at C "feels", so to speak, the possibility of a "B"-trajectory. As stated above, it continues its trajectory depending also on the family of "B"-trajectories running through C. If the partition in the tube would be elongated and the point C correspondingly shifted to the right, irrespective of how much, the "A"- and "B"subset of trajectories would now be different, but the scattering probability at C of a particle that has moved along an "A"(or "B")-trajectory would still be influenced by possible "B" (or "A")-trajectories. Furthermore, if one would place some electrostatic array into the upper part of the setup which would cause a spatially confined accelerating electic field the "A"-trajectories would change accordingly and give rise to a different interference pattern within the "C"-range.
To make the surprising content of this observation even more striking we consider a situation where one has particles enter the setup one by one from the left so that only one particle traverses the setup at a time. First, we switch the accelerating array off so that there is no extra potential along the "A"-trajectory. If one has placed a detector, an electron multiplier, for example, at some position $\boldsymbol{r}_{screen}$ on the screen, it would monitor the incoming electrons at a certain rate. These electrons come either along an 'A"- or a "B"-trajectory. Once the extra potential has been turned on, the count rate at $\boldsymbol{r}_{screen}$ changes. Although an electron may have moved along the unmodified "B"-portion of the setup, it feels the modification of the "A"-portion when it arrives at "C". As explained above, this is due to the change of the vacuum scattering probability at C. Electrons that have arrived at some elementary volume within C and have so far preferentially been scattered into $\boldsymbol{r}_{screen}$ are now also scattered to other positions on the screen, thereby changing the count rate at $\boldsymbol{r}_{screen}$.
If the electrostatic array in the "A"-portion would simply consist of two planar parallel grids perpendicular to the average particle motion, and if one applies an accelerating voltage $V$ between the grids, the particles' kinetic energy $\epsilon_0$ increases by an amount $\Delta\epsilon = e\,V$ where $e$ denotes the particle charge. The wave function $\psi_{screen}(\boldsymbol{r}, t)$ at the screen is the sum of the "A"- and "B"-related contributions:

$$= \tfrac{1}{\sqrt{2}} \left[ \hat{\psi}_A(\boldsymbol{r}_{screen})\, e^{-i\omega_A\, t} + \hat{\psi}_B(\boldsymbol{r}_{screen})\, e^{-i\omega_B\, t} \right] \tag{73}$$

where

$$\hat{\psi}_{A/B}(\boldsymbol{r}_{screen}) = \tfrac{1}{\sqrt{\mathcal{V}}}\, e^{ik_{A/B}\, r_{screen}}$$

and

$$\hbar\,\omega_A = \epsilon_0 + \Delta\epsilon\,;\, \hbar\,\omega_B = \epsilon_0\,,$$

and with $1/\sqrt{\mathcal{V}}$ denoting an appropriate normalization factor. The function $\psi(\boldsymbol{r},t)$ solves the time-dependent Schrödinger equation (61) for the particular array under study. If we introduce $\overline{\epsilon} = \epsilon_0 + \frac{1}{2}\,\Delta\epsilon$ we may cast $\hbar\,k_{A/B}$ as $\hbar\,k_{A/B} \approx \sqrt{2m_0\,\overline{\epsilon}}\left(1 \pm \frac{1}{2}\,\frac{\Delta\epsilon}{\overline{\epsilon}}\right)$ if $\frac{\Delta\epsilon}{\overline{\epsilon}} << 1$ where $m_0$ denotes the rest mass of the particle. Eq.(73) can then be rewritten

$$\psi(\boldsymbol{r}_{screen},t) = \tfrac{1}{\sqrt{\mathcal{V}}}\,e^{i(\overline{k}\,r_{screen} - \overline{\omega}\,t)}$$
$$\times\tfrac{1}{\sqrt{2}}\,\left[e^{i(\Delta k\,r_{screen} - \Delta\omega\,t)} + e^{-i(\Delta k\,r_{screen} - \Delta\omega\,t)}\right]$$

where $\hbar\,\overline{k} = \sqrt{2m_0\,\overline{\epsilon}}$, $\Delta k = k_A - k_B$ and $\hbar\,\Delta\omega = \frac{1}{2}\,\Delta\epsilon$. Hence we have for the current density $\boldsymbol{j}(\boldsymbol{r},t) \propto$ count rate at $\boldsymbol{r}_{screen}$

$$\boldsymbol{j}(\boldsymbol{r}_{screen},t) = \tfrac{\hbar\overline{\boldsymbol{k}}}{m_0}\,|\psi(\boldsymbol{r}_{screen},t)|^2 = \tfrac{1}{4\mathcal{V}}\,\tfrac{\hbar\overline{\boldsymbol{k}}}{m_0}\,[1 + \cos(2\Delta k\,r_{screen} - 2\Delta\omega\,t)]\,. \quad (74)$$

That means: the count rate oscillates at a period of $T = \frac{2\pi\hbar}{\Delta\epsilon}$. This most surprising effect of "quantum beats" has, in fact, been observed by Rauch and collaborators (s. Badurek et al. [92]) who used spin polarized neutrons instead of electrons. The energy change $\Delta\epsilon$ in the "A"-section of the setup was in that case imparted to the respective neutron by flipping its spin within a spatially confined magnetic field along the "A"-trajectory. (In practice one used a spin flipper also in the "B"-portion of the setup where the corresponding magnetic field was slightly lower than in the "A"-portion so that $\Delta\epsilon$ referred to the difference of two spin flip energies in this case. Another spin-flip was necessary anyway to enable the two beams to interfere with each other.)

It is worth noticing that $\boldsymbol{j}(\boldsymbol{r}_{screen},t)$ displays - apart from its oscillatory time dependence - an oscillatory behavior also in space, i. e. in the plane of the screen. This is due to the occurrence of $\Delta k\,r_{screen}$ in the argument of the cosine. Hence, in the plane of the screen the current density displays an interference pattern which moves perpendicular to the interference lines with a velocity $\Delta\omega/\Delta k$. If one would replace the screen by a one-slit diaphragm of adjustable width, a detector behind the slit would monitor the incoming electrons one by one. According to Eq.(74) the current density oscillates at the frequency $2\Delta\omega$ about the value $\frac{1}{4\mathcal{V}}\,\frac{\hbar\overline{\boldsymbol{k}}}{m_0}$. If the capture width of the detector, i. e. the slit of the diaphragm comprises a bright and a dark interference line, there is no oscillation of the count rate any more. If the width is narrower than that, oscillations occur which indicate the presence of the interference pattern. This situation will (very likely) not be affected, that is, the oscillations will persist, if one places an energy analyzer between the diaphragm and the detector. The analyzer can be set such that only electrons that have the energy of the "A-trajectory" are allowed to pass.

As the oscillations still occur, one is led to conclude then that tracing the electron's path does not destroy the interference.

## 11 The time-dependent Schrödinger equation

In the most general case $\boldsymbol{v}$ and hence $\varphi$ are time-dependent. As already pointed out in Section 7 the substitution of $\rho(\boldsymbol{r})$ has to be modified then in the form

$$\psi(\boldsymbol{r},t) = \pm\sqrt{\rho(\boldsymbol{r},t)}\, e^{i\varphi\,(\boldsymbol{r},\,t)} \tag{75}$$

which was introduced by Madelung in 1926 [34].
It cannot be overemphasized that this transform achieves actually a miracle. The equation of motion (41), (42) that we have obtained by allowing for additional stochastic vacuum forces is unpleasantly non-linear. This results from the peculiar occurrence of $\rho(\boldsymbol{r},t)$ in the quantum potential (42) whereby Newton's modified second law (41) attains the form

$$m_0 \frac{d}{dt}\boldsymbol{v}(\boldsymbol{r},t) = -\nabla\left(V(\boldsymbol{r}) + \tfrac{\hbar^2}{4\,m_0}\left[\frac{1}{2}\left(\frac{\nabla\rho}{\rho}\right)^2 - \frac{\nabla^2\rho}{\rho}\right]\right).$$

Moreover, there is an additional non-linearity connected with the second term on the right-hand side of

$$\frac{d}{dt}\boldsymbol{v}(\boldsymbol{r},t) = \frac{\partial}{\partial t}\boldsymbol{v}(\boldsymbol{r},t) + \left(\boldsymbol{v}(\boldsymbol{r},t)\cdot\nabla\right)\boldsymbol{v}(\boldsymbol{r},t))$$

which persists, of course, if $\boldsymbol{v}(\boldsymbol{r},t)$ is replaced with its potential

$$\boldsymbol{v}(\boldsymbol{r},t) = \frac{\hbar}{m_0}\,\nabla\varphi(\boldsymbol{r},t)\,.$$

The function $\psi(\boldsymbol{r},t)$ in (75) absorbs the two real-valued functions $\rho(\boldsymbol{r},t)$ and $\varphi(\boldsymbol{r},t)$ to form a complex-valued one. It is this combination which makes quantum mechanics in a peculiar way different from classical mechanics and electrodynamics where all fields are real-valued. Most surprisingly the above non-linearities disappear when $\rho(\boldsymbol{r},t)$ and $\varphi(\boldsymbol{r},t)$ are eliminated by using (75) which leads to the time-dependent Schrödinger equation as will become apparent below. This fortunate situation remains when electromagnetic fields come into play. This will be the subject of Section 15.

The $\pm$-sign in Eq.(75) requires a comment. As discussed in Section 4, $\rho(\boldsymbol{r},t)$ will generally be presupposed as a smooth function. The zeros of $\rho(\boldsymbol{r},t)$ pose a particular problem that occurred already in Section 7, but was not explicitly mentioned. The admissible type of zeros limits the set of functions $\rho(\boldsymbol{r})$ that can be mapped onto $\psi(\boldsymbol{r})$ according to Eq.(55). For simplicity we

confine ourselves to the time-independent case and assume that the zeros of $\rho(\boldsymbol{r})$ lie on the faces of a rectangular parallelepiped defined by the equations $x_\nu = x_{\nu 0}$ with $x_\nu$ and $\nu = 1, 2, 3$ denoting Cartesian coordinates. Hence close to $x_\nu = x_{\nu 0}$ and perpendicular to the respective face the density varies as $(x_\nu - x_{\nu 0})^2$. Since we have everywhere $\rho(\boldsymbol{r}) \geq 0$ its square root varies as $|x_\nu - x_{\nu 0}|$ and thus would not be differentiable at $x_\nu = x_{\nu 0}$. In defining the map $\rho(\boldsymbol{r}) \to \psi(\boldsymbol{r})$ one is forced hence to choose the positive sign in front of $\sqrt{\rho(\boldsymbol{r})}$ outside the rectangular parallelepiped if one has chosen the minus sign inside (or vice versa) to ensure that $\psi(\boldsymbol{r})$ stays differentiable across the face of the rectangular parallelepiped. Hence, mapping functions $\rho(\boldsymbol{r})$ onto differentiable functions $\psi(\boldsymbol{r})$ is only possible if the zeros of $\rho(\boldsymbol{r})$ subdivide the space of volume $\mathcal{V}$ into cells without leaving empty space. At first sight it appears that this limitation in the set of admissible functions $\rho(\boldsymbol{r})$ constitutes a serious drawback of the entire concept. One has to bear in mind, however, that the functions $\psi(\boldsymbol{r})$ are not determined as a map of $\rho(\boldsymbol{r})$ but rather by solving the Schrödinger equation (50) which has been the objective of the derivation. Physical meaningful solutions to Eq.(50) have automatically the required spatial structure of their zeros.

We now move on to derive the time-dependent Schrödinger equation under the supposition that the above considerations apply to the time-dependent case as well.
If one uses instead of Eq.(41) the arithmetic mean of the original Eq.(25) and its "anti-Brownian" analogue where the sign of $\nu$ and $\boldsymbol{u}(\boldsymbol{r}, t)$ is reversed, one obtains

$$\frac{\partial}{\partial t}\,\boldsymbol{v} + (\boldsymbol{v}\cdot\nabla)\,\boldsymbol{v} - (\boldsymbol{u}\cdot\nabla)\,\boldsymbol{u} + \frac{\hbar}{2\,m_0}\,\Delta\boldsymbol{u} = \frac{1}{m_0}\,\boldsymbol{F}(\boldsymbol{r})\,. \tag{76}$$

This can be simplified in the form:

$$\frac{\partial}{\partial\, t}\boldsymbol{v} = -\frac{1}{m_0}\,\nabla V - \frac{1}{2}\,\nabla\boldsymbol{v}^2 + \frac{1}{2}\,\nabla\boldsymbol{u}^2 - \frac{\hbar}{2\,m_0}\,\Delta\boldsymbol{u}\,, \tag{77}$$

where we have made use of the relations

$$\boldsymbol{v}\cdot\nabla\boldsymbol{v} = \frac{1}{2}\nabla\boldsymbol{v}^2\,; \quad \boldsymbol{u}\cdot\nabla\boldsymbol{u} = \frac{1}{2}\nabla\boldsymbol{u}^2 \quad \text{and} \quad \nu = \frac{\hbar}{2m_0}\,.$$

With the first two equations it has been observed that $\boldsymbol{v}$ and $\boldsymbol{u}$ are irrotational. On differentiating $\boldsymbol{u}$ with respect to time and using Eq.(26) one obtains

$$\frac{\partial}{\partial\, t}\,\boldsymbol{u} = -\frac{\hbar}{2\,m_0}\,\nabla\,(\frac{\partial\,\rho}{\partial\, t}/\rho)\,, \tag{78}$$

Invoking the equation of continuity

$$\partial\,\rho/\partial\, t + \nabla\cdot(\rho\,\boldsymbol{v}) = 0 \tag{79}$$

that is

$$\partial\,\rho/\partial\,t + \rho\,\nabla\cdot\boldsymbol{v} + \boldsymbol{v}\cdot\nabla\rho = 0$$

$\frac{\partial\,\rho}{\partial\,t}/\rho$ can be replaced with $-\nabla\cdot\boldsymbol{v} - \boldsymbol{v}\cdot\frac{1}{\rho}\,\nabla\rho$ which yields

$$-\frac{\hbar}{2\,m_0}\,\nabla\,(\frac{\partial\,\rho}{\partial\,t}/\rho) = \frac{\hbar}{2\,m_0}\,\nabla\,(\nabla\cdot\boldsymbol{v}) - \nabla\left[\boldsymbol{v}\cdot\left(-\frac{\hbar}{2\,m_0}\,\frac{1}{\rho}\,\nabla\rho\right)\right]\,. \qquad (80)$$

Using Eq.(26) we may substitute $\boldsymbol{v}\cdot\boldsymbol{u}$ for the expression in the [...]-brackets on the right-hand side. Hence Eq.(80) takes the form

$$\frac{\partial}{\partial\,t}\,\boldsymbol{u} = \frac{\hbar}{2\,m_0}\,\nabla(\nabla\cdot\boldsymbol{v}) - \nabla(\boldsymbol{u}\cdot\boldsymbol{v})\,. \qquad (81)$$

On multiplying the equation of motion (77) by the imaginary unit $i$ and subtracting Eq.(81) we obtain

$$\frac{\partial}{\partial\,t}\,(-\boldsymbol{u} + i\,\boldsymbol{v}) =$$
$$-\frac{i}{m_0}\,\nabla V - \frac{i}{2}\,\nabla\boldsymbol{v}^2 + \frac{i}{2}\,\nabla\boldsymbol{u}^2 - i\,\frac{\hbar}{2\,m_0}\,\Delta\boldsymbol{u} - \frac{\hbar}{2\,m_0}\,\nabla(\nabla\cdot\boldsymbol{v}) + \nabla(\boldsymbol{u}\cdot\boldsymbol{v})\,.$$

After reordering the terms on the right-hand side this becomes

$$\frac{\partial}{\partial\,t}\,(-\boldsymbol{u} + i\,\boldsymbol{v}) = \frac{i}{2}\,\nabla(-\boldsymbol{u} + i\,\boldsymbol{v})^2 + \frac{i\,\hbar}{2\,m_0}\nabla\,[\nabla\cdot(-\boldsymbol{u} + i\,\boldsymbol{v})] - \frac{i}{m_0}\,\nabla V\,. \qquad (82)$$

Here we insert Eqs.(31), (65) and (75) in the form

$$-\boldsymbol{u} + i\,\boldsymbol{v} = \frac{\hbar}{m_0}\,\nabla\ln\,[\psi/\sqrt{\rho_0}]\,. \qquad (83)$$

After interchanging the operators $\partial/\partial\,t$ and $\nabla$ one obtains

$$\nabla\left(\frac{\hbar}{m_0}\frac{1}{\psi}\,\frac{\partial\,\psi}{\partial\,t}\right) = \nabla\left[\frac{i}{2}\,\frac{\hbar^2}{m_0^2}\left\{\left(\frac{1}{\psi}\,\nabla\psi\right)^2 + \nabla\cdot\left(\frac{1}{\psi}\,\nabla\psi\right)\right\} - \frac{i}{m_0}\,V\right]\,.$$

If the gradient of some function equals that of another function the two functions can only differ by a real-space independent function of time which we denote by $\beta(t)$. Hence, if one divides the above equation by the imaginary unit the result may be cast as

$$-i\,\frac{\hbar}{m_0}\frac{1}{\psi}\,\frac{\partial\,\psi}{\partial\,t} = \frac{1}{2}\,\frac{\hbar^2}{m_0^2}\left[\left(\frac{1}{\psi}\,\nabla\psi\right)^2 + \nabla\cdot\left(\frac{1}{\psi}\,\nabla\psi\right)\right] - \frac{1}{m_0}\,V - i\,\beta(t)\,. \qquad (84)$$

One can now make use of the identity

$$\nabla\cdot\left(\frac{1}{\psi}\,\nabla\psi\right) = -\left(\frac{1}{\psi}\,\nabla\psi\right)^2 + \frac{1}{\psi}\,\nabla^2\psi$$

and multiply Eq.(84) by $-m_0\,\psi$. This yields

$$i\hbar\,\frac{\partial\,\psi}{\partial\,t} = -\frac{\hbar^2\nabla^2}{2\,m_0}\,\psi + V\,\psi + \gamma(t)\,\psi \tag{85}$$

where

$$\gamma(t) = i\,m_0\,\beta(t)\,.$$

If $\psi(\boldsymbol{r},t)$ is replaced by $\widehat{\psi}(\boldsymbol{r},t)$ defined through

$$\psi(\boldsymbol{r},t) = \widehat{\psi}(\boldsymbol{r},t)\,\exp\left[-\frac{i}{\hbar}\int_{t_0}^{t}\gamma(t')\,dt'\right]\,,$$

Eq.(85) becomes an equation for $\widehat{\psi}(\boldsymbol{r},t)$:

$$i\hbar\,\frac{\partial\,\widehat{\psi}(\boldsymbol{r},t)}{\partial\,t} = \left[\frac{\widehat{\boldsymbol{p}}^2}{2\,m_0} + V(\boldsymbol{r})\right]\,\widehat{\psi}(\boldsymbol{r},t)\,, \tag{86}$$

where

$$\widehat{\boldsymbol{p}} \equiv -i\hbar\nabla\,. \tag{87}$$

The two functions $\psi(\boldsymbol{r},t)$ and $\widehat{\psi}(\boldsymbol{r},t)$ differ only in a time-dependent phase factor without physical relevance. Only the functions

$$\rho(\boldsymbol{r},t) = \psi^*(\boldsymbol{r},t)\,\psi(\boldsymbol{r},t) \qquad \text{(density)} \tag{88}$$

and the current density:

$$\boldsymbol{j}(\boldsymbol{r},t) = \rho(\boldsymbol{r},t)\,\frac{\hbar}{m_0}\,\nabla\,\varphi(\boldsymbol{r},t)\,, \tag{89}$$

refer to relevant quantities of the system which obviously do not depend on this phase factor. For this reason we may set $\gamma(t) \equiv 0$, that is, replace $\widehat{\psi}(\boldsymbol{r},t)$ in Eq.(86) with $\psi(\boldsymbol{r},t)$ without loss of generality. To simplify the notation we introduce the so-called Hamiltonian defined by

$$\widehat{H} \equiv \frac{\widehat{\boldsymbol{p}}^2}{2\,m_0} + V(\boldsymbol{r})\,. \tag{90}$$

Eq.(86) then takes the familiar form of the Schrödinger equation

$$i\hbar\,\frac{\partial\,\psi(\boldsymbol{r},t)}{\partial\,t} = \widehat{H}(\boldsymbol{r})\,\psi(\boldsymbol{r},t) \tag{91}$$

which is linear in $\psi(\boldsymbol{r},t)$, as announced in the beginning of this section.
The first order time derivative on the left-hand side can be traced back to

the acceleration $(\partial/\partial t)\,\boldsymbol{v}$ in Newton's modified second law (76).
Using

$$\psi(\boldsymbol{r},t) = |\psi(\boldsymbol{r},t)|\, e^{i\,\varphi(\boldsymbol{r},t)}$$

and inserting this into Eqs.(88) and (89) one obtains the familiar expression

$$\boldsymbol{j}(\boldsymbol{r},t) = \rho(\boldsymbol{r},t)\,\boldsymbol{v}(\boldsymbol{r},t) = \frac{\hbar}{2i\,m_0}\,[\psi^*(\boldsymbol{r},t)\nabla\,\psi(\boldsymbol{r},t) - \psi(\boldsymbol{r},t)\nabla\,\psi^*(\boldsymbol{r},t)] \quad (92)$$

which on real-space integration and multiplication by $m_0$ yields

$$m_0\,\langle \boldsymbol{v}(t)\rangle = \int \psi^*(\boldsymbol{r},t)\,\widehat{\boldsymbol{p}}\,\psi(\boldsymbol{r},t)\,d^3r \equiv \langle\widehat{\boldsymbol{p}}\rangle \quad (93)$$

where $\psi(\boldsymbol{r},t)$ has been required to satisfy the usual boundary conditions at the surface of the normalization box. Because of Eq.(93) one is justified in terming $\widehat{\boldsymbol{p}}$ "momentum operator".
In Bohm's version of quantum mechanics [28] Eq.(92) is recast to define the velocity field

$$\boldsymbol{v}(\boldsymbol{r},t) = \frac{\hbar}{m_0}\,\Im\left(\frac{\nabla\psi(\boldsymbol{r},t)}{\psi(\boldsymbol{r},t)}\right).$$

The flowlines of this field are interpreted as true particle trajectories. From our point of view this appears to be rather absurd because the explicit $\boldsymbol{r}$-dependence of $\boldsymbol{v}$ comes about by forming the ensemble average over the (in principle infinite) family of true trajectories as defined in Eq.(21). Bohm's definition of $\boldsymbol{v}$ as describing the true velocity of the particle leads inescapably to strange results, notably with stationary real-valued wave functions $\psi(\boldsymbol{r})$ for which $\boldsymbol{v}(\boldsymbol{r}) \equiv 0$. Hence, the particle appears to be at rest although the kinetic energy of the particle

$$\langle\widehat{T}\rangle = \int \psi^*(\boldsymbol{r})\,\frac{\widehat{\boldsymbol{p}}^2}{2\,m_0}\,\psi(\boldsymbol{r})\,d^3r \equiv \frac{\langle\widehat{\boldsymbol{p}}^2\rangle}{2\,m_0} \quad (94)$$

is definitely different from zero.
The time-dependent Schrödinger equation represents the center of non-relativistic quantum mechanics. Fundamentally different from the present approach where it is derived from a new vacuum concept, in conventional quantum mechanics it falls out of the blue, and this applies to Bohm's theory as well. As the latter associates the pattern of smooth flowlines with the set of true particle trajectories, it is forced to explain the probabilistic character of the information contained in $\psi(\boldsymbol{r},t)$ by an additional "quantum equilibrium"- hypothesis. It is therefore hard to see that anything can be gained from "going Bohmian". The "process of measurement" in which a particle moves from a source to the detector where it fires a counter, is in our view described by one of the irregular trajectories which is terminated at the detector. Due to the stochastic forces that cause this irregularity, the

information on the ensemble properties is naturally probabilistic.
A frequently raised objection against Bohm's theory concerns the asymmetric way in which it deals with the particle's real-space position and its momentum. In fact, the real-space position $\boldsymbol{r}$ plays a pivotal role in Bohm's theory compared to the other observables which are "contextualized" by resorting to the wave function $\psi(\boldsymbol{r},t)$ that solves the Schrödinger equation for the system under study. By contrast, in our approach the ensemble's $i$-th particle position $\boldsymbol{r}_i$ and its velocity $\boldsymbol{v}_i(t)$ enter into the theory as autonomous quantities. This is reflected in the occurrence of two independent functions $\rho(\boldsymbol{r},t)$ and $\boldsymbol{v}(\boldsymbol{r},t) = \frac{\hbar}{2\,m_0}\,\nabla\varphi(\boldsymbol{r}\,t)$. As stated above, it is this pair of information $\rho(\boldsymbol{r},t)\,;\varphi(\boldsymbol{r},t)$ that necessitates the description of the one-particle system by a **complex**-valued function

$$\psi(\boldsymbol{r},t) = \pm\sqrt{\rho(\boldsymbol{r},t)}\,e^{i\,\varphi(\boldsymbol{r},t)}\,.$$

## 12 The uncertainty relation and the issue of "measurement"

By performing a Fourier transform on $\psi(\boldsymbol{r},t)$

$$\psi(\boldsymbol{r},t) = \frac{1}{(2\,\pi)^{3/2}}\int C(\boldsymbol{k},t)\,e^{i\,\boldsymbol{k}\cdot\boldsymbol{r}}\,d^3k \tag{95}$$

Eqs.(93) and (94) may alternatively be written

$$\begin{aligned}\langle\widehat{\boldsymbol{p}}\rangle &= \int\psi^*(\boldsymbol{r},t)\,\widehat{\boldsymbol{p}}\,\psi(\boldsymbol{r},t)\,d^3r = \int C^*(\boldsymbol{k},t)\,(\hbar\,\boldsymbol{k})\,C(\boldsymbol{k},t)\,d^3k\\ \langle\widehat{\boldsymbol{p}}^2\rangle &= \int\psi^*(\boldsymbol{r},t)\,\widehat{\boldsymbol{p}}^2\,\psi(\boldsymbol{r},t)\,d^3r = \int C^*(\boldsymbol{k},t)\,(\hbar\,\boldsymbol{k})^2\,C(\boldsymbol{k},t)\,d^3k\end{aligned} \tag{96}$$

where

$$C^*(\boldsymbol{k},t)\,C(\boldsymbol{k},t)\,\Delta^3k = P(\boldsymbol{k},t)\,\Delta^3k \tag{97}$$

describes the probability of the particle possessing a momentum that lies within $\Delta^3k$ about $\boldsymbol{k}$ in the $\boldsymbol{k}$-space. We temporarily label the coordinate-components of the particle in the two spaces by an index $\nu$:

$$\nu = 1,2,3\,.$$

The mean square departures of the position coordinates $x_\nu$ and $k_\nu$, respectively, from their arithmetic means $\bar{x}_\nu$ and $\bar{k}_\nu$ are given by

$$\langle(x_\nu-\bar{x}_\nu)^2\rangle_t = \int\psi^*(\boldsymbol{r},t)\,(x_\nu-\bar{x}_\nu)^2\,\psi(\boldsymbol{r},t)\,d^3r$$

and

$$\langle (k_\nu - \bar{k}_\nu)^2 \rangle_t = \int C^*(\boldsymbol{k},t)\,(k_\nu - \bar{k}_\nu)^2\, C(\boldsymbol{k},t)\, d^3k\,.$$

Since $C(\boldsymbol{k},t)$ is the Fourier transform of $\psi(\boldsymbol{r},t)$ we have as a fundamental mathematical theorem

$$\langle (x_\nu - \bar{x}_\nu)^2 \rangle_t \, \langle (k_\nu - \bar{k}_\nu)^2 \rangle_t \geq \frac{1}{4}$$

that is

$$\langle (x_\nu - \bar{x}_\nu)^2 \rangle_t \, \langle (\hbar\, k_\nu - \hbar\, \bar{k}_\nu)^2 \rangle_t \geq \frac{\hbar^2}{4}\,. \tag{98}$$

Following the standard notation by setting $\Delta x_\nu = \sqrt{\langle (x_\nu - \bar{x}_\nu)^2 \rangle_t}$ and $\Delta p_\nu = \sqrt{\langle (\hbar\, k_\nu - \hbar\, \bar{k}_\nu)^2 \rangle_t} = \sqrt{\langle (\widehat{\boldsymbol{p}} - \langle \widehat{\boldsymbol{p}} \rangle)^2 \rangle_t}$ the latter relation may be cast as

$$\Delta x_\nu \, \Delta p_\nu \geq \frac{\hbar}{2} \tag{99}$$

which constitutes the celebrated uncertainty relation. It is commonplace to interpret this relation, loosely speaking, by saying: "momentum and position of a particle cannot be measured simultaneously with any desirable precision".
From our point of view it does in no way refer to any measurement on the position or momentum of the particle in question. It is nothing more than the theorem Eq.(98) on the product of two quantities that are interconnected by a Fourier transform. Furthermore, since this relation is - besides the Schrödinger equation - just another consequence of our concept, it cannot possibly conflict with the existence of trajectories which constitute a fundamental element of that concept.
Eq.(99) is considered ground-laying for the Copenhagen interpretation of quantum mechanics. The latter is based on the conviction that it is the measurement that causes the indeterminacy in quantum mechanics and necessitates a probabilistic description of microscopic mechanical systems. In a highly respected article [35] Heisenberg gives a revealing example of such a measurement. To pinpoint an electron moving along the $x$-axis within an experimental setup he considers a $\gamma$-ray source, that illuminates the electron beam, and a hypothetical $\gamma$-ray microscope that possesses a sufficiently high resolution in detecting the position of that electron up to an error of $\Delta x$. He demonstrates that the $\gamma$-ray photon that "hits the electron" and is subsequently scattered into the microscope, transfers a momentum $\Delta p_x$ to the electron so that

$$\Delta x \, \Delta p_x \approx \hbar\,. \tag{100}$$

The above result reflects only a property of the microscope

$$\Delta x\,\Delta k_x \approx 2\,\pi$$

which interrelates the resolved linear dimensions $\Delta x = \lambda/\sin\alpha$ of an object and the admissible maximum angle $\alpha$ required to ensure that the scattered wave (of wavelength $\lambda$) is still captured by the front lens of the microscope, and $\Delta k_x = k\,\sin\alpha$ which describes the $k_x$-change of the wave vector of the scattered wave. But this interrelation expresses only the content of Eq.(98) in a different form. The measurement, however, is completely fictional for two reasons. Firstly, imaging systems within that regime of wavelength are for fundamental reasons unfeasible. Secondly, different from the picture insinuated by Heisenberg's phrasing, the interaction does not take place as an instantaneous collision process where a point-like particle (the photon) hits another point-like particle, the electron. Instead the transition probability of the electron for attaining a different momentum is given by the mod squared of the transition matrix element $M_{opt}$, a real-space integral that extends over a range of many light wave lengths in diameter. Moreover, the transition is not instantaneous but rather takes some time of the order $\hbar/|M_{opt}|$. Within this transition time the electron moves a distance $\Delta x'$ which has nothing to do with $\Delta x$ in Eq.(100). Other examples of "measurement", e. g. diffraction at slits of a certain width $\Delta x$ show even more directly that the probabilistic information on the (non-relativistic) motion of a particle is exhaustively described by the Schrödinger equation and boundary conditions for $\psi(\boldsymbol{r})$, and hence this information merely reflects our vacuum concept, irrespective of whether or not results on the diffraction are verified by measurements.
The host of considerations invoking the uncertainty relation (99) refers to situations where a particle is located within an interval $\Delta x$ and one interprets this confinement of the particle indiscriminately in terms of a "measurement" of its coordinate $x$ with limited accuracy. One concludes then from the uncertainty relation that $\Delta x$ correlates unavoidably with a diperson $\overline{\Delta p_x^2}$ of its momentum such that $\Delta x\,\Delta p_x \gtrapprox \frac{\hbar}{2}$ where $\Delta p_x \stackrel{\text{def}}{=} \sqrt{\overline{\Delta p_x^2}}$. In reality neither a measurement on $\Delta x$ nor on $\overline{\Delta p^2}$ is truly executable. The uncertainty relation merely states that a solution of the one-dimensional Schrödinger equation for a particle in a box of length $\Delta x$ yields a ground state energy $\Delta E = \frac{\Delta p^2}{2\,m_0}$ where $\Delta p^2 = \left(\hbar\,\frac{\pi}{\Delta x}\right)^2$. Hence one obtains simply as a consequence of solving the Schrödinger equation for that case "without observer"(!) $\Delta x\,\Delta p = \pi\,\hbar$. One cannot help but quote John Bell's question phrased in his stirring article "Against Measurement"[36]

*"What exactly qualifies some physical systems to play the role of 'measurer'?"*

The above considerations are in line with a discussion of Heisenberg's paper by Wigner [37].

## 13 Averaging over the total ensemble

In forming the arithmetic mean of the two equations (35) and (38) we omitted to mention a problem that we wish to discuss here in more detail.
We temporarily decompose the entire ensemble considered so far into a "Brownian" and "anti-Brownian" sub-ensemble, each characterized by the associated stochastic forces and comprising an equally large number of members. Accordingly we distinguish the velocities $\boldsymbol{v}(\boldsymbol{r},t)$ and the densities $\rho(\boldsymbol{r},t)$ in the respective sub-ensembles by subscripts $B$ (for "Brownian") and $A$ (for "Anti-Brownian"). If the velocities in these two equations agree at a time $t$, they are definitely different at a later time $t+\Delta t$. Yet forming the arithmetic mean of the two equations can only lead to the same average - which we could recast as "Newton's modified second law", Eq.(41) - if the two velocities $\boldsymbol{v}_B, \boldsymbol{v}_A$ and the densities $\rho_B, \rho_A$ agree also at $t+\Delta t$ and any later time. At first sight the latter appears to be irreconcilable with the former. One has to recall, however, that our subdivision of the entire ensemble into sub-ensembles $B$ and $A$ represents only a simplifying model for the actually occurring reversible scatterings. In the real system the stochastic forces of the $B$-type become automatically forces of the $A$-type and vice versa within the characteristic time $\tau$ so that the change of the velocity $\Delta\boldsymbol{v}$ in either sub-ensemble is $[\Delta\boldsymbol{v}_A+\Delta\boldsymbol{v}_B]/2$ within a time span $\Delta t \gg \tau$ which, however, must be small compared to time intervals within which the quantities of interest change sizeably. The situation is similar to that encountered in diffusion theory where we have

$$\frac{\partial\rho}{\partial t} = \nu\,\Delta\rho\,.$$

This equation is obtained from the equation of continuity for $\boldsymbol{v}_B = \boldsymbol{u}$ and $\boldsymbol{u} = -\nu\,\nabla\rho/\rho$ with the latter equation based on similar considerations as the derivation of Eq.(25) invoking Einstein's law (40) which implies $\Delta t \gg \tau$. The above equation of diffusion hence describes changes that are actually defined only on a coarse grain time scale and its validity is confined to changes that are sufficiently slow on that time scale. As we have already discussed in Section 5, this is also the assumption underlying our derivation of Newton's modified second law (41).
We temporarily rewrite the two equations (35) and (38) for an - in that sense - "appropriately long, but sufficiently short time interval" $\Delta t$ in the form

$$\Delta\boldsymbol{v}_{B/A}(\boldsymbol{r},t+\Delta t) = \boldsymbol{R}_{B/A}(\boldsymbol{r},t)\,\Delta t$$

where

$$\boldsymbol{R}_{B/A}(\boldsymbol{r},t) = \frac{1}{m_0}\left(-\nabla[V(\boldsymbol{r}) + V_{QP}(\boldsymbol{r},t)] \pm \vec{\Omega}(\boldsymbol{r},t)\right) . \tag{101}$$

and

$$\vec{\Omega} = \frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{v}\cdot\nabla)\,\boldsymbol{u} - (\boldsymbol{u}\cdot\nabla)\,\boldsymbol{v} + \nu\,\Delta\,\boldsymbol{v}\,.$$

Here we have already used $V_{QP}$ instead of $V_{stoch}$, but still denoted the prefactor of $\Delta\boldsymbol{v}$ by $\nu$ to demonstrate that $\vec{\Omega}$ (and consequently $\boldsymbol{u}$) changes sign when $\nu$ changes sign. It should be noticed that according to Eq.(42) $V_{QP}$ has the property $V_{QP}(\rho_B(\boldsymbol{r},t)) = V_{QP}(\rho_A(\boldsymbol{r},t)) = V_{QP}(\rho(\boldsymbol{r},t))$ since at the time $t$ under consideration we have $\rho_A(\boldsymbol{r},t) = \rho_B(\boldsymbol{r},t) = \frac{1}{2}\,\rho(\boldsymbol{r},t)$.
Within a time span $\Delta t$ the velocities $\boldsymbol{v}_B(\boldsymbol{r},t)$ and $\boldsymbol{v}_A(\boldsymbol{r},t)$ change according to

$$\boldsymbol{v}_B(\boldsymbol{r},t+\Delta t) = \boldsymbol{v}(\boldsymbol{r},t) + R_B(\boldsymbol{r},t)\,\Delta t\,,$$

$$\boldsymbol{v}_A(\boldsymbol{r},t+\Delta t) = \boldsymbol{v}(\boldsymbol{r},t) + R_A(\boldsymbol{r},t)\,\Delta t\,.$$

At the end of this time interval one forms according to the definition (21) the average over the total ensemble, that is the arithmetic mean of $\boldsymbol{v}_B(\boldsymbol{r},t+\Delta t)$ and $\boldsymbol{v}_A(\boldsymbol{r},t+\Delta t)$

$$\boldsymbol{v}(\boldsymbol{r},t+\Delta t) \stackrel{def}{=} \tfrac{1}{2}\,[\boldsymbol{v}_A(\boldsymbol{r},t+\Delta t) + \boldsymbol{v}_B(\boldsymbol{r},t+\Delta t)] = \boldsymbol{v}(\boldsymbol{r},t) + \underbrace{\tfrac{1}{2}\,[\boldsymbol{R}_A(\boldsymbol{r},t) + \boldsymbol{R}_B(\boldsymbol{r},t)]}_{=\frac{1}{m_0}(-grad\,[V(\boldsymbol{r})+V_{stoch}(\boldsymbol{r},t)])}\;\Delta t\,.$$

We consider this equation as implicitly defining "motion under reversible scattering". In the subsquent time interval each of the $N/2$ particles changes its affiliation (B from A or vice versa).
Subtracting $\boldsymbol{v}(\boldsymbol{r},t)$ on either side and dividing by $\Delta t/m_0$ one obtains for sufficiently small $\Delta t$

$$m_0\frac{d}{dt}\boldsymbol{v}(\boldsymbol{r},t) = \boldsymbol{F}(\boldsymbol{r})\underbrace{-grad\,V_{QP}(\boldsymbol{r},t)}_{\stackrel{Def}{=}\boldsymbol{F}_{QP}(\boldsymbol{r},t)}\,.$$

We want to demonstrate that the densities behave analogously. For this reason we resort to the equation of continuity (79) which holds for each sub-ensemble

$$\frac{\partial \rho_{B/A}}{\partial t} + \nabla\cdot(\rho_{B/A}\,\boldsymbol{v}_{A/B}) = 0\,. \tag{102}$$

It describes the conservation of the number of particles in each of the two subsystems. We conclude from this equation that $\dot{\rho}_B(\boldsymbol{r},t) = \dot{\rho}_A(\boldsymbol{r},t)$, if

$\rho_B(\boldsymbol{r},t) = \rho_A(\boldsymbol{r},t)$ and $\boldsymbol{v}_B(\boldsymbol{r},t) = \boldsymbol{v}_A(\boldsymbol{r},t)$. If one differentiates Eq.(102) with respect to time and uses $\dot{\boldsymbol{v}}_B(\boldsymbol{r},t) = \dot{\boldsymbol{v}}_A(\boldsymbol{r},t) = \dot{\boldsymbol{v}}(\boldsymbol{r},t)$ as a result of the preceding considerations, we may conclude $\ddot{\rho}_B(\boldsymbol{r},t) = \ddot{\rho}_A(\boldsymbol{r},t)$. One can carry this conclusion further to any order of time derivative. Thus, the Taylor-expansions of $\rho_B(\boldsymbol{r},t+\Delta t)$ and $\rho_A(\boldsymbol{r},t+\Delta t)$ agree for any length of the time interval $\Delta t$ if $\rho_B, \rho_A$ and $\boldsymbol{v}_B, \boldsymbol{v}_A$ agree at time $t$.

## 14 Conservative diffusion. Ehrenfest's theorem

We want to prove the validity of Eq.(46) which constitutes a necessary condition for the preservation of classical motional behavior on the average. To see this more clearly, we first consider one particle (the $i$-th) in the cube $\Delta^3 r$ about $\boldsymbol{r}$ acted upon by the external force $\boldsymbol{F}(\boldsymbol{r})$ and the stochastic force $\boldsymbol{F}_{s\,i}(t)$. According to Newton's second law we have

$$\frac{d}{dt}\, m_0\, \boldsymbol{v}_i(t) = \boldsymbol{F}(\boldsymbol{r}_i) + \boldsymbol{F}_{s\,i}(t)\,.$$

If we sum this equation over the $n(\boldsymbol{r},t)$ particles contained in $\Delta^3 r$, divide by $N$ and form ensemble averages similar to Eqs.(19) and (21) we obtain

$$\frac{\partial}{\partial t}\, m_0\, \frac{1}{N} \underbrace{\sum_{i=1}^{n(\boldsymbol{r},t)} \boldsymbol{v}_i(t)}_{=n(\boldsymbol{r},t)\,\boldsymbol{v}(\boldsymbol{r},t)} = \frac{1}{N} \underbrace{\sum_{i=1}^{n(\boldsymbol{r},t)} \boldsymbol{F}(\boldsymbol{r}_i)}_{=n(\boldsymbol{r},t)\,\boldsymbol{F}(\boldsymbol{r})} + \frac{1}{N} \underbrace{\sum_{i=1}^{n(\boldsymbol{r},t)} \boldsymbol{F}_{s\,i}(t)}_{=n(\boldsymbol{r},t)\,\boldsymbol{F}_s(\boldsymbol{r},t)}\,. \tag{103}$$

Here the summation runs over all particles in the cell irrespective of whether they belong to the first or second sub-ensemble.
The idea of "conservative diffusion" implies that the $N = \sum_{\boldsymbol{r}}^{N_{\boldsymbol{r}}} n(\boldsymbol{r},t)$ particles of the entire ensemble do not feel a stochastic force on average although $\boldsymbol{F}_s(\boldsymbol{r},t)$ does locally not vanish in general. Thus, $\boldsymbol{F}_s(\boldsymbol{r},t)$ is required to have the property

$$\sum_{\boldsymbol{r}}^{N_{\boldsymbol{r}}} \frac{n(\boldsymbol{r},t)}{N}\, \boldsymbol{F}_s(\boldsymbol{r},t) = \int_{\mathcal{V}} \rho(\boldsymbol{r},t)\, \underbrace{\boldsymbol{F}_{QP}(\boldsymbol{r},t)}_{\equiv \boldsymbol{F}_s(\boldsymbol{r},t)}\, d^3 r = 0\ \forall\, t\,, \tag{104}$$

as a result of which Eq.(103) yields after summation over all elementary cells

$$\frac{\partial}{\partial t} \sum_{\boldsymbol{r}}^{N_{\boldsymbol{r}}} m_0\, \frac{n(\boldsymbol{r},t)}{N}\, \boldsymbol{v}(\boldsymbol{r},t) = \frac{d}{dt} \underbrace{\int_{\mathcal{V}} \rho(\boldsymbol{r},t)\, m_0\, \boldsymbol{v}(\boldsymbol{r},t)\, d^3 r}_{\equiv \langle \boldsymbol{p}(t) \rangle} = \underbrace{\sum_{\boldsymbol{r}}^{N_{\boldsymbol{r}}} \frac{n(\boldsymbol{r},t)}{N}\, \boldsymbol{F}(\boldsymbol{r})}_{= \int \rho(\boldsymbol{r},t)\, \boldsymbol{F}(\boldsymbol{r})\, d^3 r = \langle \boldsymbol{F} \rangle}\,.$$

We thus obtain as a consequence of the required property of $\boldsymbol{F}_s(\boldsymbol{r},t)$

$$\frac{d}{dt}\,\langle \boldsymbol{p}(t)\rangle = \langle \boldsymbol{F}\rangle \tag{105}$$

which is Ehrenfest's first theorem[38].
In case of a force-free particle for which $\langle \boldsymbol{F}\rangle = 0$, Eq.(105) yields

$$\langle \boldsymbol{p}(t)\rangle = const.$$

which demonstrates that a free particle exposed to Brownian/anti-Brownian stochastic forces does not change its momentum on the average, as opposed to a particle that moves in a classical "Brownian" environment.

We now want to show that the expectation value of "Newton's modified second law" that we have derived in the form of Eq.(41), attains, in fact, exactly the form of Eq.(105). To this end it is convenient to recast Eq.(42) as

$$V_{QP} = \frac{\hbar^2}{4\,m_0}\,\left[\frac{1}{2}\left(\frac{\nabla\rho}{\rho}\right)^2 - \frac{\nabla^2\rho}{\rho}\right] = m_0\,\left[-\frac{\boldsymbol{u}^2(\boldsymbol{r},t)}{2} + \frac{\hbar}{2m_0}\,\nabla\cdot\boldsymbol{u}(\boldsymbol{r},t)\right]$$

where we have used Eq.(26) defining $\boldsymbol{u}(\boldsymbol{r},t)$. Hence

$$\int \rho(\boldsymbol{r},t)\,\boldsymbol{F}_{QM}(\boldsymbol{r},t)\,d^3r =$$

$$m_0\int\left[\frac{1}{2}\rho(\boldsymbol{r},t)\nabla\boldsymbol{u}^2(\boldsymbol{r},t) - \frac{\hbar}{2m_0}\,\rho(\boldsymbol{r},t)\Delta\boldsymbol{u}(\boldsymbol{r},t)\right]\,d^3r\,. \tag{106}$$

We rewrite the integral over the second term on the right-hand side using Gauss' theorem

$$\int_{\mathcal{V}}\rho\,\underbrace{\nabla\cdot(\nabla\boldsymbol{u})}_{=\Delta\boldsymbol{u}}\,d^3r = \underbrace{\int_{\mathcal{V}}\nabla\cdot(\rho\,\nabla\boldsymbol{u})\,d^3r}_{=\int_{\mathcal{F}}\rho\,\nabla\boldsymbol{u}\cdot d^2\boldsymbol{r}} - \int_{\mathcal{V}}\nabla\rho\cdot\nabla\boldsymbol{u}\,d^3r\,.$$

We assume that $\rho(\boldsymbol{r},t)$ differs sizeably from zero only within a volume that lies completely within the finite space and drops sufficiently fast to zero toward infinity so that the surface integral vanishes. Using again Eq.(26) we hence arrive at

$$-\int_{\mathcal{V}}\nabla\rho\cdot\nabla\boldsymbol{u}\,d^3r = \frac{2m_0}{\hbar}\,\int_{\mathcal{V}}\rho\,\underbrace{(\boldsymbol{u}\cdot\nabla)\boldsymbol{u}}_{=\frac{1}{2}\,\nabla\boldsymbol{u}^2}\,d^3r$$

which shows that, in fact, the right-hand side of Eq.(106) equals zero. Thus, the expectation value of the right-hand side of "Newton's modified second law", Eq.(41), becomes equal to $\langle \boldsymbol{F}\rangle$. However, we have on the left-hand side

$\langle \frac{d}{dt}\, m_0\, \boldsymbol{v}\rangle$ instead of $\frac{d}{dt}\,\langle m_0\, \boldsymbol{v}\rangle$. Nevertheless, the two expressions are equal as follows from multiplying $\frac{d}{dt}\, m_0\, \boldsymbol{v}$ by $\rho(\boldsymbol{r},t)$ and observing that $\boldsymbol{v}(\boldsymbol{r},t)$ is irrotational. Because of the latter we have

$$\frac{d}{dt}\,\boldsymbol{v} = \frac{\partial}{\partial t}\boldsymbol{v} + \frac{1}{2}\nabla \boldsymbol{v}^2$$

which can be recast as

$$m_0\,\rho\,\frac{d}{dt}\,\boldsymbol{v} = m_0\,\rho\,\frac{\partial}{\partial t}\boldsymbol{v} + \left[m_0\,\boldsymbol{v}\,\frac{\partial \rho}{\partial t} - m_0\,\boldsymbol{v}\,\frac{\partial \rho}{\partial t}\right] + \frac{m_0}{2}\,\rho\,\nabla \boldsymbol{v}^2$$

where we have added zero in the form of the bracketed expression. The real-space integral over this equation may be written after reordering

$$\underbrace{\frac{\partial}{\partial t}\int_{\mathcal{V}} \rho(\boldsymbol{r},t)\, m_0\, \boldsymbol{v}(\boldsymbol{r},t)\, d^3r}_{=\frac{d}{dt}\,\int_{\mathcal{V}}\rho(\boldsymbol{r},t)\, m_0\, \boldsymbol{v}(\boldsymbol{r},t)\, d^3r} = \langle \frac{d}{dt}\, m_0\, \boldsymbol{v}\rangle + \frac{m_0}{2}\int_{\mathcal{V}}\left[2\boldsymbol{v}\,\frac{\partial \rho}{\partial t} - \rho\,\nabla \boldsymbol{v}^2\right] d^3r \quad (107)$$

The integral on the right-hand side vanishes because of the equation of continuity

$$\frac{\partial \rho}{\partial t} + \nabla\cdot(\rho\,\boldsymbol{v}) = 0\,. \quad (108)$$

This follows from multiplying this equation by $\boldsymbol{v}$ and performing a real-space integration. We then have

$$\int_{\mathcal{V}} \boldsymbol{v}\,\frac{\partial \rho}{\partial t}\, d^3\, r = -\sum_{\nu=1}^{3} \boldsymbol{e}_\nu \int_{\mathcal{V}} v_\nu\, \nabla\cdot(\rho\,\boldsymbol{v})\, d^3\, r =$$

$$-\sum_{\nu=1}^{3} \boldsymbol{e}_\nu \underbrace{\int_{\mathcal{V}} \nabla\cdot(v_\nu\,\rho\,\boldsymbol{v})\, d^3\, r}_{=\int_{\mathcal{A}} v_\nu\,\rho\,\boldsymbol{v}\cdot d^2\,\boldsymbol{r}} + \underbrace{\sum_{\nu=1}^{3} \boldsymbol{e}_\nu \int_{\mathcal{V}} \rho\,\boldsymbol{v}\cdot\nabla v_\nu\, d^3\, r}_{=\int_{\mathcal{V}}\rho\,(\boldsymbol{v}\cdot\nabla)\,\boldsymbol{v}\, d^3\, r} \quad (109)$$

with $\boldsymbol{e}_\nu$ denoting unit vectors. The surface integral has been obtained by invoking Gauss' theorem. It vanishes since we may assume $\rho\,|\boldsymbol{v}|$ to vanish sufficiently toward infinity. Again exploiting the property of $\boldsymbol{v}$ being irrotational the second integral on the right-hand side can be written

$$\int_{\mathcal{V}} \rho\,(\boldsymbol{v}\cdot\nabla)\,\boldsymbol{v}\, d^3\, r = \frac{1}{2}\int_{\mathcal{V}} \rho\,\nabla \boldsymbol{v}^2\, d^3\, r\,.$$

It follows then from Eq.(109) that the integral on the right-hand side of Eq.(107) is, in fact, equal to zero. Thus we have shown that the expectation value of the "vacuum force" $\boldsymbol{F}_{QM}(\boldsymbol{r},t)$ vanishes

$$\int \rho(\boldsymbol{r},t)\,\boldsymbol{F}_{QM}(\boldsymbol{r},t)\, d^3r = 0$$

which plays also a central role in information theory (s. e. g. Garbaczewski [39]).

# 15 The time-dependent Schrödinger equation in the presence of an electromagnetic field

In going through the various steps that led from Eq.(41) ("Newton's modified second law") to the time-dependent Schrödinger equation (91) one recognizes that we implied nowhere that $\boldsymbol{F}$ has to be time-independent. Hence one is justified in allowing $\boldsymbol{F}$ in Eq.(41) to be time-dependent and attain the particular form

$$\boldsymbol{F}(\boldsymbol{r},t) = -\nabla V_{cons}(\boldsymbol{r}) + e\,\widehat{\boldsymbol{E}}(\boldsymbol{r},t) + e\,\boldsymbol{v}(\boldsymbol{r},t)\times\boldsymbol{B}(\boldsymbol{r},t) \tag{110}$$

if the particle under study possesses the charge $e$ and is acted upon by an electric field $\widehat{\boldsymbol{E}}(\boldsymbol{r},t)$ and a magnetic field $\boldsymbol{B}(\boldsymbol{r},t)$. The quantity $V_{cons}(\boldsymbol{r})$ denotes the potential of an additional conservative field (e. g. the gravitational field) which we include to ensure full generality, and $\boldsymbol{v}(\boldsymbol{r},t)$ is the ensemble average defined by Eq.(21). From $\boldsymbol{B} = \nabla\times\boldsymbol{A}$ and Faraday's law of induction we have $\nabla\times(\widehat{\boldsymbol{E}} + \dot{\boldsymbol{A}}) = 0$, and hence $\widehat{\boldsymbol{E}} + \dot{\boldsymbol{A}}$ may be expressed as a gradient of a scalar function which we denote by $-\frac{1}{e}\,V_{el}(\boldsymbol{r},t)$. Thus

$$e\,\widehat{\boldsymbol{E}}(\boldsymbol{r},t) = -e\,\dot{\boldsymbol{A}}(\boldsymbol{r},t) - \nabla V_{el}(\boldsymbol{r},t)\,. \tag{111}$$

If the magnetic field is switched on, it induces a voltage $V_R$ along any circular path $C$

$$V_R = \oint_C \widehat{\boldsymbol{E}}_{ind.}(\boldsymbol{r}',t)\cdot d\boldsymbol{r}' = -\frac{\partial}{\partial\,t}\int_{\mathcal{A}}\boldsymbol{B}(\boldsymbol{r}',t)\cdot d^2\boldsymbol{r}'$$

where $C$ is the rim of the surface $\mathcal{A}$. On multiplying this equation by $e$ and observing that $e\,\widehat{\boldsymbol{E}}_{ind.}$ represents an additional force that changes the momentum of the particle, we obtain

$$\oint_C \dot{\boldsymbol{p}}(\boldsymbol{r}',t')\cdot d\boldsymbol{r}' = \oint_C e\,\widehat{\boldsymbol{E}}_{ind.}(\boldsymbol{r}',t')\cdot d\boldsymbol{r}' = -\frac{\partial}{\partial\,t'}\oint_C e\,\boldsymbol{A}(\boldsymbol{r}',t')\cdot d\boldsymbol{r}'\,.$$

Integrating this equation from $t_0$ to $t$ and assuming $\boldsymbol{A}(\boldsymbol{r}',t_0)\equiv 0$ we obtain

$$-\oint_C \boldsymbol{p}(\boldsymbol{r}',t_0)\cdot d\boldsymbol{r}' + \oint_C \boldsymbol{p}(\boldsymbol{r}',t)\cdot d\boldsymbol{r}' = -\oint_C e\,\boldsymbol{A}(\boldsymbol{r}',t)\cdot d\boldsymbol{r}'\,.$$

where

$$\oint_C \boldsymbol{p}(\boldsymbol{r}',t_0)\cdot d\boldsymbol{r}' = m_0\oint_C \boldsymbol{v}(\boldsymbol{r}',t_0)\cdot d\boldsymbol{r}' = 0\,,$$

which follows from Eq.(64). Thus

$$\oint_C\left[\boldsymbol{v}(\boldsymbol{r}',t) + \frac{e}{m_0}\,\boldsymbol{A}(\boldsymbol{r}',t)\right]\cdot d\boldsymbol{r}' = 0 \quad \forall\, t$$

which means that the curl of the integrand vanishes:

$$\nabla\times\left[\boldsymbol{v}(\boldsymbol{r},t) + \frac{e}{m_0}\,\boldsymbol{A}(\boldsymbol{r},t)\right] \equiv 0\,. \tag{112}$$

Consequently, it can be expressed as a gradient of a scalar function which we denote by $(\hbar/m_0)\,\varphi(\boldsymbol{r},t)$. Hence we arrive at

$$\boldsymbol{v}(\boldsymbol{r},t) + \frac{e}{m_0}\,\boldsymbol{A}(\boldsymbol{r},t) = \frac{\hbar}{m_0}\,\nabla\varphi(\boldsymbol{r},t)\,. \tag{113}$$

which now stands in place of Eq.(65).
We note here only in passing that we have because of $\psi(\boldsymbol{r}) = |\psi(\boldsymbol{r})|e^{i\varphi(\boldsymbol{r})}$

$$\frac{1}{2i}\,[\psi^*\nabla\psi - \psi\nabla\psi^*] = |\psi(\boldsymbol{r})|^2\,\nabla\varphi\,.$$

Using Eq.(113) one can recast this as

$$\frac{\hbar}{2m_0}\,[\psi^*\nabla\psi - \psi\nabla\psi^*] = \rho\,\boldsymbol{v} + \frac{e}{m_0}\,|\psi|^2\boldsymbol{A}$$

or equivalently

$$\rho\,\boldsymbol{v} = \frac{1}{2m_0}\,[\psi^*\widehat{\boldsymbol{P}}\psi + c.c.]$$

where $\widehat{\boldsymbol{P}}$ is short-hand for $\widehat{\boldsymbol{p}} - e\,\boldsymbol{A}$. After real-space integration and an integration by parts one arrives at

$$\langle\boldsymbol{v}\rangle = \frac{1}{m_0}\int \psi^*(\boldsymbol{r},t)\widehat{\boldsymbol{P}}\,\psi(\boldsymbol{r},t)\,. \tag{114}$$

Because of Eq.(112) the expression $(\boldsymbol{v}\cdot\nabla)\,\boldsymbol{v}$ which appears in

$$m_0\,\frac{d}{dt}\,\boldsymbol{v}(\boldsymbol{r},t) = m_0\left[\frac{\partial}{\partial t}\,\boldsymbol{v} + (\boldsymbol{v}\cdot\nabla)\,\boldsymbol{v}\right] = \boldsymbol{F}(\boldsymbol{r},t) + \boldsymbol{F}_{QP}(\boldsymbol{r},t) \tag{115}$$

cannot be replaced with $\frac{1}{2}\nabla\boldsymbol{v}^2$ any more. Because of the generally valid relation

$$(\boldsymbol{a}\cdot\nabla)\,\boldsymbol{a} = \nabla\,\frac{\boldsymbol{a}^2}{2} - \boldsymbol{a}\times(\nabla\times\boldsymbol{a})$$

and because of Eq.(112) we now have

$$(\boldsymbol{v}\cdot\nabla)\,\boldsymbol{v} = \frac{1}{2}\nabla\boldsymbol{v}^2 - \boldsymbol{v}\times(\nabla\times\boldsymbol{v}) = \frac{1}{2}\nabla\boldsymbol{v}^2 + \frac{e}{m_0}\boldsymbol{v}\times(\nabla\times\boldsymbol{A})\,.$$

Using $\nabla\times\boldsymbol{A} = \boldsymbol{B}$ we may recast this as

$$(\boldsymbol{v}\cdot\nabla)\,\boldsymbol{v} = \frac{1}{2}\nabla\boldsymbol{v}^2 + \frac{e}{m_0}\boldsymbol{v}\times\boldsymbol{B}\,.$$

Inserting this result together with Eq.(110) and $\boldsymbol{F}_{QP} = -\nabla V_{QP}$ into Eq.(115) we notice that the Lorentz-force $e\,\boldsymbol{v}(\boldsymbol{r},t)\times\boldsymbol{B}(\boldsymbol{r},t)$ drops out in favor of $\boldsymbol{A}(\boldsymbol{r},t)$, and we get

$$\frac{\partial}{\partial\,t}(\boldsymbol{v} + \frac{e}{m_0}\,\boldsymbol{A}) = -\frac{1}{m_0}\nabla V - \frac{1}{2}\nabla\boldsymbol{v}^2 + \frac{1}{2}\,\nabla\boldsymbol{u}^2 - \frac{\hbar}{2\,m_0}\Delta\boldsymbol{u} \tag{116}$$

where we have introduced

$$V(\boldsymbol{r},t) = V_{cons}(\boldsymbol{r}) + V_{el}(\boldsymbol{r},t)\,. \tag{117}$$

We now multiply Eq.(116) by the imaginary unit $i$ and subtract Eq.(81) which gives by complete analogy with Eq.(82)

$$\frac{\partial}{\partial\, t}\left[-\boldsymbol{u} + i(\boldsymbol{v} + \frac{e}{m_0}\,\boldsymbol{A})\right] =$$
$$\frac{i}{2}\,\nabla(-\boldsymbol{u} + i\,\boldsymbol{v})^2 + \frac{i\,\hbar}{2\,m_0}\nabla\left[\nabla\cdot(-\boldsymbol{u} + i\,\boldsymbol{v})\right] - \frac{i}{m_0}\,\nabla V. \tag{118}$$

We mention here only in passing that Eq.(81) is equivalent to Fick's law and is hence not affected by the presence of an electromagnetic field as long as Einstein's law (40) remains unchanged which is obvious from his derivation. (S. also Fritsche and Haugk [113].)
As in the case without electromagnetic field we absorb the two independent scalar informations $\rho(\boldsymbol{r},t)$ and $\varphi(\boldsymbol{r},t)$ into one complex-valued function

$$\psi(\boldsymbol{r},t) = \pm\sqrt{\rho(\boldsymbol{r},t)}\,e^{i\varphi(\boldsymbol{r},t)}\,. \tag{119}$$

As $\boldsymbol{v}$ is no longer equal to $\frac{\hbar}{m_0}\nabla\varphi$ we have now in place of Eq.(83)

$$\frac{\hbar}{m_0}\,\nabla(\ln\psi/\sqrt{\rho_0}) = -\boldsymbol{u} + i(\boldsymbol{v} + \frac{e}{m_0}\,\boldsymbol{A})\,. \tag{120}$$

The left-hand side of Eq.(118) is obviously the time-derivative hereof. It will be useful to notice that

$$\frac{\partial}{\partial\, t}\,\frac{\hbar}{m_0}\,\nabla(\ln\psi/\sqrt{\rho_0}) = \nabla(\frac{1}{m_0\,\psi}\,\hbar\frac{\partial}{\partial\, t}\psi)\,. \tag{121}$$

We may also use Eq.(120) to recast the first expression on the right-hand side of Eq.(118)

$$\frac{i}{2}\,\nabla(-\boldsymbol{u} + i\,\boldsymbol{v})^2 =$$
$$\frac{i}{2}\frac{\hbar^2}{m_0^2}\nabla[\nabla\ln(\psi/\sqrt{\rho_0})]^2 + \frac{\hbar}{m_0}\,\frac{e}{m_0}\nabla[\boldsymbol{A}\cdot\nabla\ln(\psi/\sqrt{\rho_0})] - \frac{i}{2}\nabla(\frac{e}{m_0}\boldsymbol{A})^2\,.$$

If one observes that

$$\nabla[\nabla\ln(\psi/\sqrt{\rho_0})] = \frac{1}{\psi}\,\Delta\psi - [\nabla\ln(\psi/\sqrt{\rho_0})]^2\,, \tag{122}$$

the second expression on the right-hand side of Eq.(118) can be written

$$i\frac{\hbar}{2\,m_0}\nabla\left[\nabla\cdot(-\boldsymbol{u} + i\,\boldsymbol{v})\right] = -\frac{i}{2}\,\frac{\hbar^2}{m_0^2}\,\nabla[\nabla\ln(\psi/\sqrt{\rho_0})]^2$$
$$+i\nabla\left[\frac{1}{\psi}\left(\frac{1}{2}\,\frac{\hbar^2}{m_0^2}\,\Delta\psi - \frac{\hbar}{2\,m_0}\,\frac{e}{m_0}\,\underbrace{\psi\,\nabla\cdot\boldsymbol{A}}_{=(\nabla\cdot\boldsymbol{A})\psi - (\boldsymbol{A}\cdot\nabla)\psi}\right)\right]\,.$$

Hence we obtain

$$\frac{i}{2}\,\nabla(-\boldsymbol{u}+i\,\boldsymbol{v})^2+\frac{i\,\hbar}{2\,m_0}\nabla\left[\nabla(-\boldsymbol{u}+i\,\boldsymbol{v})\right]=-i\,\nabla\left[\frac{1}{m_0\,\psi}\mathcal{G}\,\psi\right]$$

where

$$\mathcal{G}=-\frac{\hbar^2}{2\,m_0}\,\Delta+i\,\frac{\hbar}{2}\frac{e}{m_0}\,\nabla\cdot\boldsymbol{A}+i\,2\,\frac{\hbar}{2}\,\frac{e}{m_0}\boldsymbol{A}\cdot\nabla+\frac{1}{2\,m_0}\,(e\,\boldsymbol{A})^2\,.$$

The right-hand side of this equation may be compactified by using the momentum operator (87) as a convenient short-hand notation

$$\frac{i}{2}\,\nabla(-\boldsymbol{u}+i\,\boldsymbol{v})^2+\frac{i\,\hbar}{2\,m_0}\nabla\left[\nabla(-\boldsymbol{u}+i\,\boldsymbol{v})\right]=-i\,\nabla\left[\frac{1}{m_0\,\psi}\frac{(\widehat{\boldsymbol{p}}-e\,\boldsymbol{A})^2}{2\,m_0}\,\psi\right]\,.$$

Inserting this result into Eq.(118) which derives from Eq.(115) ("Newton's modified second law") and Eq.(27) ($\equiv$ Fick's law) and exploiting the Eqs.(121) and (122) we arrive at

$$i\hbar\,\frac{\partial\,\psi(\boldsymbol{r},t)}{\partial\,t}=\widehat{H}(\boldsymbol{r},t)\,\psi(\boldsymbol{r},t) \tag{123}$$

where

$$\widehat{H}(\boldsymbol{r},t)=\frac{\widehat{\boldsymbol{P}}^{\,2}}{2\,m_0}+V(\boldsymbol{r},t)\quad\text{and}\quad\widehat{\boldsymbol{P}}=\widehat{\boldsymbol{p}}-e\,\boldsymbol{A}(\boldsymbol{r},t)\,.$$

# 16 A model for non-Markovian diffusion illustrating the origin of non-locality

It is instructive to consider a model illustrating "conservative diffusion". The latter is a consequence of forming the arithmetic mean of Eqs.(35) and (38) which leads to Eq.(39). If one were to follow the motion of an individual particle, just one member out of the total ensemble, one would directly see the effect of stochastic forces changing back and forth from "Brownian" to "anti-Brownian" with the latter causing a motion enhancement after the former have effected a slow down of the particle motion. Figure 8 shows three situation of the (free) particle which moves within a two-dimensional frame where a two-slit diaphragm has been inserted on the left-hand side. The "walls" of the frame are assumed elastically reflecting. The stochastic forces acting on the particle are simulated by a two-dimensional gas of $N$ identical point masses ($N\gg 1$) that interact via Lennard-Jones pair-potentials with each other and with the particle under study as well. The latter will henceforth be referred to as "test particle". It is this situation which the original derivation of Einstein's law (40) refers to where the motion of the test particle is described by a Langevin equation into which the embedding of the

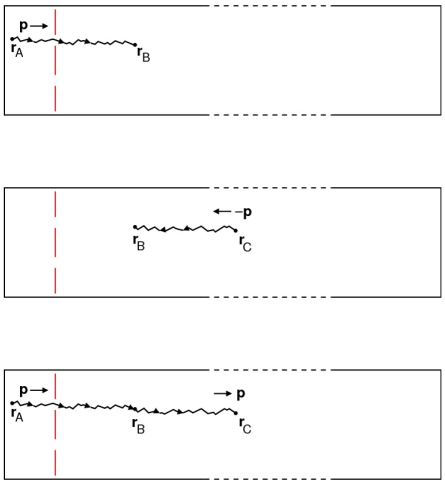


Figure 8: Trajectory of the test particle undergoing reversible scatterings

particle enters through a stochastic force. (The practical calculations have been performed with slightly modified Lennard-Jones potentials that were truncated at twice the average particle distance.) In our model the particle motion of the embedding gas results from a molecular dynamics simulation which one starts by first keeping the test particle fixed at the point $\boldsymbol{r}_A$ and letting the $N$ gas particles start from some corner of the frame with equal absolute values of their momenta. Thereby one defines a certain value of their total kinetic energy $E_{kin}^{gas}$. After a short simulation time the gas particles are uniformly distributed within the frame and their distribution in the momentum space has become Maxwellian. The latter is associated with a certain temperature such that the thermodynamical expectation value of the kinetic energy equals $E_{kin}^{gas}$. It is this temperature which finally shows up in Einstein's law (40). After the embedding gas has "thermalized" one imparts a certain momentum $\boldsymbol{p}$ on the test particle and continues the molecular dynamics simulation with the test particle now included. As indicated in the upper panel of the figure, it performs an irregular (Brownian) motion and loses momentum to the embedding gas whose particles are not shown in the figure. We have chosen the starting point $\boldsymbol{r}_A$ such that the particle moves through the upper slit of the diaphragm and reaches the point $\boldsymbol{r}_B$ after a simulation time $\Delta t$ of the order of $\tau$ which is the time constant of a freely moving particle in a gaseous medium with friction. We now look for a point $\boldsymbol{r}_C$ further to the right in the forward direction of the test particle (s. panel in the middle of the figure). At this point we impart a momentum $-\boldsymbol{p}$ on the particle (after thermalization of the embedding gas), i.e. just the reverse of the momentum at $\boldsymbol{r}_A$.
The point $\boldsymbol{r}_C$ is chosen such that the trajectory ends - again after an identical simulation time of $\Delta t$ seconds - at point $\boldsymbol{r}_B$. At this point the test

particle has lost its original momentum $-\boldsymbol{p}$ almost completely. If one now turns the velocities of **all** particles around by $180^0$ and starts the simulation again with the time running forward as before, the test particle continues its motion from point $\boldsymbol{r}_B$ and moves exactly along the trajectory it had formerly followed in the opposite direction coming from $\boldsymbol{r}_C$. When it has reached $\boldsymbol{r}_C$ again, it has regained the previously lost momentum, but this time with the sign reversed. Hence, in moving from $\boldsymbol{r}_A$ to $\boldsymbol{r}_C$ the particle undergoes scattering processes that are in alternating succession Brownian and anti-Brownian within a time interval of the order $\tau$. Thereby the average momentum of the particle is conserved. This is illustrated in the third panel (bottom). A striking feature of the momentum reconstruction by the above scattering processes is the occurrence of non-locality. This can be demonstrated by repeating the procedure that led to the trajectory portion from $\boldsymbol{r}_C$ to $\boldsymbol{r}_B$ with a crucial modification: If one closes the lower slit of the diaphragm and starts then with **the same position/velocity configuration** of all particles as before, the trajectory of the test particle evolves now differently and does no longer join the previously generated trajectory portion at $\boldsymbol{r}_B$. This is what the molecular dynamics simulation clearly yields. On the other hand, this is to be expected anyway because every momentum transfer from the test particle to the gas spreads with sound velocity throughout the entire structure and probes the change that has been introduced. The stochastic forces acting on the test particle are modified by such a change when these sound waves are reflected back on the particle. If one wants the modified trajectory to join the first trajectory portion at $\boldsymbol{r}_B$ again, one has to choose a different starting point $\boldsymbol{r}'_C$. Once the test particle has arrived at $\boldsymbol{r}_B$, one inverts all the velocities as before, and the particle will now recover the momentum $\boldsymbol{p}$ on its modified trajectory toward $\boldsymbol{r}'_C$. Note: this change in the course of the particle motion results just from closing the **lower** slit although the particle definitely traverses the **upper** slit. One is tempted to surmise that this mechanism of probing the environment "in real life" as the particle exchanges temporarily momentum with the **vacuum**, occurs at light velocity. The latter would impose a limit on the distance beyond which a previously passed potential structure can no longer affect the evolution of the particle's trajectory at its current position.

If one were dealing with Brownian scattering only, the succession of scattering events could be classed as "Markovian". (Shorthand definition: given the presence, future and past are independent.) However, the overall character of the combined Brownian/anti-Brownian scattering processes is obviously non-Markovian. It is true that the particle has almost completely lost its memory of its original momentum when it arrives at $\boldsymbol{r}_B$, but its future time evolution while moving toward $\boldsymbol{r}_C$ reconstructs, so to speak, past scattering events. The particle's momentum $\boldsymbol{p}(0)$ when it is at $\boldsymbol{r}_A$, and its momentum $\boldsymbol{p}(t)$ at $\boldsymbol{r}_C$ are **strongly correlated**.

This does not apply to the positions $\boldsymbol{r}_A(0)$ and $\boldsymbol{r}_C(t)$: if one repeats the

experiment and lets the particle start at $\boldsymbol{r}_A$ with the same momentum $\boldsymbol{p}(0)$ as before, but with the thermalization process of the embedding gas started some time interval earlier, the particle's trajectory will now be different and lead to a point different from $\boldsymbol{r}_C$ though it regains its original momentum after (approximately) the same traveling time.
Obviously, the non-Markovian (reversible) character of particle motion which results from such a combination of scattering processes can only show up on a coarse grain time scale which is the crucial assumption underlying our derivation of Newton's modified second laws Eqs.(41) and (115) together with (110).

# 17 Operators and commutators

An important advantage of our approach may be seen in the derivability of Hermitian operators which in standard quantum mechanics can merely be obtained from educated guessing employing Jordan's replacement rules. In Section 11 we have already derived the momentum operator

$$\widehat{\boldsymbol{p}} = -i\,\hbar\nabla$$

exploiting our expression (65) for $\boldsymbol{v}(\boldsymbol{r},t)$ and $\boldsymbol{j}(\boldsymbol{r},t) = \rho(\boldsymbol{r},t)\,\boldsymbol{v}(\boldsymbol{r},t)$. The same arguments used in deriving $\widehat{\boldsymbol{p}}$ apply to the angular momentum operator $\widehat{\boldsymbol{L}}$ which occurs on forming the expectation value of the angular momentum of a particle with respect to a center located at $\boldsymbol{r} = 0$. This expectation value $\langle \boldsymbol{L} \rangle$ is primarily defined as a real-space integral over the angular momentum density $\boldsymbol{r} \times m_0\,\boldsymbol{j}$:

$$\langle \boldsymbol{L}(t) \rangle = \int \boldsymbol{r} \times m_0\,\boldsymbol{j}(\boldsymbol{r},t)\,d^3r \tag{124}$$

If one here inserts $\boldsymbol{j}$ from Eq.(92), integrates by parts and requires $\psi(\boldsymbol{r},t)$ to vanish sufficiently toward infinity, the result may be written

$$\langle \boldsymbol{L}(t) \rangle = \int \psi^*(\boldsymbol{r},t)\,(\boldsymbol{r} \times \widehat{\boldsymbol{p}})\,\psi(\boldsymbol{r},t)\,d^3r \tag{125}$$

which justifies terming $\widehat{\boldsymbol{L}} \equiv \boldsymbol{r} \times \widehat{\boldsymbol{p}}$ "angular momentum operator".
The kinetic energy of an individual particle, labeled by the index j, is defined as the work performed on that particle by the external force $\boldsymbol{F}$ in accelerating it from zero velocity at time $t = 0$ to its velocity $\boldsymbol{v}_{cj}(t)$ at time $t$, which yields

$$E^j_{kin} = \frac{m_0}{2}\,\boldsymbol{v}^2_{cj}(t)\,.$$

Forming the ensemble average according to Eq.(21) one obtains $E_{kin} = \frac{m_0}{2}\,\boldsymbol{v}^2_c(\boldsymbol{r},t)$. Thus, the density of the kinetic energy is given by

$$\epsilon_{kin}(\boldsymbol{r},t) = \frac{m_0}{2}\,\rho(\boldsymbol{r},t)\,[\boldsymbol{v}_c(\boldsymbol{r},t)]^2\ .$$

In the two subsystems "B" and "A" we generally assume the associated velocities $\boldsymbol{v}$ to be identical, whereas the convective velocities $\boldsymbol{v}_c$ are different, and therefore we distinguish $\boldsymbol{v}_c^B$ from $\boldsymbol{v}_c^A$ and form the ensemble average over the two subensembles:

$$\epsilon_{kin}(\boldsymbol{r},t) = m_0 \, \tfrac{\rho(\boldsymbol{r},t)}{2} \, \tfrac{1}{2} \left( \left[\boldsymbol{v}_c^B(\boldsymbol{r},t)\right]^2 + \left[\boldsymbol{v}_c^A(\boldsymbol{r},t)\right]^2 \right) \tag{126}$$

According to Eq.(24) which still refers to the "B"-system, we have

$$\boldsymbol{v}_c^B = \boldsymbol{v} - \boldsymbol{u} \quad \text{and therefore} \quad \boldsymbol{v}_c^A = \boldsymbol{v} + \boldsymbol{u} \, .$$

Consequently Eq.(126) may be cast

$$\epsilon_{kin}(\boldsymbol{r},t) = m_0 \, \frac{\rho(\boldsymbol{r},t)}{2} \, \left( \left[\boldsymbol{v}(\boldsymbol{r},t)\right]^2 + \left[\boldsymbol{u}(\boldsymbol{r},t)\right]^2 \right) \, . \tag{127}$$

From Eq.(83) we have

$$-\boldsymbol{u} + i \, \boldsymbol{v} = \frac{\hbar}{m_0} \, \frac{1}{\psi} \, \nabla \psi \, .$$

The modulus square of this equation times $m_0 \, \rho/2$ is equal to the right-hand side of Eq.(127), that is

$$\epsilon_{kin.}(\boldsymbol{r},t) = \frac{\hbar^2}{2\, m_0} \, |\nabla \psi(\boldsymbol{r},t)|^2 \, .$$

Taking the real-space integral of this expression one obtains the kinetic energy

$$E_{kin} \equiv \langle T(t) \rangle = \int_{\mathcal{V}} \frac{\hbar^2}{2\, m_0} \, \nabla \psi^*(\boldsymbol{r},t) \cdot \nabla \psi(\boldsymbol{r},t) \, d^3 r \tag{128}$$

which by employing Green's theorem may be given the familiar form

$$\int_{\mathcal{V}} \frac{\hbar^2}{2\, m_0} \, \nabla \psi^*(\boldsymbol{r},t) \cdot \nabla \psi(\boldsymbol{r},t) \, d^3 r = \int_{\mathcal{V}} \psi^*(\boldsymbol{r},t) \, \left[ -\frac{\hbar^2 \, \nabla^2}{2\, m_0} \right] \, \psi(\boldsymbol{r},t) \, d^3 r \, ,$$

and hence

$$\langle T(t) \rangle = \int_{\mathcal{V}} \psi^*(\boldsymbol{r},t) \, \frac{\widehat{\boldsymbol{p}}^2}{2\, m_0} \, \psi(\boldsymbol{r},t) \, d^3 r \, ,$$

which justifies terming $\widehat{\boldsymbol{p}}^2/2\, m_0$ "kinetic energy operator".
In practical calculations one often benefits from the fact that $E_{kin}$ may alternatively be cast as in Eq.(128) where the integrand is real-valued and may immediately be interpreted as "kinetic energy density".

The statistical operator is a particular example of derivability from a simple concept. We confine ourselves here to the case of a quantum mechanical

system of a bound particle in contact with a heat bath of temperature $T$. In a stationary state the latter constantly exchanges energy with the system, in the simplest case photons. Hence, the wave function of that system cannot be one of its eigenstates any more, but rather represents a solution to the time-dependent Schrödinger equation and can be expanded in terms of eigenfunctions $\psi_n(\boldsymbol{r})$

$$\psi(\boldsymbol{r},t) = \sum_n c_n(t)\,\psi_n(\boldsymbol{r})\,e^{-\frac{i}{\hbar}E_n\,t} \tag{129}$$

where $E_n$ denotes eigenvalues of the unperturbed one-particle Hamiltonian $\widehat{H}$.
To make the external system classifiable as a heat bath, the time-averaged coupling energy of the two systems must be negligibly small compared to the difference $E_{n'} - E_n$ of any two eigenvalues. The particle's thermodynamical expectation value of its energy (indicated by double brackets) is given by

$$\langle\langle \widehat{H} \rangle\rangle \equiv U = \frac{1}{\tau}\int_t^{t+\tau}\left[\int \psi^*(\boldsymbol{r},t')\,\widehat{H}\,\psi(\boldsymbol{r},t')\,d^3r\right]dt' \tag{130}$$

where $\tau$ (not to be confused with the slow-down time in Section 5) has to be chosen sufficiently large such that $U$ does not depend on $t$ any more. Quantities that derive from $U$ like the specific heat, are only defined as time-averages of this kind.
Inserting Eq.(129) into (130) we obtain

$$U = \sum_n E_n\,\{\frac{1}{\tau}\int_t^{t+\tau}|c_n(t')|^2\,dt'\}\,. \tag{131}$$

The expression in curly brackets may be interpreted as the relative frequency of the system of being in the $n$-th eigenstate.
Straight-forward thermodynamics yields for a system that possesses energy levels $E_n$

$$U = \sum_n E_n\,\frac{1}{\sigma}\,e^{-\beta\,E_n}\,, \quad \beta = \frac{1}{k_B\,T} \tag{132}$$

where

$$\sigma = \sum_n e^{-\beta\,E_n}\,.$$

Thus, we have from Eq.(131)

$$\frac{1}{\tau}\int_t^{t+\tau}|c_n(t')|^2\,dt' = \frac{1}{\sigma}\,e^{-\beta\,E_n}\,.$$

If one defines a statistical operator

$$\widehat{\rho} = \frac{1}{\sigma}\,e^{-\beta\,\widehat{H}}$$

Eq.(132) can alternatively be cast as

$$U = \sum_n \langle \psi_n | \widehat{\rho}\, \widehat{H} | \psi_n \rangle \equiv \mathrm{Tr}(\widehat{\rho}\, \widehat{H})\,.$$

**Commutation rules** for the operators apply when the potential $V(\boldsymbol{r})$ in the time-independent Schrödinger equation (50) possesses a certain symmetry. If $V(\boldsymbol{r})$ is spherically symmetric, for example, one verifies simply by performing partial differentiations that

$$\left(\widehat{H}\widehat{\boldsymbol{L}}^2 - \widehat{\boldsymbol{L}}^2\widehat{H}\right)\, \psi_n(\boldsymbol{r}) \equiv [\widehat{H}, \widehat{\boldsymbol{L}}^2]\, \psi_n(\boldsymbol{r}) = 0$$

and similarly

$$[\widehat{H}, \widehat{\boldsymbol{L}}_z]\, \psi_n(\boldsymbol{r}) = 0$$

if $\psi_n(\boldsymbol{r})$ is an eigenfunction of $\widehat{H}$.

If one is dealing with some operator $\widehat{A}$ which represents just some analytical expression in $\boldsymbol{r}$ and $\widehat{\boldsymbol{p}}$, the time dependence of its expectation value $\langle \widehat{A} \rangle$ can be determined by employing the time-dependent Schrödinger equation which gives

$$\frac{d}{dt} \int \psi^*(\boldsymbol{r},t)\, \widehat{A}\, \psi(\boldsymbol{r},t)\, d^3r = \int \psi^*(\boldsymbol{r},t) \frac{i}{\hbar} [\widehat{H}, \widehat{A}]\, \psi(\boldsymbol{r},t)\, d^3r\,,$$

in short-hand notation

$$\frac{d}{dt}\, \widehat{A} = \frac{i}{\hbar} [\widehat{H}, \widehat{A}]\,. \tag{133}$$

Commutation rules of the above kind, again in short-hand notation

$$[\widehat{H}, \widehat{\boldsymbol{L}}^2] = 0\,; \quad [\widehat{H}, \widehat{\boldsymbol{L}}_z] = 0\,,$$

similarly

$$[\widehat{H}, \widehat{\boldsymbol{p}}] = 0 \;\text{ if }\; V(\boldsymbol{r}) = \text{const.}\,,$$

but also

$$[\widehat{p}_j, x_k] = \frac{\hbar}{i}\, \delta_{j\,k} \quad \text{where} \quad j = 1,2,3\,;\; k = 1,2,3$$

constitute fundamental elements of standard quantum mechanics and are discussed as pivotal in the context of measurement. From our point of view they are just byproducts of the Schrödinger equation and do not contain any more physics than has already gone into the derivation of the Schrödinger equation. In practice it is impossible to find quantum systems where eigenvalues of $\widehat{H}$ and $\widehat{L}_z$, for example, can be measured simultaneously although

there is a widespread belief to the contrary. It is not even possible, for example, to measure the eigenvalues of $\widehat{H}$ for a hydrogen atom which - in clamped proton approximation - represents the archetypal one-particle system and the starting point of quantum mechanics. The lines one observes in its discrete optical spectrum refer to eigenvalue differences and possess - different from true eigenvalues - a natural line width which goes to zero only in the hypothetical case of zero radiation coupling, that is when the lines cannot be observed any more.
There is a remark by Wigner [41] which reveals exactly that lack of stringency and consistency in the foundation of orthodox quantum mechanics:

*" All these are concrete and clearly demonstrated limitations on the measurability of operators. They should not obscure the other, perhaps even more fundamental weakness of the standard theory, that it postulates the measurability of operators but does not give directions as to how the measurement should be carried out."*

## 18 Collaps of the wave function and the node problem

A vital point of the Copenhagen interpretation consists in the notion that the wave function of a stationary one-particle state collapses on performing a measurement on the position of the particle, for example. Within our approach a phenomenon of this kind cannot occur. First of all, in our view "measurement" is not a process of something foreign intruding the realm of quantum mechanics but is rather a part of it. If one calculates, for example, the time-independent wave function $\psi(\boldsymbol{r})$ for a stationary situation where electrons in a diffraction chamber leave a tunneling cathode, sufficiently far behind each other, run through a two-slit diaphragm and finally hit a fluorescent screen, $|\psi(\boldsymbol{r})|^2$ will display the familiar diffraction pattern behind the diaphragm and in particular on the screen. But clearly, the structure of this pattern reflects the distribution of the entire ensemble of electrons that leave the cathode, and a particular electron, that hits the screen some place, is only one member out of this ensemble. Hence its capture at the screen does not destroy the properties of the ensemble. The electron capture by an atom of the screen constitutes a process that has only marginally to do with the diffraction state in that the latter determines the probability of the electron being at that particular atom. Otherwise the capture process is governed by the time dependent Schrödinger equation and the perturbation caused by the electromagnetic field of the outgoing photon. All this is completely independent of the possible presence of an "observer" who might see that photon.

Despite deceptive similarities the situation becomes conceptually different

when one replaces the tunneling tip in the otherwise unchanged diffraction chamber by a light source that emits, again in sufficiently large time intervals, photons of the same wave length as the previously considered electrons. Since the space-time structure of the wave (in principle $\propto \cos[\boldsymbol{k}\cdot\boldsymbol{r}-\omega\,t]$) with which each photon is associated, is not defined as the property of an ensemble of mechanical objects but rather by classical electrodynamics (Maxwell's equations), it will, in fact, disappear on the disappearance of the photon in question. There are a couple of properties by which photons differ crucially from massive particles: They move always at light velocity along straight lines in vacuo and the associated waves are vector-valued functions. By contrast, the de Broglie waves of massive particles are in general complex-valued functions, and the average velocity of the particles is given by the gradient of the functions' phase. Their interaction with other particles and parts of an experimental setup is described by the Schrödinger equation and the potentials therein. On the other hand, the interaction of photons with polarizers, mirrors, quaterwave plates, filters etc. is governed by classical electrodynamics. Malus' law, for example, constitutes a law of classical optics. Because of these rather fundamental differences any analysis of photon correlation experiments, for example, should critically be scrutinized whether a transfer to analogous experiments with massive particles is truly justified. In Section 33 we shall draw on the familiar example of the Stern-Gerlach experiment to demonstrate that the selection mechanism for up-spin and down-spin particles in the Stern-Gerlach magnet has nothing to do with the mechanism separating horizontally and vertically polarized photons in a polarizing beam splitter.

According to Mielnik and Tengstrand [31] excited stationary states appear to pose a serious problem in that $\psi(\boldsymbol{r})$ possesses nodal surfaces at which the normal derivative $\frac{\partial}{\partial n}\rho(\boldsymbol{r})$ vanishes but the normal component of the osmotic velocity

$$\boldsymbol{u}_n(\boldsymbol{r}) = -\frac{\hbar}{2m_0}\,\frac{\frac{\partial}{\partial n}\rho(\boldsymbol{r})}{\rho(\boldsymbol{r})}\,\boldsymbol{e}_n$$

becomes formally infinite. Moreover, at surfaces across which $\rho(\boldsymbol{r})$ attains a maximum, $\frac{\partial}{\partial n}\rho(\boldsymbol{r})$ vanishes as well, but $\boldsymbol{u}_n(\boldsymbol{r})$ becomes now zero. If $\psi(\boldsymbol{r})$ is real-valued then $\boldsymbol{v}(\boldsymbol{r})$ vanishes everywhere, and therefore we have on such surfaces with maximum probability density

$$\boldsymbol{v} = \boldsymbol{u}_n = 0\,.$$

In the 2s-state of a hydrogen electron, for example, one has a spherical surface of this kind. Hence, it seems that this sphere separates two regions of space that are mutually inaccessible for the electron. But the above velocities are only ensemble averages or - in the spirit of the definition (23) - averages of non-vanishing velocities $\boldsymbol{v}(t_i), \boldsymbol{u}_n(t_i)$ of different directions over a sufficiently long time $T$.

As for $|\boldsymbol{u}_n(\boldsymbol{r})|$, going to infinity on crossing a nodal surface of $\psi(\boldsymbol{r})$, one has to keep in mind that stationary excited states (excited eigenstates) are highly fictional and do actually not exist in nature. Because of $\Delta E\,\Delta t \approx \hbar$ and $\Delta E = 0$ for an eigenstate it would take an infinite time to prepare them. Hence, truly existing excited states do not possess nodal surfaces where $\psi(\boldsymbol{r})$ vanishes exactly. But even if one would allow them to exist, the kinetic energy density $\frac{m_0}{2}\,\rho(\boldsymbol{r})\,\boldsymbol{u}^2(\boldsymbol{r}) = \frac{\hbar^2}{2m_0}|\nabla\psi(\boldsymbol{r})|^2$ remains finite and hence ensures a physically meaningful behavior even for this idealized situation.

# 19 The Feynman path integral

As our concept builds on the existence of particle trajectories one might surmise that there should be some affinity to Feynman's path integral method [42] which also relates to possible paths a particle might take. We shall outline that there is neither any formal kinship nor does Feynman name any cause for the possible occurrence of non-classical trajectories. In so doing we limit ourselves, as Feynman in his article, to the one-dimensional case of a particle that moves non-relativistically in a potential $V(x)$. Feynman's considerations are based on two hypotheses that may be summarized by stating that the wave function $\psi(x, t+\Delta t)$ of the particle at some point $x$ and time $t+\Delta t$ is connected with the wave function $\psi(x-\sigma, t)$ at a previous point $x-\sigma$ and earlier time $t$ by an integral equation similar to the Smoluchowski equation (344) in (Section 39), viz.

$$\psi(x, t+\Delta t) = \int \psi(x-\sigma, t)\, F(x, x-\sigma, t, \Delta t)\, d\sigma \tag{134}$$

where $F(x, x-\sigma, t, \Delta t)$ is the function that brings in classical mechanics. It is defined as

$$F(x, x-\sigma, t, \Delta t) = \frac{1}{A}\; e^{\frac{i}{\hbar}\,S(x,\,x-\sigma,\,t,\,\Delta t)}$$

where

$$A = \left(\frac{2\pi\hbar\, i\,\Delta t}{m_0}\right)^{\frac{1}{2}}\,.$$

Here $S(x, x-\sigma, t, \Delta t)$ denotes Hamilton's first principle function for a particle moving classically in a potential $V(x)$ along a trajectory from a point $x-\sigma$ to $x$ within an infinitesimally small time span $\Delta t$. Hence

$$S(x, x-\sigma, t, \Delta t) = \\ \text{Min.} \int_t^{t+\Delta t} \left[\frac{m_0}{2}\,\dot{\sigma}^2 - V(x-\sigma(t'))\right] dt'$$

where

$$L(\dot{\sigma}(t), \sigma(t)) = \frac{m_0}{2}\,\dot{\sigma}^2 - V(x-\sigma(t))$$

denotes the Lagrangean.
As $\Delta t$ is infinitesimally small $S(x, x-\sigma, t, \Delta t)$ may be approximated

$$S = \Delta t \left[ \frac{m_0}{2} \left( \frac{\sigma}{\Delta t} \right)^2 - V(x) \right] .$$

Hence one has

$$F = \frac{1}{A} \left[ e^{\frac{i\, m_0}{2\hbar\, \Delta t}\, \sigma^2} \cdot e^{-\frac{i\, V(x)\, \Delta t}{\hbar}} \right] .$$

The first exponential oscillates rapidly as a function of $\sigma$ because of the prefactor $1/\Delta t$ in the exponent, whereas, by comparison, $\psi(x-\sigma, t)$ may be assumed slowly varying as a function of $\sigma$. The value of the integral in Eq.(134) depends therefore only on a small interval of $\sigma$ about the point $x$. Within this interval $\psi(x-\sigma, t)$ may be expanded as

$$\psi(x-\sigma, t) = \psi(x, t) - \frac{d\psi}{dx}\, \sigma + \frac{1}{2}\, \frac{d^2\psi}{dx^2}\, \sigma^2 .$$

If one inserts this into Eq.(134), observes

$$\frac{1}{A} \int_{-\infty}^{\infty} e^{\frac{i\, m_0}{2\hbar\, \Delta t}\, \sigma^2}\, d\sigma = 1 ;$$

(note that this equation defines $A$!), further

$$\frac{1}{A} \int_{-\infty}^{\infty} e^{\frac{i\, m_0}{2\hbar\, \Delta t}\, \sigma^2}\, \sigma\, d\sigma = 0 ,$$

$$\frac{1}{A} \int_{-\infty}^{\infty} e^{\frac{i\, m_0}{2\hbar\, \Delta t}\, \sigma^2}\, \sigma^2\, d\sigma = \frac{i\hbar}{m_0}\, \Delta t$$

and uses

$$e^{-\frac{i\, V(x)\, \Delta t}{\hbar}} \approx 1 - \frac{i\, V(x)\, \Delta t}{\hbar} ,$$

one obtains

$$\psi(x, t+\Delta t) = \psi(x, t) \left( 1 - \frac{i}{\hbar}\, V(x)\, \Delta t \right) + \frac{1}{2}\, \frac{d^2\psi}{dx^2} \cdot \frac{i\hbar}{m_0}\, \Delta t \left( 1 - \frac{i\, V(x)\, \Delta t}{\hbar} \right) .$$

Multiplying this equation by $\frac{i\hbar}{\Delta t}$ and letting $\Delta t$ tend to zero one arrives at the time dependent Schrödinger equation

$$i\hbar \frac{\partial}{\partial t}\, \psi(x, t) = \left[ -\frac{\hbar^2}{2\, m_0}\, \frac{\partial^2}{\partial x^2} + V(x) \right] \psi(x, t) .$$

Though the Schrödinger equation is obviously recovered following this line of argument, it remains unclear why Hamilton's classical first principle function should appear in the exponent of $F(x, x-\sigma, t, \Delta t)$. Feynman's considerations lean closely on arguments of measurement typical of the Copenhagen

school of thought, cast into an axiomatic framework notably by v. Neumann [43]. But $\psi(x,t)$ may, for example, describe the motion of a harmonic oscillator in the absence of any measurement. In fact, if one were to perform a measurement on the harmonic oscillator the Schrödinger equation would contain a perturbative extra term that would give rise to a different wave function. Clearly, as already stated in Section1 the probabilistic character of $\psi(x,t)$ does not originate from indeterminacies caused by the process of measurement. The complex-valuedness of the wave function in the form $\psi(x,t) = |\psi(x,t)|\, e^{i\varphi(x,t)}$ comes about by incorporating two autonomous real-valued informations: the probability density $|\psi(x,t)|^2$ of the particle being at $x$ and time $t$ and the ensemble average $v(x,t) = \frac{\hbar}{m_0}\frac{d}{dx}\,\varphi(x,t)$ of its velocity. For that reason our derivation of the Schrödinger equation requires two Smoluchowski equations for the real-valued functions $\rho(\boldsymbol{r},t)$ and $\boldsymbol{v}(\boldsymbol{r},t)$ instead of Feynman's single Eq.(134). In summary, we believe that our derivation provides a much clearer insight into the connection between classical mechanics and quantum mechanics and is not flawed by highly artificial assumptions.

## 20 Spontaneous light emission

Understanding the discrete spectrum of light emitting atoms had been the primary motivation for developing a theory beyond classical mechanics and electrodynamics. It was far from being likely that Planck's constant $h$ which he introduced to explain the continuous spectrum of light emitting incandescent "black bodies" could have anything to do with those discrete spectra. By hindsight it must be seen as a surprise when Niels Bohr [44] could explain the well studied spectrum of the hydrogen atom by requiring the associated electron to orbit around the nucleus on concentric circles where its angular momentum $L$ equals integer multiples of Planck's reduced constant $\hbar = \frac{h}{2\pi}$: $L = n\,\hbar$ and $n = 1, 2, \ldots$. In each of the orbitals the electron was considered to be in a stable state, but it was allowed to jump spontaneously to another orbital of lower energy and convert the energy difference into light. Those "quantum jumps" still belong to the vocabulary of present-day quantum mechanics (see e. g.[45]) although their existence lacks any foundation as we shall demonstrate.
In Bohr's theory the electron always possesses a non-vanishing angular momentum so that the centrifugal force keeps it well separated from the nucleus and thereby ensures a well defined size of the hydrogen atom for $n = 1$, its state of lowest energy. In reality, i. e. according to our approach, the particle under study, the electron, is driven by the combined action of the static classical Coulomb force exercised by the nucleus and by the stochastic forces of the vacuum. As a consequence, its probability amplitude obeys the Schrödinger equation, the time-independent solutions of which, $\hat{\psi}_{nlm}(\boldsymbol{r})$, are

characterized by integer quantum numbers $n, l, m$ where $\boldsymbol{r}$ is referenced to the position of the nucleus. The latter is considered to be a clamped point charge for simplicity. The state $\hat{\psi}_{100}(\boldsymbol{r})$ refers to the groundstate where $\langle \boldsymbol{L} \rangle = 0$, distinctly different from Bohr's theory. Only excited states ($n > 1$) for which $l$ equals $|m|$ display a toroidal probability density and resemble diffuse circular Bohr orbitals.
The energies that are associated with the eigensolutions $\hat{\psi}_{nlm}(\boldsymbol{r})$ are given by

$$E_{nlm} = -\frac{R}{n^2} \quad \text{where} \quad n > l + |m| \quad l = 0, 1, 2, \dots\,, \; m = -l, \dots 0 \dots + l \tag{135}$$

and

$$R = \tfrac{1}{2}\,\alpha^2 m_0\, c^2 = \text{Rydberg constant}\,; \quad R = 13.6059\, eV\,.$$

Here $m_0$ denotes the electron's rest mass, $c$ the velocity of light in vacuo and $\alpha$ the fine structure constant:

$$\alpha = \frac{e^2}{4\pi\varepsilon_0\,\hbar c} = \frac{1}{137.036}\,.$$

The quantity $\varepsilon_0$ represents, as before, the permittivity of the vacuum and $e$ is the elementary charge.
As has already been discussed in Section 12, it is one of the fundamental credos of conventional quantum mechanics that eigenvalues of the energy as in (135) constitute results of appropriate measurements, more precisely, as Mermin [46] states in a widely recognized article:

"...quantum mechanics requires that the result of measuring an observable be an eigenvalue of the corresponding Hermitian operator....."

Although this statement belongs to the seemingly ineradicable rituals in conversing about quantum mechanics, it is void of meaning. Of course, there has always been the discrete hydrogen spectrum in the back of the minds of the founding fathers, and that spectrum seemed to be clearly some map of the eigenvalues (135). But in actual fact one commonly measures the wave length of the emitted light by a spectrometer about or more than $10^{10}$ atomic diameters away from the emitter. When the packet of the light wave enters the "measurement process", i e. the spectrometer, the atom has long left its original state. The phraseology "measuring eigenvalues" invites the impression as if it would compare to measuring somebody's collar size. Moreover, as we shall show, in the emission process the energy of the atom attains all values between the eigenvalues that are involved in the transition, but the frequency and the measured associated wavelength of the emitted light remain constant.
Before we go into the details of our approach we want to emphasize that its

basic idea is almost identical with what has been popularized by E. T. Jaynes already in 1963 [47] and in the following years [48], [49] under the name "neoclasical theory (NCT)". The terminology is rather misleading. In the present theory (and in Jaynes' theory as well) the electromagnetic field is generated by an oscillating electronic current density which sets up a vector potential and this, in turn, appears in the kinetic energy operator of the electronic Hamiltonian. What should be considered "neoclassical" in using this interrelation? Quantum mechanical current densities are foreign objects to classical electrodynamics.
Although we arrive at a time evolution of the light emission that differs in crucial details from a purely exponential decay as obtained by Weisskopf and Wigner [50], the decay times are in agreement with each other. This applies to Jaynes' theory as well. Most of the criticism voiced against Jaynes' work revolves around his non-exponential time evolution. He tries to defend this result by considering ineffective excitations in which the atom acquires only a small portion of the full excitation energy. He argues that this will normally happen in reality, and therefore only the tail of his transition curve can show up in the experiment. This tail is essentially an exponential function.
We fundamentally disagree with this notion. If the atom re-emits light with a frequency $\omega$ the associated wave packet contains a photon of energy $\hbar\omega$ and not a fraction of it. Hence the atom must have definitely been in its excited state prior to the emission process.

How does spontaneous light emission fit into the framework that we have developed so far? Our point of departure from the standard approach consists in questioning the assumption that eigenstates "can be prepared". How should such a "preparation" be achieved? By definition, an eigenstate is associated with zero dispersion of its energy. Hence, because of

$$\Delta E\,\Delta t \approx \hbar \quad \text{where} \quad \Delta E = \sqrt{\overline{(E - E_{nlm})^2}} \tag{136}$$

the preparation time $\Delta t$ is infinite for an eigenstate.[2] That is, in reality, an excited state can only be a solution to the **time-dependent** Schrödinger equation and hence may be cast as

$$\psi(\boldsymbol{r}, t) = \sum_{n,l,m} c_{nlm}\,\hat{\psi}_{nlm}(\boldsymbol{r})\,e^{-i\frac{E_{nlm}}{\hbar}\,t} \tag{137}$$

where

$$\int \hat{\psi}^*_{n'l'm'}(\boldsymbol{r})\,\hat{\psi}_{nlm}(\boldsymbol{r})\,d^3r = \delta_{n'n}\,\delta_{l'l}\,\delta_{m'm} \tag{138}$$

[2] A similar situation occurs if one wants to excite a superconducting cavity in one of its modes. If the cavity can lose energy to the outside at a small rate it behaves as if it were slightly attenuated. The time it takes to arrive at a stationary state grows longer and longer the weaker the energy loss becomes. The excitation time tends to infinity as the loss rate tends to zero.

and because of

$$\int |\psi(\boldsymbol{r},t)|^2\, d^3r = 1 \quad \text{one has} \quad \sum_{n,l,m} |c_{nlm}|^2 = 1\,. \tag{139}$$

Each term under the sum in Eq.(137) satiesfies individually the time-dependent Schrödinger equation of the hydrogen electron since by definition

$$\hat{H}\hat{\psi}_{nlm}(\boldsymbol{r}) = E_{nlm}\,\hat{\psi}_{nlm}(\boldsymbol{r}) \quad \text{where} \quad \hat{H} = \frac{\widehat{\boldsymbol{p}}^{\,2}}{2\,m_0} - \frac{e^2}{4\pi\varepsilon_0\, r} \quad \text{and} \quad \widehat{\boldsymbol{p}} = -i\hbar\,\nabla \tag{140}$$

A realistic "eigenstate" is characterized by the property that the square modulus of one the coefficients $c_{nlm}$ in Eq.(137) is close to unity, that of the others correspondingly small.
In the following we consider the situation in which the hydrogen atom has been excited from the ground state 1s to the state 2p where $m = 0$. The excitation may have been caused by absorbing linearly polarized light. As stated above, it is, as a matter of fact, impossible that the atom in the excitation process really ends up in the eigenstate 2p. Its state will rather have the form

$$\psi(\boldsymbol{r},t) = c_0\,\hat{\psi}_{1s}(\boldsymbol{r})\,e^{-i\frac{E_{1s}}{\hbar}\,t} + c_1\,\hat{\psi}_{2p}(\boldsymbol{r})\,e^{-i\frac{E_{2p}}{\hbar}\,t}$$
$$\text{where} \quad 0 < |c_0| \ll |c_1| < 1\,. \tag{141}$$

Using Eq.(141) we obtain

$$\int \psi^*(\boldsymbol{r},t)\,\hat{H}\,\psi(\boldsymbol{r},t)\,d^3r = \underbrace{|c_1|^2}_{=1-|c_0|^2}\; E_{2p} + |c_0|^2\,E_{1s}$$
$$\text{that is} \quad E = E_{2p} - \widetilde{E}\,|c_0|^2 \tag{142}$$

where

$$\widetilde{E} = E_{2p} - E_{1s}\,. \tag{143}$$

The expression $\widetilde{E}\,|c_0|^2$ represents obviously the uncertainty $\Delta E$ with which the 2p-state has been "prepared".
From Eq.(141) we may form the electronic charge density $\rho(\boldsymbol{r},t) = e\,|\psi(\boldsymbol{r},t)|^2$ which we cast as

$$\rho(\boldsymbol{r},t) = \rho_0(\boldsymbol{r}) + \widetilde{\rho}(\boldsymbol{r},t) \tag{144}$$

where

$$\rho_0(\boldsymbol{r}) = e\,\left[|c_0|^2\,\hat{\psi}^2_{1s}(\boldsymbol{r}) + |c_1|^2\,\hat{\psi}^2_{2p}(\boldsymbol{r})\right] \tag{145}$$

and

$$\widetilde{\rho}(\boldsymbol{r},t) = |c_0^*\, c_1|\, e\, \hat{\psi}_{1s}(\boldsymbol{r})\, \hat{\psi}_{2p}(\boldsymbol{r}) \left[ e^{i\left[\frac{E_{2p}-E_{1s}}{\hbar}\, t+\varphi\right]} + e^{-i\left[\frac{E_{2p}-E_{1s}}{\hbar}+\varphi\right]} \right] . \quad (146)$$

where $\varphi$ is defined through

$$c_0^* c_1 = |c_0^* c_1|\, e^{i\varphi} . \quad (147)$$

Here we have exploited the fact that $\hat{\psi}_{1s}(\boldsymbol{r})$ and $\hat{\psi}_{2p}(\boldsymbol{r})$ are real-valued functions. Eq.(144) may hence be rewritten

$$\rho(\boldsymbol{r},t) = \rho_0(\boldsymbol{r}) + 2\,|c_0^*\, c_1|\, \widetilde{\rho}_0(\boldsymbol{r}) \cos(\omega t + \varphi) \quad (148)$$

where

$$\widetilde{\rho}_0(\boldsymbol{r}) = e\, \hat{\psi}_{1s}(\boldsymbol{r})\, \hat{\psi}_{2p}(\boldsymbol{r}) \quad \text{and} \quad \omega = \frac{E_{2p}-E_{1s}}{\hbar} \quad \text{i. e.} \quad \hbar\,\omega = E_{2p} - E_{1s} \quad (149)$$

The following figure shows four snapshots of the time evolution of $\rho(\boldsymbol{r},t)$

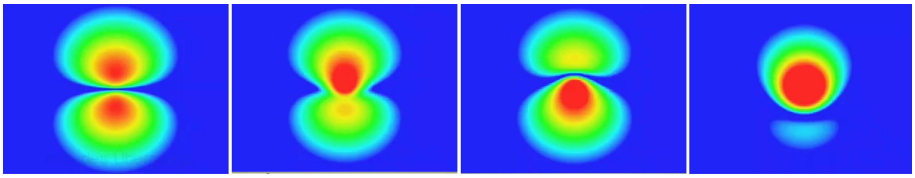

Figure 9: Four snapshots of the color coded density of a H-atom in the transition 2p→1s

As one can see from Eq.(142):

$$E = |c_0|^2\, E_{1s} + |c_1|^2\, E_{2p} \quad \text{and} \quad 0 \le |c_0|\,;\, 0 \le |c_1| \quad |c_0|^2 + |c_1|^2 = 1$$

the energy of the electron can have any value between $E_{2p}$ and $E_{1s}$. **Regardless of the value of** $E$ its charge density oscillates sharply at $\omega$! In the following calculation we shall derive a transition time which the electron takes to change its state from (141) with $0 < |c_0| \ll |c_1| < 1$ to a form of $\psi(\boldsymbol{r},t)$ where $|c_0| \approx 1$ and $|c_1| \approx 0$. This transition time turns out to be of the order of $10^{-9}\,s$, that is, **there are no quantum jumps**! At this point it should be remembered that the article by Dehmelt and collaborators [45] "..on the observation of quantum jumps" shows a plot of these jumps on a time scale of 20 s unit length!

The function $\psi(\boldsymbol{r},t)$ defined by Eq.(141) is a solution to the time-dependent Schrödinger equation

$$\hat{H}\psi(\boldsymbol{r},t) = i\,\hbar \frac{\partial}{\partial t}\, \psi(\boldsymbol{r},t) \quad (150)$$

only as long as the coefficients $c_0, c_1$ are constant. However, even when $c_0$ is very small compared to unity, $\rho(\boldsymbol{r}, t)$ oscillates at the frequency $\omega$ and thus gives rise to the emission of an electromagnetic wave. The latter is polarized in the direction of the quantization axis of $\hat{\psi}_{2p}(\boldsymbol{r})$ which also defines the symmetry axis of $\hat{\psi}_{1s}(\boldsymbol{r})\,\hat{\psi}_{2p}(\boldsymbol{r})$ in Eq.(149). As the atom loses energy in building up the electromagnetic wave, $E$ in Eq.(142) decreases, and hence $c_0$ must now increase as a function of time. This is a consequence of the fact that the radiation field acts back on the atom, and therefore the Hamiltonion in Eq.(150) is now modified:

$$\hat{H}'\psi(\boldsymbol{r}, t) = i\,\hbar\frac{\partial}{\partial t}\,\psi(\boldsymbol{r}, t) \quad \text{where} \quad \hat{H}' = \frac{(\hat{\boldsymbol{p}} - e\boldsymbol{A}(\boldsymbol{r}, t))^2}{2\,m_0} - \frac{e^2}{4\pi\varepsilon_0\,r} \tag{151}$$

where $\boldsymbol{A}(\boldsymbol{r}, t)$ denotes the vector potential of the radiation field. It is set up by the quantum mechanical current density $\boldsymbol{j}(\boldsymbol{r}, t)$. As we expect and what the calculation actually comes up with is an outgoing wave packet with a thickness of $c\,\hat{\tau}$ where $\hat{\tau}$ is the transition time. At a distance of some wavelength away from the center of the atom there is still a longitudinal component in the oscillating electric field in the wave packet. Moreover, the current density of the energy flow, $\boldsymbol{S}(\boldsymbol{r}, t)$, will display the characteristic feature of a Hertzian dipole.
In the article by Weisskopf and Wigner [50] the radiation field is quantized which suggests that their derivation qualifies to be more fundamental. The authors consider a transition between two states, an initial state defined by the electrons of the atom being in an excited eigenstate with no photon present and a final state that describes the electrons being in the lower eigenstate and a linear combination of quantized electromagnetic modes in a cube of volume $\mathcal{V}$ with ideally reflecting walls. Hence, these modes represent standing waves. The sum of the mod squared of the coefficients in the linear combination equals unity. All modes that pertain to the final state are assumed to have equal weight and are associated with essentially the same frequency $\omega = \frac{E_i - E_f}{\hbar}$. Here $E_i$ and $E_f$ refer to the energy of the electronic initial and final state, respectively.

From a principal point of view this field-theoretical description appears to be rather absurd. The final state does not represent an outgoing electromagnetic wave of a certain thickness which forms a hollow sphere about the emitter, as with our theory, but rather a set of standing waves which penetrate the emitter undisturbed. They penetrate the atom completely unmodified also during the entire transition process. There is nowhere a longitudinal electric field component. It seems to border on magic that a calculation of this kind still arrives at a result that is in agreement with the experiment, although the time evolution is hardly accessible and therefore still open to discussion.

We now turn back to our derivation. To obtain $\boldsymbol{A}(\boldsymbol{r}, t)$ we first determine

the current density

$$\boldsymbol{j}(\boldsymbol{r},t) = \frac{e\,\hbar}{2i\,m_0}\left[\psi^*(\boldsymbol{r},t)\nabla\,\psi(\boldsymbol{r},t) - \psi(\boldsymbol{r},t)\nabla\,\psi^*(\boldsymbol{r},t)\right]. \tag{152}$$

On inserting $\psi(\boldsymbol{r},t)$ from Eq.(141) the current density takes the form

$$\boldsymbol{j}(\boldsymbol{r},t) = \frac{e\,\hbar}{m_0}\,|c_0^*\,c_1|\,[\hat{\psi}_{1s}(\boldsymbol{r})\nabla\,\hat{\psi}_{2p}(\boldsymbol{r}) - \hat{\psi}_{2p}(\boldsymbol{r})\nabla\,\hat{\psi}_{1s}(\boldsymbol{r})]\,\sin(\omega\,t+\varphi)\,. \tag{153}$$

The vector potential $\boldsymbol{A}(\boldsymbol{r},t)$ and $\boldsymbol{j}(\boldsymbol{r},t)$ are interconnected by

$$\boldsymbol{A}(\boldsymbol{r},t) = \frac{\mu_0}{4\pi}\int\frac{\boldsymbol{j}(\boldsymbol{r}',t-\frac{|\boldsymbol{r}'-\boldsymbol{r}|}{c})}{|\boldsymbol{r}'-\boldsymbol{r}|}\,d^3r' \quad \text{where} \quad \mu_0 = \frac{1}{\varepsilon_0\,c^2}\,. \tag{154}$$

Because of Eq.(152) $\boldsymbol{A}(\boldsymbol{r},t)$ is a functional of $\psi(\boldsymbol{r},t)$. It follows then from inspection of Eq.(151) that this modified Schrödinger equation constitutes now a **non-linear** partial differential equation since the Hamiltonian $\hat{H}'$ depends on $\psi(\boldsymbol{r},t)$. Below we shall derive a detailed solution to this equation. If one is not interested in the details of the time dependence one can take a short-cut:
First we give the expressions

$$\hat{\psi}_{1s}(\boldsymbol{r})\nabla\,\hat{\psi}_{2p}(\boldsymbol{r}) \quad \text{and} \quad \hat{\psi}_{2p}(\boldsymbol{r})\nabla\,\hat{\psi}_{1s}(\boldsymbol{r})$$

a different form by using the identity (which is just an application of the chain rule):

$$[\hat{H}\,\boldsymbol{r} - \boldsymbol{r}\,\hat{H}]\,\hat{\psi}(\boldsymbol{r}) = -i\,\frac{\hbar}{m_0}\,\hat{\boldsymbol{p}}\,\hat{\psi}(\boldsymbol{r}) = -\frac{\hbar^2}{m_0}\,\nabla\,\hat{\psi}(\boldsymbol{r})\,. \tag{155}$$

This yields

$$\hat{\psi}_{1s}(\boldsymbol{r})\nabla\,\hat{\psi}_{2p}(\boldsymbol{r}) = \frac{m_0}{\hbar^2}\,[\hat{\psi}_{1s}(\boldsymbol{r})\,\boldsymbol{r}\,\hat{H}\,\hat{\psi}_{2p}(\boldsymbol{r}) - \hat{\psi}_{1s}(\boldsymbol{r})\,\hat{H}\,\boldsymbol{r}\,\hat{\psi}_{2p}(\boldsymbol{r})]$$

and

$$\hat{\psi}_{2p}(\boldsymbol{r})\nabla\,\hat{\psi}_{1s}(\boldsymbol{r}) = \frac{m_0}{\hbar^2}\,[\hat{\psi}_{2p}(\boldsymbol{r})\,\boldsymbol{r}\,\hat{H}\,\hat{\psi}_{1s}(\boldsymbol{r}) - \hat{\psi}_{2p}(\boldsymbol{r})\,\hat{H}\,\boldsymbol{r}\,\hat{\psi}_{1s}(\boldsymbol{r})]\,.$$

Forming the integral of Eq.(153), exploiting the hermitiaty of $\hat{H}$, using Eq.(208) and $\hbar\,\omega = E_{2p} - E_{1s}$ we thus obtain

$$I(t)\,\boldsymbol{e}_z = 2\,|c_0^*\,c_1|\,e\,\omega\int\hat{\psi}_{1s}(\boldsymbol{r})\,\boldsymbol{r}\,\hat{\psi}_{2p}(\boldsymbol{r})\,d^3r\,\sin(\omega\,t+\varphi) \quad \text{where} \quad \boldsymbol{e}_z||z-\text{axis} \tag{156}$$

The quantity $I(t)$ denotes the alternating current that is set up in the atom as a result of $c_0$ not being zero. The quantization axis of $\hat{\psi}_{2p}(\boldsymbol{r})$ is taken along the $z$-axis. We may rewrite the above integral

$$\int\hat{\psi}_{1s}(\boldsymbol{r})\,\boldsymbol{r}\,\hat{\psi}_{2p}(\boldsymbol{r})\,d^3r = \int\rho_{dipole}(\boldsymbol{r})\,\boldsymbol{r}\,d^3r = \overline{\boldsymbol{r}}$$

where we have expressed the fact that $\hat{\psi}_{1s}(\boldsymbol{r})\,\hat{\psi}_{2p}(\boldsymbol{r})$ represents a dipole-type probability density. Hence, Eq.(156) can be cast as

$$I(t)\,\boldsymbol{e}_z = -\frac{d}{dt}\,\boldsymbol{p}(t) \quad \text{where} \quad \boldsymbol{p}(t) = g(t)\,|e|\,\overline{\boldsymbol{r}}\,\cos\omega\,t \quad \text{and} \quad g(t) = 2\,|c_0^*(t)\,c_1(t)|\,.$$

As the emission of the electromagnetic wave proceeds, the coefficient $c_0$ becomes larger and will finally attain its largest value 1 at the end of the transition. According to Eq.(137) it will be equal to $\frac{1}{\sqrt{2}}$ in the middle of the transition. The coefficient $c_1$ changes in reverse since the sum of the square of the coefficients must be unity at any time. Hence, in the middle of the transition the function $g(t)$ defined above attains its maximum value 1 and drops asymptotically to zero on either side. To serve the purpose of the present short-cut, we approximate the actually bell-shape time-dependence of $g(t)$ by a rectangle of width $\hat{\tau}$ and height unity.
We now invoke Hertz's result on the density $\boldsymbol{S}(\boldsymbol{r},t)$ of the energy flow from an oscillating dipole:

$$\boldsymbol{S}(r,\theta,t) = \frac{1}{16\pi^2\,\varepsilon_0\,c^3}\,\frac{\sin^2\theta}{r^2}\,\left[\frac{d^2}{dt^2}\,\boldsymbol{p}(t)\right]^2$$

where $\theta$ is the angle that $\boldsymbol{r}$ encloses with the dipole axis.
Forming a surface integral with $\boldsymbol{S}(r,\theta,t)$ over a concentric sphere of radius r and averaging over one oscillation period one arrives at

$$S(t) = [g(t)]^2\,\frac{e^2\,\omega^4}{6\pi\,\varepsilon_0\,c^3}\,|\boldsymbol{p}_{n'n}|^2$$

$$\text{where} \quad S(t) = \pi\,r^2\int|\boldsymbol{S}(r,\theta,t)|\,\sin 2\,\theta\,d\,\theta \quad \text{and} \quad n' = 1s\,;n = 2p$$

and

$$\boldsymbol{p}_{n'n} = \int\hat{\psi}_{n'}(\boldsymbol{r})\,\boldsymbol{r}\,\hat{\psi}_n(\boldsymbol{r})\,d^3r\,; \qquad [g(t)]^2 = \begin{cases} 1 & \text{for} \quad |t| \le \hat{\tau}/2 \\ 0 & \text{for} \quad |t| > \hat{\tau}/2 \end{cases}\,. \quad (157)$$

Integration of $S(t)$ over the transition time $\hat{\tau}$ must yield $E_{2p} - E_{1s} = \hbar\,\omega$ :

$$\int_0^{\hat{\tau}} S(t)\,dt = \hbar\,\omega = \frac{e^2\,\omega^4}{6\pi\,\varepsilon_0\,c^3}\,|\boldsymbol{p}_{n'n}|^2\hat{\tau}\,.$$

From this we obtain an expression for the inverse of the transition time

$$\tfrac{1}{\hat{\tau}} = \frac{e^2\,\omega^3}{6\pi\,\varepsilon_0\,c^3\,\hbar}\,|\boldsymbol{p}_{n'n}|^2 \quad \text{or} \quad \tfrac{1}{\hat{\tau}} = \alpha\,\frac{2\,\omega^3}{3\,c^2}\,|\boldsymbol{p}_{n'n}|^2 \quad \text{where} \quad \alpha = \frac{e^2}{4\pi\varepsilon_0\,\hbar} \quad (158)$$

in agreement with the result of the standard calculation (s. e. g. [50]) which is based on a remarkably different concept, as already mentioned above. It

should be observed, however, that this calculation yields an expression for the transition rate $\frac{1}{\tau'}$ which is equated with $\frac{d}{dt}\,|c_0|^2(t)|_{t=0} = \frac{2}{\tilde{\tau}}$. Hence

$$\tfrac{1}{\tau'} = \frac{e^2\,\omega^3}{3\pi\,\varepsilon_0\,c^3\,\hbar}\,|\boldsymbol{p}_{n'n}|^2\,.$$

It is worth noting that the problem of spontaneous light emission has for the first time been treated by Fermi [51] in 1927. He chose an approach very similar to ours, but used the classical expression for the radiation back action $\propto \frac{d^3}{dt^3}\,p$ which led to a frequency shift of the emitted light depending on the transition time. However, this is at variance with the observation.

We now turn back to the problem of calculating the detailed time-dependence of $|c_0(t)|^2, |c_1(t)|^2$. To this end we first observe that

$$\hat{H}' = \hat{H} + \hat{H}_{int} = \frac{(\hat{\boldsymbol{p}} - e\boldsymbol{A}(\boldsymbol{r},t))^2}{2\,m_0} - \frac{e^2}{4\pi\varepsilon_0\,r} = \hat{H} - \frac{e}{m_0}\,\boldsymbol{A}(\boldsymbol{r},t)\cdot\hat{\boldsymbol{p}} + \ldots \quad (159)$$

where the dots stand for $\frac{(e\boldsymbol{A}(\boldsymbol{r},t))^2}{2\,m_0}$ which will be neglected for the term linear in $\boldsymbol{A}(\boldsymbol{r},t)$. Inserting (159) and $\psi(\boldsymbol{r},t)$ from (141) into the time-dependent Schrödinger equation Eq.(151), multiplying this equation by $\hat{\psi}_{2p}(\boldsymbol{r})\,e^{i\frac{E_{2p}}{\hbar}\,t}$ or alternatively by $\hat{\psi}_{1s}(\boldsymbol{r})\,e^{i\frac{E_{1s}}{\hbar}\,t}$ and performing a real-space integration one arrives at

$$i\hbar\,\dot{c}_1 = c_0\,M_{10}\,e^{i\omega\,t} + c_1\,M_{11} \quad (160)$$

where

$$M_{10} = \int \hat{\psi}_{2p}(\boldsymbol{r})\,\hat{H}_{int}\,\hat{\psi}_{1s}(\boldsymbol{r})\,d^3r \quad \text{and} \quad M_{11} = \int \hat{\psi}_{2p}(\boldsymbol{r})\,\hat{H}_{int}\,\hat{\psi}_{2p}(\boldsymbol{r})\,d^3r$$

and

$$\hat{H}_{int} = i\,\frac{e\hbar}{m_0}\boldsymbol{A}(\boldsymbol{r},t)\cdot\nabla\,. \quad (161)$$

Analogously we have, in obvious notation

$$i\hbar\,\dot{c}_0 = c_1\,M_{01}\,e^{-i\omega\,t} + c_0\,M_{00}\,. \quad (162)$$

According to Eqs.(153) and (154) one has

$$\boldsymbol{A}(\boldsymbol{r},t) = |c_0^* c_1|\,\frac{e\hbar}{4\pi\varepsilon_0\,m_0 c^2}\times \quad (163)$$

$$\int \frac{[\hat{\psi}_{1s}(\boldsymbol{r}')\nabla'\hat{\psi}_{2p}(\boldsymbol{r}') - \hat{\psi}_{2p}(\boldsymbol{r}')\nabla'\,\hat{\psi}_{1s}(\boldsymbol{r}')]\,\sin[\omega\,(t - \frac{|\boldsymbol{r}-\boldsymbol{r}'|}{c}) + \varphi]}{|\boldsymbol{r}-\boldsymbol{r}'|}\,d^3r'\,.$$

The retardation in the time dependence of the sine-function is crucial for the occurrence of an outgoing wave. If one were to neglect retardation the

atom would not undergo a change of its energy, averaged over an oscillation period.
For light frequencies $\nu = \frac{\omega}{2\pi} \approx 10^{15} s^{-1}$ and $|\boldsymbol{r} - \boldsymbol{r}'| \lessapprox 4 \cdot 10^{-8} cm$ for points within the atomic volume we have $\frac{\omega}{c}|\boldsymbol{r} - \boldsymbol{r}'| \lessapprox 10^{-2}$, and hence we may approximate:

$$\sin[\omega\,(t - \tfrac{|\boldsymbol{r}-\boldsymbol{r}'|}{c}) + \varphi] \approx \sin(\omega\,t + \varphi) - \omega\,\tfrac{|\boldsymbol{r}-\boldsymbol{r}'|}{c}\cos(\omega\,t + \varphi)$$

Inserting this into Eq.(163) one obtains

$$\boldsymbol{A}(\boldsymbol{r}, t) = \boldsymbol{A}_1(\boldsymbol{r}, t) + \boldsymbol{A}_2(\boldsymbol{r}, t) = \hat{\boldsymbol{A}}_1(\boldsymbol{r})\sin(\omega\,t + \varphi) + \hat{\boldsymbol{A}}_2\cos(\omega\,t + \varphi) \quad (164)$$

where

$$\hat{\boldsymbol{A}}_1(\boldsymbol{r}) = |c_0^* c_1|\,\frac{e\hbar}{4\pi\varepsilon_0\,m_0 c^2}\int \frac{[\hat{\psi}_{1s}(\boldsymbol{r}')\nabla'\hat{\psi}_{2p}(\boldsymbol{r}') - \hat{\psi}_{2p}(\boldsymbol{r}')\nabla'\,\hat{\psi}_{1s}(\boldsymbol{r}')]}{|\boldsymbol{r} - \boldsymbol{r}'|}\,d^3r' \quad (165)$$

and

$$\hat{\boldsymbol{A}}_2 = -|c_0^* c_1|\,\frac{e\,\hbar\,\omega}{4\pi\varepsilon_0\,m_0 c^3}\int [\hat{\psi}_{1s}(\boldsymbol{r}')\nabla'\hat{\psi}_{2p}(\boldsymbol{r}') - \hat{\psi}_{2p}(\boldsymbol{r}')\nabla'\,\hat{\psi}_{1s}(\boldsymbol{r}')]\,d^3r' \quad (166)$$

The integral in Eq.(166) can be rewritten by using the identity (155):

$$\boldsymbol{A}_2(\boldsymbol{r}, t) = \hat{\boldsymbol{A}}_2\,\cos(\omega\,t + \varphi) = \\ -2|c_0^* c_1|\,\frac{e\,\omega^2}{4\pi\varepsilon_0\,c^3}\underbrace{\int \hat{\psi}_{1s}(\boldsymbol{r}')\boldsymbol{r}'\,\hat{\psi}_{2p}(\boldsymbol{r}')\,d^3r'}_{=\boldsymbol{p}_{n'n}}\cos(\omega t + \varphi)\,. \quad (167)$$

We now form the matrix element of $\hat{H}_{int} = i\,\frac{e\hbar}{m_0}\boldsymbol{A}(\boldsymbol{r}, t)\cdot\nabla$ according to Eq.(160) using again the identity (155).

$$M_{10} = \frac{i\hbar}{m_0}\,2|c_0^*\,c_1|\,\frac{e^2\,\omega^2}{4\pi\,\varepsilon_0\,c^2}\,\boldsymbol{p}_{n'n}\cdot\underbrace{\int \hat{\psi}_{2p}\nabla\,\hat{\psi}_{1s}\,d^3r}_{=-\omega\,\frac{m_0}{\hbar}\boldsymbol{p}_{n'n}}\cos(\omega t + \varphi) \quad (168)$$

$$+\frac{i\hbar}{m_0}\int \hat{\psi}_{2p}(\boldsymbol{r})\,\frac{e}{m_0}\hat{\boldsymbol{A}}_1(\boldsymbol{r})\cdot\nabla\,\hat{\psi}_{1s}(\boldsymbol{r})\,d^3r\,\sin(\omega\,t + \varphi)$$

We multiply Eq.(160) by $c_1^*$ and form the sum with its complex conjugate. The result may be written:

$$\frac{\partial}{\partial t}|c_1(t)|^2 = -4\gamma\,|c_0^*(t)c_1(t)|^2\cos^2(\omega\,t + \varphi) + \quad (169)$$

$$2|c_0^*(t)c_1(t)| \int \hat{\psi}_{2p}(\boldsymbol{r})\,\frac{e}{m_0}\hat{\boldsymbol{A}}_1(\boldsymbol{r})\cdot\nabla\hat{\psi}_{1s}(\boldsymbol{r})\,d^3r\,\cos(\omega\,t+\varphi)\sin(\omega\,t+\varphi)$$
$$+2|c_1(t)|^2 \int \hat{\psi}_{2p}(\boldsymbol{r})\,\frac{e}{m_0}\hat{\boldsymbol{A}}_1(\boldsymbol{r})\cdot\nabla\hat{\psi}_{2p}(\boldsymbol{r})\,d^3r\,\sin(\omega\,t+\varphi)$$
$$+2|c_1(t)|^2 \int \hat{\psi}_{2p}(\boldsymbol{r})\,\frac{e}{m_0}\hat{\boldsymbol{A}}_2\cdot\nabla\hat{\psi}_{2p}(\boldsymbol{r})\,d^3r\,\cos(\omega\,t+\varphi)\,.$$

The quantity $\gamma$ in the first line of this equation stands for

$$\gamma = \frac{e^2\,\omega^3}{4\pi\,\varepsilon_0\,c^3\,\hbar}\,|\boldsymbol{p}_{n'n}|^2\,. \tag{170}$$

We now perform a time average on the right-hand side of Eq.(169) over successive oscillation periods $T = \frac{2\pi}{\omega}$ of the emitted light. Since the emission time $\hat{\tau}$ is many orders of magnitude larger than $T$, one may approximate $|c_{0/1}(t)|$ by $|c_{0/1}(\bar{t}_\nu)|$ where $\nu = 1, 2, \ldots$ counts successive oscillation intervals and $\bar{t}_\nu$ denotes an appropriately chosen time in the respective interval. On performing the time average all terms on the right-hand side of Eq.(169) now drop out except for the first one. Hence we arrive at

$$\frac{\partial}{\partial t}|c_1(t)|^2 = -2\gamma\,|c_0(t)|^2|c_1(t)|^2 \tag{171}$$

where we have used $\overline{\cos^2(\omega\,t+\varphi)} = \frac{1}{2}$ with the bar denoting time averaging. We have, furthermore, replaced the histogram-type functions of time $|c_{0/1}(\bar{t}_\nu)|^2$ on the right-hand side by their smooth least mean-square fits.
In complete analogy we obtain

$$\frac{\partial}{\partial t}|c_0(t)|^2 = 2\gamma\,|c_0(t)|^2|c_1(t)|^2\,. \tag{172}$$

Since $|c_0(t)|^2 + |c_1(t)|^2 = 1$, the time derivative of this sum must vanish. This is obviously ensured by the above two coupled equations (171) and (172). It can readily be verified that their two solutions are

$$|c_0(t)|^2 = \tfrac{1}{2}\,(1+\tanh\tfrac{2t}{\tau}) \quad \text{and} \quad |c_1(t)|^2 = \tfrac{1}{2}\,(1-\tanh\tfrac{2t}{\tau})\,. \tag{173}$$

On multiplying these two functions one gets

$$|c_0(t)|^2|c_1(t)|^2 = \tfrac{1}{4}\,\frac{1}{\cosh^2\frac{2t}{\tau}}\,.$$

From Eq.(171) we have

$$\frac{\partial}{\partial t}|c_1(t)|^2 = -2\gamma\,|c_0(t)|^2|c_1(t)|^2 = -\tfrac{1}{2}\,\gamma\,\frac{1}{\cosh^2\frac{2t}{\tau}}\,.$$

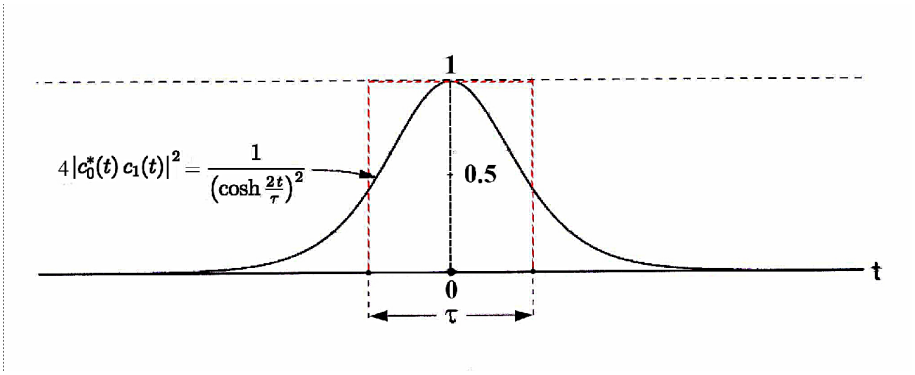


Figure 10: Optical transition: time-dependence of the "driving force" $\propto \boldsymbol{A}_2^2$

On the other hand it follows from Eq.(173) on differentiating $|c_1(t)|^2$

$$\frac{\partial}{\partial t}|c_1(t)|^2 = -\frac{1}{\tau}\,\frac{1}{\cosh^2\frac{2t}{\tau}}\,.$$

That means, the functions $|c_1(t)|^2$ and $|c_0(t)|^2$ fulfill Eqs.(171) and (172) if

$$\tfrac{1}{\tau} = \tfrac{1}{2}\,\gamma = \frac{e^2\,\omega^3}{8\pi\,\varepsilon_0\,c^3\,\hbar}\,|\boldsymbol{p}_{n'n}|^2\,.$$

Comparing this result with our "short-cut calculation" (158) we see that it is 25% smaller than the latter:

$$\frac{1}{\tau} = 0.75\,\frac{1}{\hat{\tau}}\,.$$

This difference originates in the simplification of the time dependence of $|c_1(t)|^2$ and $|c_0(t)|^2$ in taking the short-cut.
The following figure illustrates the time dependences according to Eq.(173). We have marked two points A and B on the left-hand side of the curve for $|c_1(t)|^2$. As explained in connection with Eq.(142), the quantity $[E_{2p} - E_{1s}]\,|c_0|^2$ represents the energy uncertainty with which the state $\hat{\psi}_{2p}(\boldsymbol{r})$ has been "prepared" as a result of the finite preparation time $\Delta t$. With the aid of Eq.(136) and $|c_1(t)|^2 = 1 - |c_0(t)|^2$ this can be recast

$$1 - |c_1(t)|^2 = \frac{\hbar}{[E_{2p} - E_{1s}]\,\Delta t}\,.$$

The shorter the excitation time, the more $|c_1(t)|^2$ departs from unity. Hence, point A refers to a longer excitation time than point B. Correspondingly, if the system has landed at A after the excitation process, it takes a longer time to reach the transition interval (marked by two vertical dashed lines)

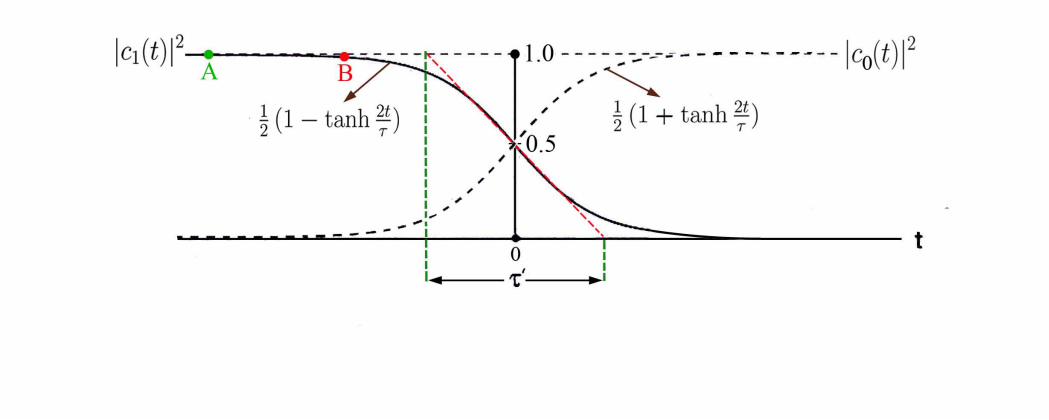


Figure 11: Optical transition between two states: Time dependence of the modulus square of the two-state related coefficients

than it would take if it would start at B. One may refer to these residence times prior to emission as "dead times". It should be noticed, however, that the "emission time", limited by the two vertical dashed lines, remains largely unaffected by the different lengths of the dead times. That is to say, largely independent of the form of the excitation one observes a spectral line of a natural width that is only determined by the two states of the atom under study.

As already alluded to, the time evolution of the transition obtained above contrasts remarkably with that of Weisskopf and Wigner [50]. Their article is still considered ground laying for the theory of spontaneous light emission. However, these authors arrive at $|c_1(t)|^2 = e^{-\frac{t}{\tau'}}$ which appears to be plausible at first sight, but is inconsistent with a solution to the time-dependent Schrödinger equation as follows from our derivation.

Another point of misunderstanding concerns "the measurement" of that exponential decay law $e^{-\frac{t}{\tau'}}$. Clearly, neither $|c_1(t)|^2$ nor any related quantity, for example $E = |c_0(t)|^2 E_{1s} + |c_1(t)|^2 E_{2p}$, is experimentally accessible in any way since one can only detect the light (i. e. the associated photon) when it has been fully emitted. What is actually done in the experiments is measuring the time-dependence of the photon-capture rate at which a photon detector fires after a large number of identical atoms has been excited by a flash. In the ensuing process the atoms re-emit the light spontaneously. The instant of time of the flash serves as a reference point with respect to which the detector records the flow of the incoming photons, and this flow is exponentially decaying in time. But each atom contributes only one single photon. Obviously, the photons are emitted at different times from different atoms. What has the time-dependence of their flow to do with the Weisskopf-Wigner decay law which refers to the time evolution of a single

atom? According to their theory all atoms start decaying immediately after the excitation by the flash. Since the photons can only be detected after the asssociated wave packets have been fully emitted, they should also be monitored by the detector at approximately the same time and not according to an exponential time law.
Our derivation relates the re-emission of photons at different times to different deadtimes which occur because of the spectral width of the light-flash. If the atom absorbs a photon of lower frequency out of the flash ($\omega < \omega_0$) it ends up in a state where $|c_1(t)|^2$ is now smaller than unity and we have because of Eq.(142)

$$\hbar\,\Delta\omega = \Delta E\,[1 - |c_1(t)|^2] \quad \text{which can be recast} \quad \hbar\,\Delta\omega = \Delta E\,|c_0(t)|^2 \tag{174}$$

with $\Delta\omega$ denoting $\omega_0 - \omega$ where $\omega_0 = \frac{E_{2p}-E_{1s}}{\hbar}$.
We temporarily abbreviate $\frac{2t}{\tau}$ into $x$ and observe

$$\tanh x = \frac{e^x - e^{-x}}{e^x + e^{-x}} \approx -1{+}e^{2x} \quad \text{if} \quad x \ll -1 \text{ and hence } \tfrac{1}{2}\,(1{+}\tanh x) \approx \tfrac{1}{2}\,e^{2x}\,.$$

Eq.(174) may therefore be rewritten (replacing $\Delta E$ with $E_{2p} - E_{1s}$ for clarity):

$$\hbar\,\Delta\omega = \tfrac{E_{2p}-E_{1s}}{2}\,e^{\frac{4t}{\tau}}\,. \tag{175}$$

Here $t \ll -\tau$ is referenced to the middle of the transition interval. If one wants to find the position of some point like A or B in the above figure for some atom that has absorbed a photon of energy $\hbar(\omega_0 - \Delta\omega)$, one has to insert the particular $\Delta\omega$ in Eq.(175) and one obtains the associated $t$ that gives the distance of that point from the middle of the transition interval. If the spectrum of the flash is rectangular the probability of an atom absorbing such a photon is equal for all frequencies of the spectrum. That means that the lengths of the dead times $t$ associated with the various values of $\Delta\omega$ are ordered in an exponential fashion.
Each atom appears with one deadtime point on its associated $|c_0(t)|^2$-curve ( Fig.(11)). These points form a dotted line along a common $|c_0(t)|^2$-curve if one projects them from their individual curves onto one plot. The density of the points is exponentially decreasing in the $(-t)$-direction. The points move at constant velocity towards the transition intervall. The time a point takes to travers the transition interval is $\tau$. If $n(t)$ is the number of atoms whose points are within that transition interval at time $t$, the transition rate is then given by $\frac{n(t)}{\tau}$ which means

$$\dot{n} = -\frac{n(t)}{\tau} \quad \hookrightarrow \quad n(t) = n_0\,e^{-\frac{t}{\tau}}\,,$$

where $t = 0$ marks the beginning of the emissions and $n_0$ is the number of originally excited atoms. It is this result which explains the observed

exponential time law of spontaneous emission.

In concluding this section we want to hint at a particular feature of our treatment that might encourage an interesting experiment: One could use the experimental setup by Dehmelt and associates [45] in which a single $Ba^+$-ion is kept in a Paul-trap. The ion contains one outer electron which behaves very similar to a hyrogen electron considered so far. One can excite this electron from its 6s-groundstate to a 6p-state by the absorption of linearly polarized light of the appropiate energy. According to our theory the ion will spontaneously emit light then which is polarized in the same plane as the light that was previously absorbed. A detector monitors the emitted photon at some fixed distance $d$. (As for the definition of a photon the ensuing section should be consulted.) The detector can be moved on a sphere of radius $d$. If the excitation has been repeated sufficiently often, the lateral distribution of detection events along the sphere should display the characteristic features of the Hertzian dipole radiation, i. e. the dependence of its electromagnetic energy density as a function of the polar angle.

## 21 Planck's radiation law

An important spin-off product of the previous section is the perception of a rigid interrelation between the energy content of an electromagnetic wavepacket that oscillates at an angular frequency $\omega$ and the concomitant energy loss $\Delta E$ of an electrically charged quantenmechanical system:

$$\hbar\omega = \Delta E\,. \tag{176}$$

"Free radiation" which all considerations in quantum electrodynamics and its formalisms of quantization start from does not exist in nature. Radiation always originates from a source where it has been generated by oscillating current densities that are associated with charged particles. Their motion is governed by quantum mechanics and therefore gives rise to an apparent quantization of the emitted electromagnetic wave according to Eq.(176).

In his paper of 1905 Einstein [52] suggested the existence of "light quanta" (later renamed "photons" by the chemist Gilbert Newton Lewis [53] and earlier already by Arthur Compton). Though this new idea was already introduced 20 years before the advent of the quantum mechanics of radiation it proved to be ground laying for today's understanding of light/matter interaction. For the first time it introduces a puzzling and seeemingly contradictory particle/wave-concept which can be summarized as follows:

1. The photon is a point-like object. It contains the full energy of the primarily generated electrodynamical wave packet emitted from some oscillating charge, in particular from an atom. Despite the fact that the electrodynamical field spreads from the atom over the entire space

as long as it is not absorbed, it is evident from the experiments that the energy of the wavepacket is in the end fully transferred to an absorber atom. This absorber may be astronomically distant. Of course, the absorption probability decreases as the inverse of the distance squared, but if the absorption takes place it is the original amount of energy. This behavior can only be explained if the lateral dimension of a photon is infinitesimally small. On its way to the absorber it never divides up even when the wavepacket is split according to the laws of electrodynamics, for example, at beam splitters or any other optical object. It stays with one part of the split wavepacket and the probability of which part it chooses is dictated by the classical reflectivity/transparency. Quite generally, the laws of electrodynamics governing the propagation of the wavepacket stay intact everywhere. The polarization of the photon is that of the wave packet.

2. The probability density of finding the photon of frequency $\omega$ in the associated propagating wave field is given by[3]

$$\rho(\boldsymbol{r},t) = \frac{u(\boldsymbol{r},t)}{\hbar\,\omega} \tag{177}$$

where $u(\boldsymbol{r},t) = \epsilon_0\, c\, \overline{|\vec{E}_\gamma(\boldsymbol{r},t)|^2}$ denotes the electromagnetic energy density, $\vec{E}_\gamma$ the electrical field vector in the wave packet, $c$ the light velocity in vacuo, and $\epsilon_0$ the permittivity of the vacuum. The expression $\overline{|\vec{E}_\gamma(\boldsymbol{r},t)|^2}$ is a spatial average of $|\vec{E}_\gamma(\boldsymbol{r},t)|^2$:

$$\overline{|\vec{E}_\gamma(\boldsymbol{r},t)|^2} = \tfrac{1}{\delta V} \int_{\delta V} |\vec{E}_\gamma(\boldsymbol{r},t)|^2\, d^3r\,,$$

where $\delta V$ denotes a cylindrical volume about the point $\boldsymbol{r}$.
It is given by the infinitesimal cross section of an energy fluxtube in the direction of propagation times the wavelength $\lambda = 2\pi\frac{c}{\omega}$ of the wave packet. To keep the notation simple the centroid of this volume is also denoted by $\boldsymbol{r}$.
If the wavepacket has been split up but the various portions are refocused again to a confined space where they can interfere, the photon will not appear where $u(\boldsymbol{r},t)$ is zero due to destructive interference. This is despite the fact that it has been following only one of the portions to the place of interference.

It is important to note that Einstein's photon hypothesis has to be regarded as a postulate. It cannot be proved opposed to what one might erraneously be inferred from the existence of quantum electrodynamics where photons

[3]This applies to a very good approximation if the frequency spread of the wave packet is very small compared to the central frequency of its spectrum.

appear as a consequence of the formal apparatus. The formalism is contrived to yield the quantization.
Another point which is actually quite irritating concerns the size of a photon: There is still a widespread doubt as to whether or not the photon is a point-like particle as one form of its appearance in the particle/wave concept. It has been Louis de Broglie who used exactly this particle/wave duality when he layed ground to wave mechanics. He just reversed Einstein's line of thought. Ironically, today nobody has any qualms about interpreting the modulus square of the wavefunction $\psi(\boldsymbol{r})$ as the probability density of a point-like particle occurring at $\boldsymbol{r}$, but there are always doubts about the size of a photon.

Thermal ("black") radiation as a radiation standard is generated in closed cavities whose surface inside is kept at a well defined temperature. Towards the outside there is a small opening which must be small enough to ensure that the outgoing radiative energy flux whose spectral density is the object of interest, affects only negligibly the thermal equilibrium of the radiation inside.
Inside the cavity the heated walls represent oscillating charged currents which emit electromagnetic wavepackets into the hollow space of the cavity. For simplicity the hollow space is assumed to be a rectangular parallelepiped whose edge lengths are $L_j$ with $j = 1, 2, 3$ numbering the three coordinate axes which are collinear with the edges.
In a stationary state of the radiation inside the cavity the walls re-absorb as much radiation as they emit. If a photon stays within the cavity for some residence time much larger than the oscillation period of its associated wave, it can attain a quasi-stationary state only if that wave is a standing wave, i. e. a "mode" of the cavity. Each mode is characterized by a wave vektor $\boldsymbol{k}$ whose components are specified by the requirement:

$$k_j = \begin{cases} (2n_j - 1)\,\frac{\pi}{L_j}\,; & n_j = 1, 2, 3, \ldots \\ n_j\,\frac{2\pi}{L_j}\,; & n_j = 1, 2, 3, \ldots \end{cases} \tag{178}$$

This ensures that the standing wave has nodes at the inner surface of the cavity. The photons considered in the following will exclusively be linearly polarized with the two planes of polarization denoted by $\sigma = \pm 1$.
Since photons do not interact, there can be any number of photons sharing this mode. This simply amounts to increasing the amplitude of that standing wave by a faktor of $\sqrt{n_{\boldsymbol{k},\sigma}}$ if there are $n_{\boldsymbol{k},\sigma}$ photons. Recalling the interconnection (176) one obtains for the energy in that mode:

$$\mathcal{E}_{\boldsymbol{k},\sigma} = n_{\boldsymbol{k},\sigma}\,\hbar\omega_{\boldsymbol{k}} \quad \text{where} \quad n_{\boldsymbol{k},\sigma} = 0, 1, 2 \ldots . \tag{179}$$

In contact with the cavity walls which serve as a heat bath of temperature $T$ the thermal average of this energy becomes

$$\overline{\mathcal{E}}_{\boldsymbol{k},\sigma} = \frac{1}{\sigma_{\boldsymbol{k},\sigma}} \sum_{\mathcal{E}_{\boldsymbol{k},\sigma}} \mathcal{E}_{\boldsymbol{k},\sigma}\, e^{-\beta\, \mathcal{E}_{\boldsymbol{k},\sigma}}$$

where

$$\sigma_{\boldsymbol{k},\sigma} = \sum_{\mathcal{E}_{\boldsymbol{k},\sigma}} e^{-\beta\, \mathcal{E}_{\boldsymbol{k},\sigma}} \quad \text{denotes the partition function and} \quad \beta \stackrel{def}{=} \tfrac{1}{k_B\, T}\,.$$

Using Eq.(179) one can rewrite the right-hand side

$$\overline{\mathcal{E}}_{\boldsymbol{k},\sigma} = \frac{\hbar\omega_{\boldsymbol{k}}}{\sigma_{\boldsymbol{k}\sigma}} \sum_{n_{\boldsymbol{k},\sigma}} n_{\boldsymbol{k},\sigma} \left[e^{-\beta\, \hbar\omega_{\boldsymbol{k}}}\right]^{n_{\boldsymbol{k}}}\,. \tag{180}$$

The sum on the right-hand side has the form

$$\sum_{n=1}^{\infty} n\, Q^n = \frac{d}{dQ} \sum_{n=0}^{\infty} Q^n = \frac{d}{dQ}\, \frac{1}{1-Q} = \frac{Q}{(1-Q)^2} \quad \text{where} \quad Q = e^{-\beta\, \hbar\omega_{\boldsymbol{k}}}\,.$$

Correspondingly we have

$$\sigma_{\boldsymbol{k}} = \sum_{n_{\boldsymbol{k}}} \left[e^{-\beta\, \hbar\omega_{\boldsymbol{k}}}\right]^{n_{\boldsymbol{k}}} = \frac{1}{1-Q}\,. \quad \text{Hence} \quad \overline{\mathcal{E}}_{\boldsymbol{k},\sigma} = \hbar\omega_{\boldsymbol{k}}\, \frac{Q}{(1-Q)}\,,$$

One can therefore cast the average energy $\overline{\mathcal{E}}_{\boldsymbol{k},\sigma}$ as

$$\overline{\mathcal{E}}_{\boldsymbol{k},\sigma} \equiv \overline{\mathcal{E}}_{\boldsymbol{k}} = \hbar\omega_{\boldsymbol{k}}\, \overline{n}_{\boldsymbol{k}}\,, \tag{181}$$

where

$$\overline{n}_{\boldsymbol{k}} = \frac{1}{e^{\frac{\hbar\omega_{\boldsymbol{k}}}{k_B\, T}} - 1}\,. \tag{182}$$

The right-hand side represents formally a Bose-distribution function of $\hbar\omega_{\boldsymbol{k}}$ with vanishing chemical potential. This reference is, however, quite misleading because particle spin does nowhere appear along the entire derivation, and there is no symmetric $N$-particle wavefunction in the configuration space which would refer to the photons under consideration. All that has been presupposed is that the wavepackets, and consequently the modes, can linearly be superposed.
The total radiation energy within the cavity is given by

$$\mathcal{E} = \sum_{\boldsymbol{k},\sigma} \overline{\mathcal{E}}_{\boldsymbol{k}} = 2 \sum_{\boldsymbol{k}} \overline{\mathcal{E}}_{\boldsymbol{k}}\,. \tag{183}$$

Because of (178) one has

$$k_{j,n_j+1} - k_{j,n_j} \stackrel{def}{=} \Delta k_j = \frac{2\pi}{L_j}$$

and hence

$$\Delta^3 k \stackrel{def}{=} \Delta k_1\, \Delta k_2\, \Delta k_3 = \frac{2\pi}{L_1}\,\frac{2\pi}{L_2}\,\frac{2\pi}{L_3} = \frac{(2\pi)^3}{\mathcal{V}}\,, \quad \text{that is} \quad \frac{\mathcal{V}}{(2\pi)^3}\,\Delta^3 k = 1\,.$$

Eq.(183) may therefore be rewritten

$$\mathcal{E} = 2\frac{\mathcal{V}}{(2\pi)^3}\,\sum_{\boldsymbol{k}} \overline{\mathcal{E}}_{\boldsymbol{k}}\,\Delta^3 k \approx 2\frac{\mathcal{V}}{(2\pi)^3}\int \overline{\mathcal{E}}_{\boldsymbol{k}}\, d^3 k = \frac{\mathcal{V}}{\pi^2}\int_0^\infty \overline{\mathcal{E}}_k\, k^2 dk$$

where it has been exploited that $\omega_{\boldsymbol{k}}$ depends only on $k = |\boldsymbol{k}|$.
Substituting $k$ with $\frac{\omega}{c}$ and inserting $\overline{\mathcal{E}}_k$ from Eq.(181) one arrives at

$$\frac{\mathcal{E}}{\mathcal{V}} \stackrel{def}{=} u = \int_0^\infty \underbrace{\frac{\hbar}{\pi^2\, c^3}\,\omega^3 \frac{1}{e^{\frac{\hbar\omega}{k_B\, T}} - 1}}_{\stackrel{def}{=} \hat{u}_\omega}\, d\omega\,.$$

The quantity $u$ denotes the energy density, and $\hat{u}_\omega$ stands for the spectral energy density. The latter expression represents Planck's radiation law.
Although the spectral density of sunlight is exactly described by this law it remains rather unclear how nearsurface subspaces of the sun can be subdivided into cavities and their interior. This applies similarly to the light emitted from incandescent material.

# 22 The time-dependent N-particle Schrödinger equation

So far we have merely been concerned with a single particle whose stochastic behavior was described by regarding it as a member of $N$ identically prepared, but statistically independent one-particle systems under the supposition that $N$ be sufficiently large. To avoid confusion we shall henceforth rename that number by $\mathcal{N}$. Instead of a single particle we now consider $N$ particles that interact via pair-forces. Each of these particles is individually a member of $\mathcal{N}$ statistically independent one-particle systems where the $N-1$ remaining particles appear at fixed positions $\boldsymbol{r}_2, \boldsymbol{r}_2, \ldots \boldsymbol{r}_N$ if the particle under consideration, picked at will, just happens to be "number 1". The considerations of Sections 11 and 15 carry over to this $N$-particle system. To see that one simply has to replace the 3-dimensional real-space

of the single particle discussed as yet by a $3N$-dimensional space where the $N$ particles appear as one point again. Instead of the probability density $\rho(\boldsymbol{r},t)$ one is now dealing with

$$\rho(\boldsymbol{r}_1,\boldsymbol{r}_2,\ldots\boldsymbol{r}_N,t)=\rho(\boldsymbol{r}^N,t)$$

$$\text{where}\qquad \int\rho(\boldsymbol{r}^N,t)\,d^3r_1\,d^3r_2\,\ldots d^3r_N=1 \tag{184}$$

and

$$\boldsymbol{r}^N=(\boldsymbol{r}_1,\boldsymbol{r}_2,\ldots\boldsymbol{r}_N)=\sum_{j=1}^{N}\sum_{k=1}^{3}x_{j\,k}\,\boldsymbol{e}_{j\,k}$$

with $j=1,2,\ldots N$ numbering the particles and $x_{j\,k}$ denoting Cartesian coordinates which are associated with orthogonal unit vectors $\boldsymbol{e}_{j\,k}$. The quantities $\nabla^N$, $\boldsymbol{u}^N$ and $\boldsymbol{v}^N$ are defined analogously.
Instead of $\varphi(\boldsymbol{r},t)$ we now have $\phi(\boldsymbol{r}^N,t)$. Thus

$$\boldsymbol{v}^N(\boldsymbol{r}^N,t)=\frac{\hbar}{m_0}\,\nabla^N\,\phi(\boldsymbol{r}^N,t)\,. \tag{185}$$

Correspondingly, the $3N$-dimensional osmotic velocity has the form

$$\boldsymbol{u}^N(\boldsymbol{r}^N,t)=-\frac{\hbar}{2\,m_0}\,\nabla^N\,\ln[\rho(\boldsymbol{r}^N,t)/\rho_0]\,, \tag{186}$$

and hence we have similar to the single-particle case

$$\frac{\partial\boldsymbol{u}^N}{\partial t}=-\frac{\hbar}{2\,m_0}\,\nabla^N\frac{\partial}{\partial t}\,[\ln\rho/\rho_0]=-\frac{\hbar}{2\,m_0}\,\nabla^N\,\left[\frac{1}{\rho}\,\frac{\partial\rho}{\partial t}\right]\,. \tag{187}$$

Invoking the equation of continuity

$$\frac{\partial\rho}{\partial t}+\underbrace{\nabla^N\cdot(\rho\,\boldsymbol{v}^N)}_{=\rho\,\nabla^N\cdot\boldsymbol{v}^N+\boldsymbol{v}^N\cdot\nabla^N\rho}=0$$

and using the definition (186), Eq.(187) can be cast as

$$\frac{\partial\boldsymbol{u}^N}{\partial t}=-\frac{\hbar}{2\,m_0}\,\nabla^N\,[(\nabla^N\cdot\boldsymbol{v}^N)-(\boldsymbol{u}^N\cdot\boldsymbol{v}^N)]\,. \tag{188}$$

In the following we first confine ourselves to time-independent conservative forces which - in the spirit of our notation - may be written

$$\boldsymbol{F}^N_{ext.}(\boldsymbol{r}^N)=\sum_{j=1}^{N}\sum_{k=1}^{3}F^{ext.}_k(\boldsymbol{r}_j)\,\boldsymbol{e}_{j\,k}$$

where

$$F_k^{ext.}(\boldsymbol{r}_j) = -\frac{\partial}{\partial x_{j\,k}}\, V_{ext.}(\boldsymbol{r}_j)$$

with $V_{ext.}(\boldsymbol{r})$ denoting an external potential. Hence $\boldsymbol{F}_{ext.}^N$ may alternatively be written

$$\boldsymbol{F}_{ext.}^N(\boldsymbol{r}^N) = -\nabla^N \widehat{V}_{ext.}(\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots \boldsymbol{r}_N)$$

where

$$\widehat{V}_{ext.}(\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots \boldsymbol{r}_N) = \sum_{j=1}^{N} V_{ext.}(\boldsymbol{r}_j)\,.$$

The force exerted on the $j$-th particle due to pair-interaction with the $N-1$ remaining particles is given by

$$F_{j\,k}^{inter}(\boldsymbol{r}_j) = -\frac{\partial}{\partial\, x_{j\,k}} \sum_{\substack{i=1 \\ i\neq j}}^{N} V(|\boldsymbol{r}_j - \boldsymbol{r}_i|)\,,$$

where $V(|\boldsymbol{r}_j - \boldsymbol{r}_i|)$ denotes the interaction potential. The generalized total force in the $3N$-dimensional space may therefore be cast as

$$\boldsymbol{F}^N(\boldsymbol{r}^N) = -\nabla^N \widehat{V}(\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots \boldsymbol{r}_N)\,,$$

where $\widehat{V}(\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots \boldsymbol{r}_N)$ is defined by

$$\widehat{V}(\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots \boldsymbol{r}_N) = \sum_{j=1}^{N} V_{ext.}(\boldsymbol{r}_j) + \frac{1}{2}\sum_{j=1}^{N}\sum_{\substack{i=1 \\ i\neq j}}^{N} V(|\boldsymbol{r}_j - \boldsymbol{r}_i|)\,. \tag{189}$$

Newton's modified second law (77) hence attains the form

$$\frac{\partial\, \boldsymbol{v}^N}{\partial\, t} = -\nabla^N \left[\frac{1}{m_0}\,\widehat{V} + \frac{1}{2}\,(\boldsymbol{v}^N)^2 - \frac{1}{2}\,(\boldsymbol{u}^N)^2 + \frac{\hbar}{2\, m_0}\,\nabla^N \cdot\, \boldsymbol{u}^N\right]. \tag{190}$$

As in the one-particle case the two scalar functions $\rho^N(\boldsymbol{r}^N, t)$ and $\phi(\boldsymbol{r}^N, t)$ can be absorbed into a complex-valued function $\Psi(\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots \boldsymbol{r}_N, t)$ defined by

$$\Psi(\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots \boldsymbol{r}_N, t) = \pm\sqrt{\rho(\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots \boldsymbol{r}_N, t)} \times \exp\left[i\,\phi(\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots \boldsymbol{r}_N, t)\right].$$

This is equivalent to

$$-\boldsymbol{u}^N(\boldsymbol{r}^N, t) + i\,\boldsymbol{v}^N(\boldsymbol{r}^N, t) = \frac{\hbar}{m_0}\,\nabla^N(\ln\Psi(\boldsymbol{r}^N, t)/\sqrt{\rho_0}) = \frac{\hbar}{m_0}\,\frac{\nabla^N\Psi}{\Psi}$$

which is the analogue to Eq.(83), and we obtain accordingly

$$\frac{\partial}{\partial t}(-\boldsymbol{u}^N + i\,\boldsymbol{v}^N) = \nabla^N\left(\frac{\hbar}{m_0}\,\frac{1}{\Psi}\,\frac{\partial\Psi}{\partial t}\right).$$

If we here insert Eqs.(188) and(190) for $\frac{\partial \boldsymbol{v}^N}{\partial t}$ and $\frac{\partial \boldsymbol{u}^N}{\partial t}$ and proceed exactly as in the single-particle case we arrive at the $N$-particle Schrödinger equation

$$\underbrace{\left[\widehat{H}_0 + \frac{1}{2}\sum_{\substack{i,j \\ i\neq j}} V(|\boldsymbol{r}_j - \boldsymbol{r}_i|)\right]}_{=\widehat{H}} \Psi(\boldsymbol{r}_1, \ldots \boldsymbol{r}_N, t) = i\,\hbar\,\frac{\partial}{\partial\, t}\Psi(\boldsymbol{r}_1, \ldots \boldsymbol{r}_N, t)\,. \quad (191)$$

Here $\widehat{H}_0$ denotes the "free Hamiltonian"

$$\widehat{H}_0 = \sum_{j=1}^{N} \widehat{H}_j \quad \text{where} \quad \widehat{H}_j = \left[\frac{\widehat{\boldsymbol{p}}_j^2}{2\,m_0} + V_{ext.}(\boldsymbol{r}_j)\right]. \quad (192)$$

Because of Eq.(185) the phase of the wave function may still depend on time when $\rho$ and $\boldsymbol{v}^N$ are time-independent:

$$\phi(\boldsymbol{r}^N, t) = \phi_0(\boldsymbol{r}^N) + f(t)\,.$$

Thus we have in this case

$$\begin{aligned} \Psi(\boldsymbol{r}^N, t) &= \Psi_0(\boldsymbol{r}^N)\, e^{-if(t)}\,; \\ \Psi_0(\boldsymbol{r}^N) &= \pm\sqrt{\rho(\boldsymbol{r}^N)}\,\exp\left[i\,\phi_0(\boldsymbol{r}^N)\right] \end{aligned}$$

which on insertion into Eq.(191) yields

$$\widehat{H}\,\Psi_0(\boldsymbol{r}^N) = \hbar\,\dot{f}\,\Psi_0(\boldsymbol{r}^N) \quad \hookrightarrow \quad \hbar\,\dot{f} = const. = E \quad \hookrightarrow f(t) = \frac{E}{\hbar}\,t\,,$$

whereby Eq.(191) becomes the time-independent Schrödinger equation

$$\widehat{H}\,\Psi_0(\boldsymbol{r}^N) = E\,\Psi_0(\boldsymbol{r}^N)\,. \quad (193)$$

## 23 States of identical particles and entanglement

If the particles are non-interacting, one would naïvely expect their motions to be completely uncorrelated which means

$$\rho(\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots \boldsymbol{r}_N, t) = \prod_{j=1}^{N} \rho_j(\boldsymbol{r}_j, t)\,, \quad (194)$$

and

$$\phi(\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots \boldsymbol{r}_N, t) = \sum_{j=1}^{N} \varphi_j(\boldsymbol{r}_j, t)\,. \quad (195)$$

In that case Eq.(185) attains the form

$$(\boldsymbol{v}_1(\boldsymbol{r}_1,t),\boldsymbol{v}_2(\boldsymbol{r}_2,t),\dots\boldsymbol{v}_N(\boldsymbol{r}_N,t)) = \frac{\hbar}{m_0}\,(\nabla_1\varphi_1(\boldsymbol{r}_1,t),\nabla_2\varphi_2(\boldsymbol{r}_2,t),\dots\nabla_N\varphi_N(\boldsymbol{r}_N,t))\ .$$

Likewise, Eq.(186) becomes

$$(\boldsymbol{u}_1(\boldsymbol{r}_1,t),\boldsymbol{u}_2(\boldsymbol{r}_2,t),\dots\boldsymbol{u}_N(\boldsymbol{r}_N,t)) =$$
$$-\frac{\hbar}{2\,m_0}\,(\nabla_1\ln[\rho_1(\boldsymbol{r}_1,t)/\rho_{01}],\ \nabla_2\ln[\rho_2(\boldsymbol{r}_2,t)/\rho_{02}],\dots\nabla_N[\ln\rho_N(\boldsymbol{r}_N,t)/\rho_{0N}])\ .$$

Newton's modified second law (190) decomposes accordingly into $N$ analogous equations for single particles, as has to be expected. Each of these equations can be subjected to a Madelung transform which yields time-dependent one-particle Schrödinger equations solved by one-particle wave functions $\psi_j(\boldsymbol{r}_j,t)$. If one multiplies

$$\widehat{H}_j(\boldsymbol{r}_j)\,\psi_j(\boldsymbol{r}_j,t) = i\hbar\,\frac{\partial}{\partial\,t}\,\psi_j(\boldsymbol{r}_j,t) \tag{196}$$

by $\prod_{\substack{i=1\\ i\neq j}}^{N}\psi_i(\boldsymbol{r}_i,t)$ one obtains

$$\widehat{H}_j(\boldsymbol{r}_j)\prod_{i=1}^{N}\psi_i(\boldsymbol{r}_i,t) = \prod_{\substack{i=1\\ i\neq j}}^{N}\psi_i(\boldsymbol{r}_i,t)\,i\hbar\,\frac{\partial}{\partial\,t}\,\psi_j(\boldsymbol{r}_i,t)$$

which on forming the sum $\sum_{j=1}^{N}$ yields, in fact,

$$\widehat{H}_0\,\Psi(\boldsymbol{r}_1,\boldsymbol{r}_2,\dots\boldsymbol{r}_N,t) = i\hbar\,\frac{\partial}{\partial\,t}\,\Psi(\boldsymbol{r}_1,\boldsymbol{r}_2,\dots\boldsymbol{r}_N,t)$$
$$\text{where}\quad \Psi(\boldsymbol{r}_1,\boldsymbol{r}_2,\dots\boldsymbol{r}_N,t) = \prod_{j=1}^{N}\psi_j(\boldsymbol{r}_j,t)\,. \tag{197}$$

Hence, the above time-dependent $N$-particle Schrödinger equation is solved by the product of individually time-dependent wave functions $\psi_j(\boldsymbol{r}_j,t)$.

Obviously, the density (194) that results from this wave function is **not** invariant against interchange of any two particles if they are in different states, say $\psi_{k_n}(\boldsymbol{r}_k,t)$ and $\psi_{l_m}(\boldsymbol{r}_l,t)$ where $k_n \neq l_m$.
It is not exactly physical wisdom but rather firm belief that even non-interacting massive particles, though non-existing in nature, do not perform an uncorrelated motion and can, therefore, not be described by the wave function (197). This belief is based on the idea that the particles cannot be tracked individually as they move (contrary to classical particles) because the uncertainty relation "forbids" the existence of trajectories. Our

approach to the many-particle problem is characterized by the plausible assumption that each particle can be identified any time by an affix if it has been assigned to a certain number at some chosen instant since each particle follows an individual trajectory. The quantity $\boldsymbol{v}_1(\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots \boldsymbol{r}_N, t)$, for example, represents the average over all particle velocities at $\boldsymbol{r}_1$ and time $t$ of the ensemble associated with particle "number 1". In forming this average the positions $\boldsymbol{r}_2, \boldsymbol{r}_3, \ldots \boldsymbol{r}_N$ of the $N-1$ remaining particles are kept fixed, that is, the average results from the entire set of "number 1"-trajectories that occur in the "number 1"-ensemble while the particles "number 2, 3 ...$N$" are at fixed positions. Clearly, if one or more of those particles are kept at different positions and if all particles interact, $\boldsymbol{v}_1$ will in general be different at $\boldsymbol{r}_1$ and time $t$. Hence in our view there is no extra quantum phenomenon of indiscernibility. As in classical mechanics it is entirely sufficient to characterize identical particles merely by their property of having the same mass and charge.

If one insists, however, on "quantum indiscernibility" also for non-interacting particles, that is, on the invariance of $\rho(\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots \boldsymbol{r}_N)$ against interchange of any two particles, one has to replace (197) with a renormalized linear combination of all $N!$ products that differ in the interchange of two particles

$$\Psi(\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots \boldsymbol{r}_N) = \frac{1}{\sqrt{N!}} \sum_{P=1}^{N!} (\pm 1)^P \hat{P}(k,l) \prod_{j=1}^{N} \psi_{n_j}(\boldsymbol{r}_j)\,. \tag{198}$$

where $\hat{P}(k,l)$ is the permutation operator exchanging the particle referring to $j=k$ with that for $j=l$, and $P$ numbers the permutations.

**If the particles interact** and are bound in an external potential or move in a parallelepiped where $\Psi(\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots \boldsymbol{r}_N)$ is subjected to periodic boundary conditions, each particle is constantly scattered, and hence the probability of some particle, say "number k", being within an elementary volume $\Delta^3 r$ about $\boldsymbol{r}$ is given by:

$$P(\boldsymbol{r}) = \int |\Psi(\boldsymbol{r}_1, \ldots \boldsymbol{r}_{k-1}, \boldsymbol{r}, \boldsymbol{r}_{k+1} \ldots \boldsymbol{r}_N)|^2 \, d^3 r_1 \ldots d^3 r_{k-1} d^3 r_{k+1} \ldots d^3 r_N \, \Delta^3 r\,.$$

**Indiscernibility means** that $P(\boldsymbol{r})$ is the same for any particle one picks, that is, each particle appears at $\boldsymbol{r}$ with the same probability. Hence we have

$$\rho(\boldsymbol{r}) = N\, P(\boldsymbol{r})$$

with $\rho(\boldsymbol{r})\, \Delta^3 r$ denoting the probability of **any** of the $N$ electrons being in $\Delta^3 r$.
The function $\rho(\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots \boldsymbol{r}_N)$ is now naturally invariant against interchange of any two particles.
An important property of particles is their spin which will be discussed

farther below in this article. In the present context it may be sufficient to introduce

$$\boldsymbol{x} = (\boldsymbol{r}, \sigma)$$

as a generalized particle coordinate where $\sigma = \pm 1$ denotes its discrete spin coordinate and refers to parallel or anti-parallel orientation with respect to a global axis. The wave function (198) for non-interacting particles then takes the form

$$\Psi(\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots \boldsymbol{x}_N) = \\ \frac{1}{\sqrt{N!}} \sum_{P=1}^{N!} (\pm 1)^P \hat{P}(k,l) \prod_{j=1}^{N} \psi_{n_j}(\boldsymbol{x}_j)\,. \tag{199}$$

The alternative in the sign under the sum is related to the two fundamentally different species of particles: The plus sign in $(\pm 1)^P$ characterizes bosons, the minus sign fermions. Hence the latter are associated with a wave function that changes sign on interchanging any two particles. This property persists when $\Psi(\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots \boldsymbol{x}_N)$ describes $N$ interacting fermions. Antisymmetry of the wave function gives rise to a peculiar behavior of the so-called pair-density

$$\rho_2(\boldsymbol{x}, \boldsymbol{x}') \stackrel{\text{Def}}{=} N(N-1) \int |\Psi(\boldsymbol{x}, \boldsymbol{x}', \boldsymbol{x}_3, \ldots \boldsymbol{x}_N)|^2 \, d^4x_3 \ldots d^4x_N$$

where

$$\int \ldots d^4x = \sum_{\sigma} \ldots d^3r\,.$$

Obviously

$$\Psi(\boldsymbol{x}_1, \ldots \boldsymbol{x}_\nu, \boldsymbol{x}_{\nu+1}, \ldots \boldsymbol{x}_N) \equiv \Psi(\boldsymbol{x}_1, \ldots \boldsymbol{x}_{\nu+1}, \boldsymbol{x}_\nu, \ldots \boldsymbol{x}_N) \quad \text{if} \quad \boldsymbol{x}_\nu = \boldsymbol{x}_{\nu+1}\,.$$

On the other hand, $\Psi$ is required to change sign on interchanging two particles, and hence the above equation can only hold if $\Psi$ equals zero if the coordinates of any two particles are equal. Thus

$$\rho_2(\boldsymbol{x}, \boldsymbol{x}') = 0 \quad \text{if} \quad \boldsymbol{x}' = \boldsymbol{x}\,.$$

This indicates the occurrence of the so-called Fermi-hole which is absent in bose-particle systems.

The form of the wave function (199) may be cast as a determinant, named after J. C. Slater. In so-called EPRB-experiments (EPRB=Einstein, Podolsky, Rosen [54], Bohm [55]) which were originally devised to test possible correlations between two macroscopically distant fermions in a singlet state, the associated wave function is just a $2 \times 2$ determinant. The respective two one-particle states are in this context commonly referred to as "entangled states".

The requirement of antisymmetry, which is equivalent to the Pauli exclusion principle, is a strong subsidiary condition in solving the Schrödinger equation (193). Wave functions associated with fermions constitute only a small subset of the set of functions that satisfy the Schrödinger equation (193).

It should clearly be stated that the antisymmetry of the wave function is definitely not a consequence of our stochastic approach, but rather has to be required as an additional property, as in standard quantum mechanics.

The derivation of the time-dependent Schrödinger equation (191) can again be extended to the case where the particles move in an electromagnetic field. The external potential becomes time-dependent then ($V_{ext.}(\boldsymbol{r}) \to V(\boldsymbol{r},t)$) and $\widehat{\boldsymbol{p}}_j$ has to replaced with $\widehat{\boldsymbol{P}}_j(\boldsymbol{r},t) = \widehat{\boldsymbol{p}}_j - e\,\boldsymbol{A}(\boldsymbol{r}_j,t)$.

## 24 A borderline case of entanglement

We consider a hydrogen molecule whose nuclei are located at $\boldsymbol{R}_A$ and $\boldsymbol{R}_B$, respectively. The Hamiltonian of the two electrons is given by

$$\hat{H} = \sum_{k=1}^{2}\left[\frac{(-i\hbar\,\nabla_k - e\boldsymbol{A}(\boldsymbol{r}_k,t))^2}{2\,m_0} + V(\boldsymbol{r}_k)\right] + \frac{e^2}{4\pi\,\epsilon_0}\sum_{k,l\neq k}\frac{1}{|\boldsymbol{r}_k-\boldsymbol{r}_l|} \tag{200}$$

where

$$V(\boldsymbol{r}) = -\frac{e^2}{4\pi\,\epsilon_0|\boldsymbol{r}-\boldsymbol{R}_A|} - \frac{e^2}{4\pi\,\epsilon_0|\boldsymbol{r}-\boldsymbol{R}_B|}\,,$$

and $\epsilon_0$ denotes the permittivity of the vacuum.
We first assume that there is no external field ($\boldsymbol{A}(\boldsymbol{r},t)\equiv 0$) and that the 2-electron wave function has for large proton-proton separation, that is when $R_{AB} = |\boldsymbol{R}_A - \boldsymbol{R}_B| \gg$Bohr radius, still the entangled form of a **singlet state** dictated by the Pauli principle

$$\Psi(\boldsymbol{r}_1,\boldsymbol{r}_2) = \frac{1}{\sqrt{2}}\left[\underline{\psi}(\boldsymbol{r}_1\,,\uparrow)\otimes\underline{\psi}(\boldsymbol{r}_2\,,\downarrow) - \underline{\psi}(\boldsymbol{r}_1\,,\downarrow)\otimes\underline{\psi}(\boldsymbol{r}_2\,,\uparrow)\right] \tag{201}$$

where

$$\underline{\psi}(\boldsymbol{r},\sigma) = \left[a_\sigma(R_{AB})\,\varphi_A(\boldsymbol{r}) + b_\sigma(R_{AB})\,\varphi_B(\boldsymbol{r})\right]\underline{\chi}(\sigma) \tag{202}$$

and

$$\sigma = \uparrow\,(\downarrow)\,; \quad a_\sigma^2 + b_\sigma^2 = 1\,; \quad \varphi_{A/B}(\boldsymbol{r}) = \varphi(\boldsymbol{r}-\boldsymbol{R}_{A/B})$$

with the property

$$\int |\varphi(\boldsymbol{r}-\boldsymbol{R}_{A/B})|^2\,d^3r = 1\,.$$

Here the integrand denotes the electronic 1s-orbital of a single hydrogen atom, and $\rho_{A/B}(\boldsymbol{r},t) = |\varphi(\boldsymbol{r}-\boldsymbol{R}_{A/B})|^2$ is the associated probability density. Furthermore, the unit spinors $\underline{\chi}(\sigma)$ have the property

$$\underline{\chi}^{\dagger}(\sigma')\,\underline{\chi}(\sigma) = \delta_{\sigma'\sigma}\,.$$

Under the supposition that $R_{AB} = |\boldsymbol{R}_A - \boldsymbol{R}_B|$ is sufficiently large, say 10 cm or even larger, the expectation value $\langle\widehat{H}\rangle$ attains a minimum for either

$$(a_\uparrow \to 1\,, a_\downarrow \to 0) \hookrightarrow (b_\uparrow \to 0\,, b_\downarrow \to 1) \quad \text{“case l”}$$

or

$$(a_\uparrow \to 0\,, a_\downarrow \to 1) \hookrightarrow (b_\uparrow \to 1\,, b_\downarrow \to 0) \quad \text{“case r”}\,.$$

For both cases $\langle\widehat{H}\rangle$ yields the correct value, viz. -2 Ryd, as has to be expected for two hydrogen atoms, each of which possesses the energy -1 Ryd. Since the spin structure does not reflect the symmetry of the potential, one forms a symmetry-adapted linear combination

$$\Psi_i(\boldsymbol{r}_1,\boldsymbol{r}_2) = \frac{1}{\sqrt{2}}\left[\Psi_l(\boldsymbol{r}_1,\boldsymbol{r}_2) + \Psi_r(\boldsymbol{r}_1,\boldsymbol{r}_2)\right],$$

where

$$\Psi_l(\boldsymbol{r}_1,\boldsymbol{r}_2) = \frac{1}{\sqrt{2}}\begin{vmatrix} \varphi_A(\boldsymbol{r}_1)\,\underline{\chi}(\uparrow) & \varphi_A(\boldsymbol{r}_2)\,\underline{\chi}(\uparrow) \\ \varphi_B(\boldsymbol{r}_1)\,\underline{\chi}(\downarrow) & \varphi_B(\boldsymbol{r}_2)\,\underline{\chi}(\downarrow) \end{vmatrix}$$

and

$$\Psi_r(\boldsymbol{r}_1,\boldsymbol{r}_2) = \frac{1}{\sqrt{2}}\begin{vmatrix} \varphi_B(\boldsymbol{r}_1)\,\underline{\chi}(\uparrow) & \varphi_B(\boldsymbol{r}_2)\,\underline{\chi}(\uparrow) \\ \varphi_A(\boldsymbol{r}_1)\,\underline{\chi}(\downarrow) & \varphi_A(\boldsymbol{r}_2)\,\underline{\chi}(\downarrow) \end{vmatrix}.$$

The two 2-electron functions are associated with the same energy which hence applies to $\Psi_i(\boldsymbol{r}_1,\boldsymbol{r}_2)$ as well. As a consequence of the symmetry of $\Psi_i(\boldsymbol{r}_1,\boldsymbol{r}_2)$ in $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$ we have

$$\rho(\boldsymbol{r}_1) = \int |\Psi(\boldsymbol{r}_1,\boldsymbol{r}_2)|^2\, d^3r_2 = \rho_A(\boldsymbol{r}_1) + \rho_B(\boldsymbol{r}_1)$$

and

$$\rho(\boldsymbol{r}_2) = \int |\Psi(\boldsymbol{r}_1,\boldsymbol{r}_2)|^2\, d^3r_1 = \rho_A(\boldsymbol{r}_2) + \rho_B(\boldsymbol{r}_2)\,.$$

Moreover

$$\int \rho_{A/B}(\boldsymbol{r}_{1/2})\, d^3r_{1/2} = \frac{1}{2} \quad \text{and}$$

$$\int \rho_{A/B}(\boldsymbol{r}_1)\, d^3r_1 + \int \rho_{A/B}(\boldsymbol{r}_2)\, d^3r_2 = 1\,. \tag{203}$$

That means that each electron appears in each of the atoms (A and B) with the same probability. This has rather implausible consequences if one

exposes, for example, **one** of the atoms (say A) to a Laser puls of frequency $\omega$. Now $\boldsymbol{A}(\boldsymbol{r},t)$ is no longer zero. The associate perturbation operator has the form

$$V_{perturb}(\boldsymbol{r}_1,\boldsymbol{r}_2,t) = \begin{cases} \frac{ie\hbar}{m_0}\sum_{k=1}^{2}\boldsymbol{A}(\boldsymbol{r}_k,t)\cdot\nabla_k & \text{if } \boldsymbol{r}_1,\boldsymbol{r}_2 \text{ in or near atom A} \\ 0 & \text{else} \end{cases}$$

which promotes the 2-electron system to an excited state

$$\Psi_f(\boldsymbol{r}_1,\boldsymbol{r}_2) = \frac{1}{\sqrt{2}}\left[\Psi_l^{(f)}(\boldsymbol{r}_1,\boldsymbol{r}_2) + \Psi_r^{(f)}(\boldsymbol{r}_1,\boldsymbol{r}_2)\right]$$

where

$$\Psi_l^{(f)}(\boldsymbol{r}_1,\boldsymbol{r}_2) = \frac{1}{\sqrt{2}}\begin{vmatrix} \varphi_A^{(f)}(\boldsymbol{r}_1)\,\underline{\chi}(\uparrow) & \varphi_A^{(f)}(\boldsymbol{r}_2)\,\underline{\chi}(\uparrow) \\ \varphi_B(\boldsymbol{r}_1)\,\underline{\chi}(\downarrow) & \varphi_B(\boldsymbol{r}_2)\,\underline{\chi}(\downarrow) \end{vmatrix}$$

and

$$\Psi_r^{(f)}(\boldsymbol{r}_1,\boldsymbol{r}_2) = \frac{1}{\sqrt{2}}\begin{vmatrix} \varphi_B^{(f)}(\boldsymbol{r}_1)\,\underline{\chi}(\uparrow) & \varphi_B^{(f)}(\boldsymbol{r}_2)\,\underline{\chi}(\uparrow) \\ \varphi_A(\boldsymbol{r}_1)\,\underline{\chi}(\downarrow) & \varphi_A(\boldsymbol{r}_2)\,\underline{\chi}(\downarrow) \end{vmatrix}.$$

Here $\varphi_{A/B}^{(f)}(\boldsymbol{r})$ describes an outgoing wave which has in principle the asymptotic form

$$\varphi_{A/B}^{(f)}(\boldsymbol{r}) \cong \frac{1}{r_{A/B}}\,e^{ik\,r_{A/B}}\,Y_{10}(\widehat{r}_{A/B})\;; \quad r_{AB} \equiv |\boldsymbol{r}-\boldsymbol{R}_{A/B}|$$

with $Y_{10}(\widehat{r}_{A/B})$ denoting the spherical harmonic for $l=1, m=0$, and $k$ is given by $\hbar^2\,k^2/2\,m_0 = -1\,\mathrm{Ryd} + \hbar\,\omega$. We have assumed linearly polarized Laser light with the quantization axis of $Y_{10}(\widehat{r}_{A/B})$ coinciding with the axis of polarization. Moreover we have disregarded the residual charge left with each atom as part of the electronic charge is emitted.
Although only the illuminated volume of atom A can contribute to the transition matrix element

$$M_{fi} = \int_{atom\,A}\int \Psi_f^*(\boldsymbol{r}_1,\boldsymbol{r}_2)\,V_{perturb}(\boldsymbol{r}_1,\boldsymbol{r}_2)\,\Psi_i(\boldsymbol{r}_1,\boldsymbol{r}_2)\,d^3r_1\,d^3r_2$$

the final state $\Psi_f(\boldsymbol{r}_1,\boldsymbol{r}_2)$ yields a current density

$$\begin{aligned} \boldsymbol{j}(\boldsymbol{r}) &= \frac{\hbar}{i\,m_0}\int[\Psi_f^*(\boldsymbol{r},\boldsymbol{r}_2)\nabla\Psi_f(\boldsymbol{r},\boldsymbol{r}_2) - c.c.]\,d^3r_2 \\ &= \frac{\hbar}{i\,m_0}\int[\Psi_f^*(\boldsymbol{r}_1,\boldsymbol{r})\nabla\Psi_f(\boldsymbol{r}_1,\boldsymbol{r}) - c.c.]\,d^3r_1 \\ &= \boldsymbol{j}_A(\boldsymbol{r}-\boldsymbol{R}_A) + \boldsymbol{j}_B(\boldsymbol{r}-\boldsymbol{R}_B) \end{aligned}$$

where $\boldsymbol{j}_{A/B}$ is associated with $\varphi_{A/B}^{(f)}$, and hence $\boldsymbol{j}(\boldsymbol{r})$ contains also a photo emission current coming from the non-illuminated atom B at a distance of 10 cm away from A. Similar considerations apply if one excites the molecule

to a bound state which would spontaneously decay back then to the ground-state by emitting fluorescent light. If one repeats the excitation sufficiently often one would obtain as many fluorescence photons coming from the illuminated atom as from the non-illuminated one. There is no experimental evidence that anything like that could ever happen.
We are hence led to conclude that the concept of entanglement (i. e. anti-symmetry of the wavefunction when dealing with fermions) does not apply anymore when the atoms are macroscopically distant. The reason may be traced back to the definition (22) of the probability density $\rho(\boldsymbol{r})$ as the relative residence time that a particle spends in an elementary volume $\Delta^3 r$ about $\boldsymbol{r}$, provided it is bound in a potential and thus occurs repeatedly in that volume. On pulling the two atoms of a $H_2$-molecule gradually apart one arrives at a situation where one of the two electrons remains captured near the nucleus of atom A for a while, and accordingly the second electron stays captured near the nucleus of atom B for the same time. The Coulomb repulsion between the two electrons effects a correlated separation of the two electrons into the two regions.[4] If the inter-nuclear distance becomes large compared to the linear dimensions of the atoms, the time spans for tunneling of the "A-electron" (marked by the index "1") into the B-region and vice versa become enormously long compared to the time required to cross the associated atom. The time $T$ for the photo-excitation process will therefore be many orders of magnitude shorter than the tunneling time. Given this situation, the definition (22) yields

$$\rho(\boldsymbol{r}_{1/2}) = \begin{cases} \rho_{A/B}(\boldsymbol{r}_{1/2}) & \text{for } \boldsymbol{r}_{1/2} \text{ about nucleus A/B} \\ 0 & \text{else} \end{cases}$$

where - different from Eq.(203) - the densities $\rho_{A/B}(\boldsymbol{r}_{1/2})$ now integrate to unity. The two electrons do not appear entangled any more, and only the A-atom will now emit an electron under the exposure of light.

## 25 van der Waals interaction

Chemical bonding occurs when $N_{at}$ atoms get so close to each other that their total number of electrons ($N_e = \sum_{i=1}^{N_{at}} N_{e\,i}$) becomes associated with a new common wave function which is anti-symmetric with respect to the exchange of any two electrons from the entire set of $N_e$ electrons. At larger distances the atoms interact only weakly by so-called van der Waals forces. The associated interaction energy has first been treated by Eisenschitz and

[4]The possibility that both electrons accumulate in one of the atoms can safely be excluded. In such a case the other atom would be left ionized requiring an energy $\Delta E$ of about 1Ryd. Within a time $\Delta t$ that excess energy must disappear again where $\Delta t$ results from $\Delta E\,\Delta t \approx \hbar$. This yields $\Delta t \approx 5 \cdot 10^{-17}\,s$, thus excluding the possibility for one of the electrons to go back to the ionized atom 10 cm away at a speed well below light velocity.

London [58]. Further studies (s. e. g. Dzyaloshinskii et al. [59]) are based on the idea that the atoms undergo density fluctuations that give rise to temporary dipole moments. The latter cause interatomic attraction. From our point of view density fluctuations of the electronic probability density cannot occur in the groundstate of any system because it would inevitably cause radiative emission. This follows immediately from our treatment of spontaneous light emission in Section 20. We shall therefore go back to the original idea of the Eisenschitz-London paper.

We consider two atoms **A** and **B** whose electronic densities are spherical. Their nuclei are centered at $\boldsymbol{R}_A$ and $\boldsymbol{R}_B$, respectively. The individual atoms of that pair may in general be different, consist of a sodium and a potassium atom, for example. The interatomic distance is assumed larger than the sum of the atomic radii so that the overlap of the electronic densities may be regarded as zero on the scale of interest. It is this situation which we have analyzed in the previous section for two hydrogen atoms whose two-electron wave function factorizes at this distance into the wave functions of the individual atoms. Accordingly, we have in the present case for the groundstate $\Psi_0$ of the atomic pair

$$\begin{aligned}\Psi_0(\boldsymbol{r}_{A1}, \boldsymbol{r}_{A2}, \ldots \boldsymbol{r}_{AN_A}, \boldsymbol{r}_{B1}, \boldsymbol{r}_{B2}, \ldots \boldsymbol{r}_{BN_B}) = \\ \phi_0^A(\boldsymbol{r}_{A1}, \boldsymbol{r}_{A2}, \ldots \boldsymbol{r}_{AN_A})\, \phi_0^B(\boldsymbol{r}_{B1}, \boldsymbol{r}_{B2}, \ldots \boldsymbol{r}_{BN_B})\end{aligned}$$

with $N_A$ and $N_B$ denoting the number of electrons of the respective atoms, and $\phi_0^A$, $\phi_0^B$ represent antisymmetric wave functions. They are normalized to unity:

$$\int |\phi_0^A|^2 \, d^3r_{A\,1} \; d^3r_{A\,2} \ldots d^3r_{A\,N_A} = 1$$

and

$$\int |\phi_0^B|^2 \, d^3r_{B\,1} \; d^3r_{B\,2} \ldots d^3r_{B\,N_B} = 1\,.$$

For simplicity we have dropped the spin coordinates. The two wave functions are solutions to the associated Schrödinger equations

$$\widehat{H}_{A/B}\, \phi_0^{A/B} = E_0^{A/B}\, \phi_0^{A/B}$$

where

$$\widehat{H}_{A/B} = \sum_{i=1}^{N_{A/B}} \left[ -\frac{1}{2}\, \nabla^2_{A/B\,i} - \frac{Z_{A/B}}{|\boldsymbol{r}_{A/B\,i} - \boldsymbol{R}_{A/B}|} \right] + \frac{1}{2} \sum_{\substack{i,\,j \\ i \neq j}} \frac{1}{|\boldsymbol{r}_{A/B\,i} - \boldsymbol{r}_{A/B\,j}|}$$

with $Z_{A/B}$ denoting the respective atomic number. The indices $i\,, j$ in the second sum run over $N_{A/B}$ coordinates, and hence this sum describes only

the electron-electron interaction within the associated atom.
To simplify the notation we have introduced atomic Hartree units, i. e. the Bohr radius $r_B$ as the unit length and 1 Hartree as the unit of energy.
Obviously, $\Psi_0$ satifies the Schrödinger equation

$$(\widehat{H}_A + \widehat{H}_B)\Psi_0 = (E_0^A + E_0^B)\Psi_0$$

and hence

$$E = \langle \Psi_0 | \widehat{H}_A + \widehat{H}_B | \Psi_0 \rangle = E_0^A + E_0^B \,. \tag{204}$$

However, the actual Hamiltonian describing the $(N_A + N_B)$-electron system and the two nuclei is given by

$$\begin{aligned} \widehat{H}_{total} = \widehat{H}_A + \widehat{H}_B + \sum_{i=1}^{N_A} \sum_{j=1}^{N_B} \frac{1}{|\boldsymbol{r}_{A\,i} - \boldsymbol{r}_{B\,j}|} - \\ - \sum_{j=1}^{N_B} \frac{Z_A}{|\boldsymbol{r}_{B\,j} - \boldsymbol{R}_A|} - \sum_{j=1}^{N_A} \frac{Z_B}{|\boldsymbol{r}_{A\,i} - \boldsymbol{R}_B|} + \frac{Z_A\, Z_B}{|\boldsymbol{R}_A - \boldsymbol{R}_B|} \,. \end{aligned} \tag{205}$$

The electronic densities $\rho_0^A(\boldsymbol{r})$, $\rho_0^B(\boldsymbol{r})$ are defined by

$$\begin{aligned} \rho_0^A(\boldsymbol{r}) \stackrel{def}{=} \tilde{\rho}_0^A(\boldsymbol{r} - \boldsymbol{R}_A) &= N_A \int |\phi_0^A(\boldsymbol{r}, \ldots \boldsymbol{r}_{A\,N_A})|^2 \, d^3 r_{A\,2} \ldots d^3 r_{A\,N_A} \\ \rho_0^B(\boldsymbol{r}) \stackrel{def}{=} \tilde{\rho}_0^B(\boldsymbol{r} - \boldsymbol{R}_B) &= N_B \int |\phi_0^B(\boldsymbol{r}, \ldots \boldsymbol{r}_{B\,N_B})|^2 \, d^3 r_{B\,2} \ldots d^3 r_{B\,N_B} \end{aligned} \tag{206}$$

On forming the expectation value $\langle \Psi_0 | \widehat{H}_{total} | \Psi_0 \rangle$ the single sum over the $\boldsymbol{r}_B$-coordinates in Eq.(205) yields because of (206)

$$-Z_A \int \frac{\rho_0^B(\boldsymbol{r})}{|\boldsymbol{r} - \boldsymbol{R}_A|} \, d^3 r = -\frac{Z_A\, Z_B}{|\boldsymbol{R}_B - \boldsymbol{R}_A|} \,.$$

The latter holds since $N_B$ equals $Z_B$ for neutral atoms, and $\rho_0^B(\boldsymbol{r})$ is assumed spherically symmetric with respect to $\boldsymbol{R}_B$.
Similarly, when dealing with the double-sum in Eq.(205), if one first performs the integration over the $\boldsymbol{r}_B$-coordinates one obtains as an intermediate result

$$\sum_{i=1}^{N_A} \int \frac{\rho_0^B(\boldsymbol{r})}{|\boldsymbol{r}_{A\,i} - \boldsymbol{r}|} \, d^3 r = \sum_{j=1}^{N_A} \frac{Z_B}{|\boldsymbol{r}_{A\,i} - \boldsymbol{R}_B|}$$

with the latter again being a consequence of the spherical symmetry of $\rho_0^B(\boldsymbol{r})$ with respect to $\boldsymbol{R}_B$. Performing the remaining integration of this expression and of the third sum in Eq.(205) over the $\boldsymbol{r}_A$-coordinates, one recognizes

that the two expressions cancel. Hence, one has - because of perfect mutual screening - despite the occurrence of the extra sums in expression (205)

$$E = \langle \Psi_0 | \widehat{H}_{total} | \Psi_0 \rangle = E_0^A + E_0^B \tag{207}$$

as before in (204).
That means, at this level of analysis each atom remains unaffected by the presence of the other. However, because of the occurrence of the extra sums in (205) $\Psi_0$ does not satisfy the Schödinger equation

$$\widehat{H}_{total} \Psi = E_0^{total} \, \Psi \, . \tag{208}$$

As the solution to (208) yields a minimum of the expectation value of $\widehat{H}_{total}$ for the groundstate $\Psi_0^{total}$ one may equivalently state that $\langle \Psi_0 | \widehat{H}_{total} | \Psi_0 \rangle$ can be lowered to the exact total energy $E_0^{total}$, i. e. to the lowest eigenvalue of $\widehat{H}_{total}$ by appropriately distorting $\Psi_0$ toward $\Psi_0^{total}$. This can be done in a simplified way by partially including excited states of the atoms so that one is now dealing with a wave function that slightly departs from the groundstate $\Psi_0$

$$\Psi_0^{total} = c_0 \, \Psi_0 + c_1 \, \Psi_1 = c_0 \, \phi_0^A \, \phi_0^B + c_1 \, \phi_1^A \, \phi_1^B \tag{209}$$

with $c_0 \, , c_1$ denoting real-valued coefficients, and $\phi_1^A$ stands for some excited state of atom A associated with an energy $E_1^A > E_0^A$. Corresponding definitions apply to atom B. The set of electronic coordinates and their assocation with the respective wave functions remain unchanged. As we assume an only slight departure from the groundstate we have

$$|c_1| \ll 1 \, , \quad \text{and we observe} \quad c_0^2 + c_1^2 = 1 \, . \tag{210}$$

The latter reflects the unaltered norm unity of $\Psi$.
To simplify the argument, we confine ourselves to just one excited state, a lowest lying state that can be mapped onto a Slater determinant in which the excited orbital possesses a negative parity compared to the corresponding groundstate ($s$-type) orbital $\psi_0^{A/B}(\boldsymbol{r} - \boldsymbol{R}_{A/B})$ that is replaced in the excitation. We choose as the excited one-electron state $\psi_1^{A/B}(\boldsymbol{r} - \boldsymbol{R}_{A/B})$ a $p_z$-type orbital whose quantization axis, the $z$-axis, is taken along the direction $\boldsymbol{R}_A - \boldsymbol{R}_B$.
Different from $\rho_0^A(\boldsymbol{r})$ the electronic charge density in the excited state

$$\rho_1^A(\boldsymbol{r}) = N_A \int |\phi_1^A(\boldsymbol{r}, \boldsymbol{r}_{A2}, \ldots \boldsymbol{r}_{A\,N_A})|^2 \, d^3 r_{A\,2} \; d^3 r_{A\,3} \ldots d^3 r_{A\,N_A}$$

is not spherical any more, but its centroid still conicides with the nucleus, that is, its electrostatic potential does not contain a dipole-type contribution, merely a short-range quadrupole component that we shall ignore in the

following. The same applies to $\rho_1^B$.
As a result, all considerations above for the groundstate carry over to the present case except for the double-sum in Eq.(205). In forming $|\Psi_0^{total}|^2$ we obtain

$$|\Psi_0^{total}|^2 = c_0^2|\phi_0^A|^2|\phi_0^B|^2 + c_1^2|\phi_1^A|^2|\phi_1^B|^2 + 2c_0\,c_1\,\phi_0^A\,\phi_1^A\,\phi_0^B\,\phi_1^B\,.$$

It is the occurrence of the last expression which gives rise to an interatomic potential that has been absent so far.
In forming $\langle\Psi_0^{total}|\widehat{H}_{total}|\Psi_0^{total}\rangle$ one obtains

$$\langle\Psi_0^{total}|\widehat{H}_{total}|\Psi_0^{total}\rangle = c_0^2\,(E_0^A + E_0^B) + c_1^2\,(E_1^A + E_1^B) + \ldots \tag{211}$$

where the dots stand for

$$2c_0c_1 \int \psi_1^A(\boldsymbol{r}_A - \boldsymbol{R}_A)\psi_0^A(\boldsymbol{r}_A - \boldsymbol{R}_A) \times \left[\int \frac{\psi_1^B(\boldsymbol{r}_B - \boldsymbol{R}_B)\psi_0^B(\boldsymbol{r}_B - \boldsymbol{R}_B)}{|\boldsymbol{r}_A - \boldsymbol{r}_B|}\,d^3r_B\right] d^3r_A\,. \tag{212}$$

The numerator in the second integral represents a dipole-type charge density with the dipole axis lying in the $\boldsymbol{R}_A - \boldsymbol{R}_B$-direction. As $|\boldsymbol{r}_A - \boldsymbol{r}_B|$ is assumed to be large compared to the sum of the atomic radii, one may approximate the second integral

$$\int \frac{\psi_1^B(\boldsymbol{r}_B - \boldsymbol{R}_B)\psi_0^B(\boldsymbol{r}_B - \boldsymbol{R}_B)}{|\boldsymbol{r}_A - \boldsymbol{r}_B|}\,d^3r_B \approx \frac{p_B}{|\boldsymbol{r}_A - \boldsymbol{R}_B|^2} \tag{213}$$

where

$$p_B = e'\,|\delta\boldsymbol{r}_B|$$

denotes the dipole moment, and $\pm\,e'$ is the effective charge in the centroid of that charge density above and below the plane across the B-nucleus and perpendicular to the $z$-axis. The two charges are interconnected by $\delta\boldsymbol{r}_B$.
Similarly, the integral

$$\int \psi_1^A(\boldsymbol{r}_A - \boldsymbol{R}_A)\psi_0^A(\boldsymbol{r}_A - \boldsymbol{R}_A)\,\frac{p_B}{|\boldsymbol{r}_A - \boldsymbol{R}_B|^2}\,d^3r_A$$

may be approximated

$$\int \psi_1^A(\boldsymbol{r}_A - \boldsymbol{R}_A)\psi_0^A(\boldsymbol{r}_A - \boldsymbol{R}_A)\,\frac{p_B}{|\boldsymbol{r}_A - \boldsymbol{R}_B|^2}\,d^3r_A = \frac{2\,p_A\,p_B}{|\boldsymbol{R}_A - \boldsymbol{R}_B|^3}\,.$$

Because of (210) one may set $2\,c_0\,c_1 \approx 2\,c_1$ and replace $c_0^2$ by $1 - c_1^2$ so that Eq.(211), on employing (212), takes the form

$$E = \langle\Psi_0^{total}|\widehat{H}_{total}|\Psi_0^{total}\rangle = (E_0^A + E_0^B) + c_1^2\,\Delta E_1 + 2\,c_1\frac{2\,p_A\,p_B}{R^3} \tag{214}$$

where

$$\begin{aligned} \Delta E_1 &= (E_1^A + E_1^B) - (E_0^A + E_0^B) \quad \text{or} \\ \Delta E_1 &= E_1^A - E_0^A + E_1^B - E_0^B \qquad \text{and} \\ R &\stackrel{def}{=} |\boldsymbol{R}_A - \boldsymbol{R}_B| \,. \end{aligned} \tag{215}$$

The new groundstate is given then by requiring

$$\frac{dE}{dc_1} = 0 \quad \text{that is} \quad c_1 \, \Delta E_1 + \frac{2 \, p_A \, p_B}{R^3} = 0$$

which yields

$$c_1 = -\frac{1}{\Delta E_1} \, \frac{2 \, p_A \, p_B}{R^3} \,.$$

Inserting this into Eq.(214) one arrives at a total energy that is now different from (207)

$$E = (E_0^A + E_0^B) - \frac{4}{\Delta E_1} \, \frac{p_A^2 \, p_B^2}{R^6} \,. \tag{216}$$

This constitutes van der Waals' well known law on the $R$-dependence of the attractive potential between neutral atoms whose charge densities do not overlap. By breaking the spherical symmetry of the electronic densities the bi-atomic system lowers its total energy. We shall denote this $R$-dependent portion by $V_{vdW}(R)$ from now on.

As one would qualitatively expect, the attraction is large for atoms with low lying excitation energies. It is obvious from our derivation that it applies to any combination of orbitals $\psi_0^{A/B}(\boldsymbol{r} - \boldsymbol{R}_{A/B})$ and $\psi_1^{A/B}(\boldsymbol{r} - \boldsymbol{R}_{A/B})$ that lead to a product with dipole character, regardless which of the orbitals refers to the groundstate configuration. Although the groundstate charge density in the bi-atomic system may well be shaped by an incompletely filled p-, d- or f-shell of the respective atoms, it will merely give rise to negligible short range quadrupole (multipole) contributions to the interaction potential.

As indicated, the above derivation can be refined by including more than just one excited pair $\phi_1^A \, \phi_1^B$, that is by allowing for additional pairs which contain higher excited orbitals that also yield dipole-type products with the groundstate orbitals. To this end the ansatz (209) has to be generalized in the form

$$\Psi_0^{total} = c_0 \, \Psi_0 + \sum_{(n,m)} c_{n\,m} \, \Psi_{n\,m} = c_0 \phi_0^A \, \phi_0^B + \sum_n \sum_m c_{n\,m} \, \phi_n^A \, \phi_m^B \,; \quad n, m > 0 \tag{217}$$

where

$$c_0^2 + \sum_n \sum_m c_{n\,m}^2 = 1 \,.$$

Instead of (216) one then obtains the general expression

$$V_{vdW}(R) = -\left[4\sum_n\sum_m \frac{p^2_{n\,A}\,p^2_{m\,B}}{E^A_n - E^A_0 + E^B_m - E^B_0}\right]\frac{1}{R^6} \tag{218}$$

where

$$V_{vdW}(R) = E(R) - (E^A_0 + E^B_0)\,.$$

This result is essentially identical with that derived by Dzyaloshinskii et al.[59], however in an exceedingly involved, completely different way based on quantum field theory and "long-wave electrodynamical fluctuations". The paranthesized expression is commonly denoted by $C_6$. The expression obtained by Dzyaloshinskii et al. contains a factor of 6 in front of the double-sum instead of 4. Some experimental results seem to favor our smaller factor. (For details see Feibelman [60], p.394.)
If the two atoms are identical (A=B) and if one only considers the contributions for $n = m$ to the above sum Eq.(218) takes the form

$$V^{(n,n)}_{vdW}(R) = -\left[2\sum_n \frac{p^4_{n\,A}}{\Delta E_n}\right]\frac{1}{R^6}\,. \tag{219}$$

The parenthesized expression closely resembles the static polarizability $\alpha$ of the atom which - to first perturbation order - attains the form

$$\alpha = 2\sum_n \frac{p^2_{n\,A}}{\Delta E_n}\,. \tag{220}$$

The similarity of expression (219) and $\alpha$ has led to quote $-\nabla V_{vdw}(\boldsymbol{r})$ occasionally by the name "dispersion force" which is exceedingly misleading. Obviously, only the **static** polarizibility displays a certain affinity with $V_{vdW}$. Optical dispersion relates to the frequency dependence of the dynamical polarizability.
In determining $C_6$ from Eq.(218)) one can easily run into numerical inaccuracies because of the large spatial extent of excited orbitals. To get an estimate of $C_6$ we determine $p_{1\,A}$ from the polarizibility $\alpha$ of the atom under study. In Table 1 we have listed results on $V_{vdW}(R) = -C_6/R^6$ and on $\alpha$ for the noble gases where we have reduced the sums in (219) and (220) to the strongly dominating first summand and shortened the notation accordingly by setting $p_{1\,A} = p_A$. Further, we have introduced

$$p_0 = 1e \cdot 1r_B = 0.848 \cdot 10^{-29}\,C\,m$$

as a unit for the atomic dipole and observed that in familiar units ($\epsilon_0$=vacuum permittivity)

$$\alpha = \frac{2\,\hat{p}^2_A}{\Delta E_1\,4\pi\,\epsilon_0}\,; \quad \hat{p}_A = p_A\,p_0\,;$$
$$\frac{p^2_0}{4\pi\,\epsilon_0} = 0.646 \cdot 10^{-23}\,eV\,cm^3 \tag{221}$$

Table 1 Polarizabilities in $[10^{-24}cm^3]$, lowest excitation energies and the vdW-prefactor $C_6$ in units of $Hartree \cdot r_B^6$ for the noble gases $p_A = \hat{p}_A/p_0$ [Eq.(221)]

| | $\alpha_{exp}$ | $\alpha(p_A)$ | $p_A$ | $\Delta E_{1[eV]}$ | $C_6^{present}$ | $C_6^{ref}$ |
|---|---|---|---|---|---|---|
| He | 0.204 | 0.245 | 0.8 | 21.13 | 1.04 | 1.29 (1.45) |
| Ne | 0.396 | 0.47 | 1.4 | 16.84 | 6.22 | 7.5 |
| Ar | 1.645 | 1.8 | 2.3 | 11.83 | 64.0 | 71.5 |
| Kr | 2.49 | 2.76 | 2.63 | 9.99 | 128.7 | 145.5 |
| Xe | 4.05 | 4.57 | 3.09 | 8.44 | 293.5 | 331.5 |

The results denoted by $C_6^{ref}$ were obtained by Hult et al.[61], the paranthesized value is due to Kohn et al.[62]. The rather involved calculations of these authors are based on perturbational density functional theory. The experimental data on $\Delta E_1$ and $\alpha$ were taken from *Smithsonian Physical Tables* [63]. As the theoretical expressions for $\alpha$ and $C_6$ both contain $p_A$ we have chosen a compromise value for the latter quantity to reconcile the former quantities with least error. First-principles calculations on $\Delta E_n$ and $p_{n\,A}$ require considerable numerical effort because excited atomic states are not easily accessible. Their linear dimensions increase quickly with $n$. For that reason we rather rely on experimental data on $\Delta E_1$ and $\alpha$. To demonstrate the sensibility with which $C_6$ responds to errors in $p_A$ due to its appearance in fourth power, we have listed in Table 2 recalculated $C_6^{present}$-values which result from an increase of $p_A$ bei 3% compared to the $p_A$-values given in Table 1.

Table 2 $C_6$ in units of $Hartree \cdot r_B^6$ [Eq.(219), $n = 1$] for the noble gases; $p_A = \hat{p}_A/p_0$ [Eq.(221)]

| | $p_A$ | $\Delta E_{1[eV]}$ | $C_6^{present}$ | $C_6^{ref}$ |
|---|---|---|---|---|
| He | 0.82 | 21.13 | 1.17 | 1.29 (1.45) |
| Ne | 1.44 | 16.84 | 7.00 | 7.5 |
| Ar | 2.37 | 11.83 | 72.03 | 71.5 |
| Kr | 2.71 | 9.99 | 144.85 | 145.5 |
| Xe | 3.18 | 8.44 | 330.33 | 331.5 |

It is obvious from the above considerations which steps have to be taken to improve on the accuracy of our results. Furthermore, as one can see from Eq.(218), our approach is actually not restricted to atoms since it is merely based on dipole-associated virtual excitations of the interacting systems which may be molecules, clusters or even macroscopic solid objects.

# 26 Decomposing an experimental setup into the quantum system under study and an environment. Schrödinger's cat

One of the puzzling credos of the Copenhagen interpretation of quantum mechanics consists in the conviction that an experimental setup for performing measurements on microscopic particles, has to be subdivided "somehow" into the particles under study and a remainder that functions as a classical system. This decomposition is known under the name "Heisenberg-cut". Yet from an unbiased point of view it appears to be self-evident that an experimental setup as a whole represents a many-particle system each part of which is subjected to the same laws of quantum mechanics as the particular portion that constitutes the object under study, an electron in a diffraction chamber, for example. We shall use this example to demonstrate the consistency of this standpoint, but we limit ourselves to considering a system that merely consists of just one specific apparatus plus a particle undergoing diffraction in it. The generalization to the inclusion of the entire environment is obvious from the ensuing considerations.

We assume that the system is made up of $N$ particles, a subset consisting of atomic nuclei which we number by a label $\alpha$, and $N_e$ electrons, one of which representing the single particle of interest, the "test particle". To keep the notation simple, we limit ourselves to considering only electrostatic particle interactions of the kind described by the many-body potential (189). If the test particle has left the cathode of the setup it is kept by electrodes, diaphragms and lenses at a macroscopic distance away from all kinds of surfaces it might strike and where it might get captured. Thus, the associated one-particle wave function $\psi_e(\boldsymbol{r}, t)$ which describes the electron on its way through the apparatus to the screen or detector, has de facto zero overlap with the wave function of the $N-1$ remaining particles of the apparatus. Still, in standard setups it is intended that the particle hits a secluded portion of material on its way to the monitoring device, a diffracting single crystalline foil of metal, for example. But in the majority of cases the contact time is so short compared to the electronic excitation times of the material that the test electron cannot mingle with the other electrons. Below we shall briefly discuss prominent exceptions.

Similar to the case of the $H_2$-molecule with macroscopically distant nuclei, one is justified then in assuming a factorization of the total wave function

$$\Psi_N(\boldsymbol{r}, \boldsymbol{r}_2, \ldots \boldsymbol{r}_N, t) = \psi_e(\boldsymbol{r}, t)\, \Psi_{N-1}(\boldsymbol{r}_2, \boldsymbol{r}_3, \ldots \boldsymbol{r}_N, t) \tag{222}$$

where the spin coordinates have again been suppressed for simplicity. We emphasize that $\Psi_N(\boldsymbol{r}, \boldsymbol{r}_2, \ldots \boldsymbol{r}_N, t)$ in the present case constitutes the wave function of $N = N_e + N_n^{app.}$ particles: of the test electron, of the $N_e - 1$ electrons that belong to the apparatus **and in addition** of the $N_n^{app}$ nuclei

of the latter. If we insert this wave function into the associated $N$-particle Schrödinger equation (191) we obtain

$$\Psi_{N-1}\, i\hbar\, \dot{\psi}_e + \psi_e\, i\hbar\, \dot{\Psi}_{N-1} = \psi_e\, \widehat{H}_0^{(N-1)}\, \Psi_{N-1} + \Psi_{N-1}\, \widehat{H}_0^e\, \psi_e + V_{tot}\psi_e\, \Psi_{N-1} \quad (223)$$

where $V_{tot}$ denotes the total (Coulomb) interaction potential between all particles

$$V_{tot} = V_{apparatus}(\boldsymbol{r}_2, \boldsymbol{r}_3, \ldots \boldsymbol{r}_N) + V_e^{N-1}(\boldsymbol{r}, \boldsymbol{r}_2 \ldots \boldsymbol{r}_N)$$

with $V_e^{N-1}$ referring to the Coulomb interaction of the test particle with all charges of the apparatus

$$V_e^{N-1}(\boldsymbol{r}, \boldsymbol{r}_2 \ldots \boldsymbol{r}_N) = \sum_{j=2}^{N} \frac{e^2\, Z_j}{4\pi\, \epsilon_0\, |\boldsymbol{r}_j - \boldsymbol{r}|}\,. \quad (224)$$

From Eq.(192) we have

$$\widehat{H}_0 = \sum_{j=1}^{N} \left[ \frac{\widehat{\boldsymbol{p}}_j^2}{2\, m_0} + V_{ext.}(\boldsymbol{r}_j, t) \right] = \widehat{H}_0^{N-1} + \underbrace{\left[ \frac{\widehat{\boldsymbol{p}}^2}{2\, m_0} + V_{ext.}(\boldsymbol{r}, t) \right]}_{=\widehat{H}_0^e}\,.$$

where $V_{ext.}(\boldsymbol{r}, t)$ denotes some extra potential set up outside the apparatus. In general it would at least be the gravitational potential, in which case it would be time-independent In Eq.(224) $|Z_j|$ stands for the number of elementary charges, i. e.

$$Z_j = \begin{cases} -Z_\alpha & \text{if } j \text{ runs over the } \alpha^{th} \text{ nucleus} \\ 1 & \text{if } j \text{ refers to an electron}\,. \end{cases}$$

If one multiplies Eq.(223) by $\Psi_{N-1}^*$ and performs an integration with respect to $\boldsymbol{r}_2, \ldots \boldsymbol{r}_N$ one obtains

$$i\hbar\, \dot{\psi}_e + \psi_e \int \Psi_{N-1}^* \left[ i\hbar\, \frac{\partial \Psi_{N-1}}{\partial t} - \left( \widehat{H}_0^{(N-1)} + V_{apparatus} \right) \Psi_{N-1} \right] d^3r_2 \ldots d^3r_N$$

$$= \widehat{H}_0^e\, \psi_e + \widehat{V}_e\, \psi_e \quad (225)$$

where $\widehat{V}_e(\boldsymbol{r}, t)$ represents a one-electron potential defined as

$$\widehat{V}_e(\boldsymbol{r}, t) = \int \Psi_{N-1}^* \sum_{j=2}^{N} \frac{e^2\, Z_j}{4\pi\, \epsilon_0\, |\boldsymbol{r}_j - \boldsymbol{r}|}\, \Psi_{N-1}\, d^3r_2 \ldots d^3r_N\,. \quad (226)$$

Since the bracketed expression under the integral in the above equation vanishes, we arrive at

$$i\hbar\, \frac{\partial}{\partial t} \psi_e(\boldsymbol{r}, t) = [\widehat{H}_0^e + \widehat{V}_e(\boldsymbol{r}, t)]\, \psi_e(\boldsymbol{r}, t)\,. \quad (227)$$

Thus, the wave function of the electron under study obeys, in fact, a one-particle Schrödinger equation.

However, in the above derivation we have ignored the response of the wave-function $\Psi_{N-1}$ of the apparatus to the presence of the test particle. This is is hidden in $\sum_{j=2}^{N} V_{ext.}(\boldsymbol{r}_j, t)$ being a constituent of $\widehat{H}_0^{N-1}$. Not only the gravitational potential acts on the apparatus but also the "still external" test particle through its Coulomb potential. Inclusion of this effect amounts to adding this extra potential

$$\Delta V_{ext.}(\boldsymbol{r}_2, \boldsymbol{r}_3, \ldots \boldsymbol{r}_N) = \int \psi_e^*(\boldsymbol{r}, t)\, V_e^{N-1}(\boldsymbol{r}, \boldsymbol{r}_2 \ldots \boldsymbol{r}_N, t)\psi_e(\boldsymbol{r}, t)\, d^3r$$

to the unmodified expression for $\widehat{H}_0^{N-1}$ in Eq.(225). With the appearance of $\Delta V_{ext.}$ the apparatus wave function changes and becomes a functional of $\psi_e(\boldsymbol{r}, t)$. This, in turn, gives rise to a change of $\widehat{V}_e(\boldsymbol{r}, t)$ as follows from its definition Eq.(226). That means that the test particle feels the potential of the charge distribution which it induces in the apparatus. It should be clearly recognized that this - admittedly small - effect turns the one-particle Eq.(227) into a non-linear partial differential equation. That is to say that at this level of description even the simplest realistic case of a particle travelling in a vacuum chamber leads to a non-linear Schrödinger equation. In the following considerations we ignore this charge induction effect.

There are certain cases in which the contact time of the test particle is not short enough, and hence there is a non-vanishing probability that the particle mingles with those of the target. To get a rough picture of this situation, we describe the wave function instead of (222) by

$$\begin{gathered}\Psi_N(\boldsymbol{r}, \boldsymbol{r}_2, \ldots \boldsymbol{r}_N, t) = \\ c_0(t)\, \psi_e(\boldsymbol{r}, t)\, \Psi_{N-1}(\boldsymbol{r}_2, \boldsymbol{r}_3, \ldots \boldsymbol{r}_N, t) + c_1(t)\, \Psi_N^{capt}(\boldsymbol{r}, \boldsymbol{r}_2, \ldots \boldsymbol{r}_N, t)\end{gathered} \tag{228}$$

where $c_0(t)$ and $c_1(t)$ are real-valued functions with the property $|c_0(t)|^2 + |c_1(t)|^2 = 1$, in particular

$$c_0(t) = e^{-\frac{t}{2\tau}}$$

and hence

$$|c_0(t)|^2 = e^{-\frac{t}{\tau}}\,; \quad |c_1(t)|^2 = 1 - e^{-\frac{t}{\tau}}\,. \tag{229}$$

Here $\tau$ refers to a characteristic interaction time with the target, and $|c_1(t)|^2$ is the probability with which the test electron is captured by the target. Thereby it loses its identity as the "test electron". The latter effect is expressed by the property of $\Psi_N^{capt}$ being antisymmetric with respect to interchange of **any** two particles out of the set of $N_e$ electrons.

Inserting $\Psi_N$ from Eq.(228) into the Schrödinger equation (191) we obtain

$$c_0(t)\left[\Psi_{N-1}\, i\hbar\,\dot{\psi}_e + \psi_e\, i\hbar\,\dot{\Psi}_{N-1}\right] +$$
$$i\hbar\,\dot{c}_0(t)\,\psi_e\Psi_{N-1} + c_1(t)\, i\hbar\,\dot{\Psi}_N^{capt} + i\hbar\,\dot{c}_1(t)\,\Psi_N^{capt}$$
$$= c_0(t)\left[\psi_e\,\widehat{H}_0^{(N-1)}\,\Psi_{N-1} + \Psi_{N-1}\,\widehat{H}_0^e\,\psi_e + V_{tot}\psi_e\,\Psi_{N-1}\right] + c_1(t)\,\widehat{H}\,\Psi_N^{capt} \quad (230)$$

The functions $\Psi_{N-1}$ and $\Psi_N^{capt}$ satisfy the associated time-dependent Schrödinger equations

$$i\hbar\,\dot{\Psi}_{N-1} = \left[\widehat{H}_0^{(N-1)} + V_{apparatus}\right]\,\Psi_{N-1} \quad (231)$$

and

$$i\hbar\,\dot{\Psi}_N^{capt} = \widehat{H}\,\Psi_N^{capt}\,.$$

If we insert this into Eq.(230), multiply the result in front by $\Psi_{N-1}^*$ and perform an integration over $\boldsymbol{r}_2, \boldsymbol{r}_3, \ldots \boldsymbol{r}_N$, we obtain

$$c_0(t)\,\left[i\hbar\,\frac{\partial}{\partial t} - \widehat{H}_0^e - V_e'(\boldsymbol{r},t)\right]\psi_e(\boldsymbol{r},t) +$$

$$i\hbar\,\dot{c}_1(t)\int \Psi_{N-1}^*(\boldsymbol{r}_2,\ldots\boldsymbol{r}_N,t)\cdot\Psi_N^{capt}(\boldsymbol{r},\boldsymbol{r}_2\,\ldots\boldsymbol{r}_N,t)\,d^3r_2\ldots d^3r_N = 0\,. \quad (232)$$

Here we have used $i\hbar\,\frac{\partial}{\partial t}\,c_0(t) = -i\,\frac{\hbar}{2\tau}\,c_0(t)$ and set

$$V_e'(\boldsymbol{r},t) = V_e(\boldsymbol{r},t) + i\,\tilde{V}_e \quad \text{where} \quad \frac{\tilde{V}_e}{\hbar} \equiv \frac{1}{2\tau}\,.$$

The imaginary part of $V_e'(\boldsymbol{r},t)$ is commonly referred to as "optical potential".
According to our classification of the electron under study as either "distinguishable" or "non-distinguishable" the associated total probability density $\rho(\boldsymbol{r},t)$ splits (almost quantitatively) into the "either- and or-probability"

$$\rho(\boldsymbol{r},t) = \underbrace{|c_0(t)|^2\,|\psi_e(\boldsymbol{r},t)|^2}_{=\rho_0(\boldsymbol{r},t)} + \underbrace{|c_1(t)|^2\int|\Psi_N^{capt}(\boldsymbol{r},\ldots\boldsymbol{r}_N,t)|^2\,d^3r_2,\ldots d^3r_N}_{\equiv\rho_1(\boldsymbol{r},t)}$$

which means

$$S_e(\boldsymbol{r},t) = \int\Psi_{N-1}^*(\boldsymbol{r}_2,\ldots\boldsymbol{r}_N)\times\Psi_N^{capt}(\boldsymbol{r},\boldsymbol{r}_2,\ldots\boldsymbol{r}_N)\,d^3r_2,\ldots d^3r_N \approx 0\,\forall\,\boldsymbol{r},t\,.$$

It follows then from Eq.(232) that $\psi_e(\boldsymbol{r},t)$ solves the modified Schrödinger equation

$$\left[i\hbar\,\frac{\partial}{\partial t} - \widehat{H}_0^e - V_e'(\boldsymbol{r},t)\right]\psi_e(\boldsymbol{r},t) = 0\,, \quad (233)$$

which describes situations one encounters, for example, in experiments on low energy electron diffraction (LEED) at surfaces of solids.
The mod squared of the actually not completely vanishing overlap

$$S(t) = \int S_e(\boldsymbol{r}, t)\, \psi_e^*(\boldsymbol{r}, t)\, d^3r$$

determines the transition probability $1/\tau$. Eq.(228) and the resulting Eqs.(231) and (233) are pivotal in describing generic quantum mechanical processes, a subset of which plays the role of "measurements"[5]. For example, when one is dealing with a setup where an electron traverses the legendary double slit diaphragm, defined by the potential (226), the function $\Psi_N^{capt}(\boldsymbol{r}, \boldsymbol{r}_2, \ldots \boldsymbol{r}_N, t)$ describes the situation when the electron has been captured by the detector which is a part of the "apparatus". In spirit this in keeping with a statement by Hartle and Gell-Mann [56]: *"In a theory of the whole thing there can be no fundamental division into observer and observed"* Our approach reflects even more directly the standpoint taken by v. Kampen [57]: *"The measuring act is fully described by the Schroedinger equation for object and apparatus together..."*

It is the archetypal combination of a particular setup and "pointer readings" of a detector that enables the experimentalist to determine certain properties of a one-particle quantum system: The sought-for information can only be extracted from a solution to the respective Schrödinger (or Pauli) equation that yields $\boldsymbol{j}(\boldsymbol{r}) = \rho(\boldsymbol{r}, t)\, \boldsymbol{v}(\boldsymbol{r}, t)$ at $\boldsymbol{r}_{detector}$. Eigenvalues of Hermitian operators can only be obtained via this detour, and for fundamental, mostly experimental, reasons, only with limited accuracy.

The paradoxical situation which one runs into if one endows the "observer" (or "measurer") with an unrealistic meaning, is illustrated by Schrödinger's cat example [64]: An alpha-particle emitted from some radioactive material triggers a device that kills a cat in a closed box by releasing a poisonous gas. Of course, the moment of radioactive decay does in no way depend on the particular setup. Our description of this process would be based on Eq.(228) where $\Psi_N(\boldsymbol{r}, \boldsymbol{r}_2, \ldots \boldsymbol{r}_N, t)$ on the left-hand side now represents the wave function $\Psi_{gas+cat}(t)$ of the system cat plus gas, $\psi_e(\boldsymbol{r}, t)$ has to be replaced with an $N$-particle wave function $\psi_{poison}$ referring to the only weakly "cat-overlapping" molecules of the poisonous gas set free by the device, and $\Psi_{N-1}(\boldsymbol{r}_2, \boldsymbol{r}_3, \ldots \boldsymbol{r}_N, t)$ is the many-particle wave function $\Psi_{cat}$ of the live cat. After a time span of $\approx \tau$ the system's wave function $\Psi_{gas+cat}(t)$ has attained the form $\Psi_{capture}(t)$ where the poisonous molecules are now a part of the cat. It solves the time-dependent Schrödinger equation of the united system. The time-evolution of $\Psi_{capture}(t)$ describes all the atomic

[5] We side here emphatically with John Bell [36] who pleads in his article *"Against Measurement"* for more common sense in describing what is actually happening: the time evolution of a particular **experiment**.

(chemical) processes that eventually lead to the cat's death. It is this time-dependent process that is familiar from ab initio calculations on chemical reactions. The latter are completely "self-controlled". There is definitely no "observer-induced" influence. From this point of view it appears to be rather absurd that orthodox quantum mechanics interprets Eq.(228) with the explained new meaning of the wave functions as a superposition of a "live" and a "dead"-state of the cat, and only on opening the lid of the box by an observer, $\Psi_{gas+cat}$ collapses onto the wave function of a live or dead cat.

## 27 The origin of particle spin

In 1925 Uhlenbeck and Goudsmit [65] suggested in a widely recognized paper that Pauli's idea [66] of a fourth quantum number in the description of electronic states of atoms might be associated with the rotation of an electron about its own axis thus giving rise to an extra angular moment. From the analysis of atomic spectra it was clear that the magnetic moment generated by such a rotation of the electron as a charged sphere had to be equal to the Bohr magneton

$$\mu_B = \frac{e\hbar}{2m_0}\,.$$

There was also experimental evidence that the associated mechanical spin moment $\vec{S}$ - different from the atomic orbital momentum - would not obey the classical law of magneto-mechanical parallelism according to which $\mu_B$ should differ from $\vec{S}$ by a factor $\frac{e}{2m_0}$. In actual fact this factor had been found to be $\frac{e}{m_0}$ instead so that

$$|\vec{S}| = \frac{\hbar}{2}\,.$$

and hence

$$\mu_B = g\,\frac{e}{2m_0}\,\frac{\hbar}{2}\,. \tag{234}$$

We ignore here and in the following the minute departure of $g$ from 2 due to quantum electrodynamical corrections.
The radius of the rotating electron sphere was equated with the classical electron radius $2.8 \cdot 10^{-13}$ cm. As van der Waerden [67] reports, Lorentz immediately demonstrated to Uhlenbeck and Goudsmit that the electron mass would actually be larger than that of a proton if the magnetic moment of a Bohr magneton would be confined to that sphere. Moreover, the speed at the equator of the rotating sphere would by far exceed the velocity of light. Although these objections definitely disqualified the rotating

sphere as a model of electron spin, it is still used, tacitly implied or appears concealed as "intrinsic" property in the analysis of most of the present-day experiments involving spin-orientation or spin flips. There are very explicit warnings in widely used textbooks like that by Landau and Lifshitz [68]: *In particular, it would be wholly meaningless to imagine the "intrinsic" angular momentum of an elementary particle as being the result of its rotation "about its own axis".* However, all these objections have failed to prevent people from thinking in terms of this model.
If an "eigen-rotation" cannot explain the occurrence of a mechanical spin moment associated with a gyratory electronic motion, what else can be responsible for it? The following considerations are based on the idea that **"spin" is not a property of the particle** but is rather a property of its quantum mechanical state. Ohanian [69] arrives at the same conclusion summarizing an early analysis by Gordon [70] in 1928. He states:

*This means that neither the spin nor the magnetic moment are internal properties of the electron - they have nothing to do with the internal structure of the electron, but only with the structure of its wave field.*

However, as for his basic message we definitely disagree with Ohanian. He presents reasons that there is formally a strong similarity between a spin-polarized particle wave and a circularly polarized electromagnetic plane wave. His arguments are valid for the case of a longitudinally polarized free particle wave, but they do not apply to a transversally polarized particle wave.

Our description of particle motion as modified by stochastic vacuum forces makes it particularly suggestive to correlate - similar to the explanation of zero-point motion of oscillators - particle spin with the quivering motion that results from those forces and vanishes as $\hbar$ tends to zero. (This applies, of course, to all the other quantum mechanical groundstate properties as well.) Hestenes [71], [72] discussed particle spin within the same concept. To illustrate our idea in more detail we consider the simplest case of a hydrogen electron exposed to a magnetic field $\boldsymbol{B} = B_Z\,\boldsymbol{e}_z$ in its ground state $\psi_0(\boldsymbol{r})$. In Fig.12 we show a schematic distribution of positions that the electron has successively taken at times $t_i$ and equal time intervals $t_{i+1} - t_i = \Delta t$ where $\Delta t$ is very small compared to $T$. This time span has been introduced in Section 4 in connection with defining the probability density $\rho(\boldsymbol{r})$. The $z-$axis is thought to run through the atomic center perpendicular to the plotting plane. At each of the points the electron possesses a velocity which we decompose into a radial and a $z-$component, and in a component perpendicular to the $z-$axis. Only the latter components are indicated by arrows. For symmetry reasons there will be as many positive as negative radial and $z-$components in the elementary volume about each point. They average out. We subdivide the set of arrows into two subsets associated with left-hand and right-hand circular motion, respectively. One might surmise

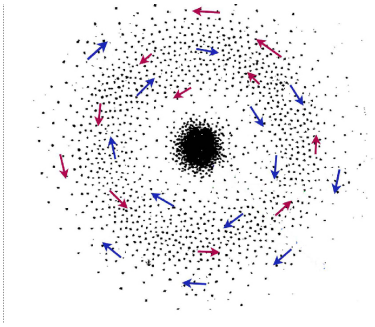

Figure 12: Spin effective components of the quivering motion

that in the presence of the magnetic field along the $z$-direction one of the sets becomes empty in favor of doubling the other set thereby giving rise to a net circular current so as to minimize the total energy in that electronic state. The gain in energy must be transferred to an external reservoir.
This energy gain is proportional to $B_z$ which is a defining property, and it vanishes as $\hbar \to 0$. As has been shown in Section 15 the magnetic field causes a current density $\boldsymbol{j}(\boldsymbol{r}) = \frac{e}{m_0}|\psi_0(\boldsymbol{r})|^2\,\boldsymbol{A}(\boldsymbol{r})$ when the particle is in the state $\psi_0(\boldsymbol{r})$ , but the energy gain from this goes as $B_z^2$ because of $\Delta E = \int \boldsymbol{j}\cdot\boldsymbol{A}\,d^3r$ and $\boldsymbol{B} = \nabla \times \boldsymbol{A}$. The omission of the empty subset of arrows does not change the distribution of points defining $\psi_0(\boldsymbol{r})$. This distribution is via the Schrödinger equation shaped by the guiding field in the system, which is the nuclear electrostatic field in the case of a hydrogen electron, or, in general, the effective field an electron feels in an atom. In the presence of a magnetic field the associated vector potential $\boldsymbol{A}(\boldsymbol{r})$ in the kinetic energy operator is a constituent of the total field shaping $\psi_0(\boldsymbol{r})$.

We thus arrive at the conclusion that the circular current which occurs on allowing the quivering motion of the electron to become asymmetric does not change the probability density which is characteristic of real-valued solutions to the Schrödinger equation. But it definitely yields a physical effect that has so far been outside our formal framework. In discussing certain properties of solutions to the Dirac equation Schrödinger [73] was led to a similar interpretation of particle spin and named the irregular particle motion causing it "Zitterbewegung". However, he presupposed the existence of the Dirac equation in his considerations as opposed to our approach where the Dirac equation will be derived.
The additional spin-dependent interaction with a magnetic field occurs also in complex-valued states $\psi(\boldsymbol{r})$ when the particle moves in a spherical or cylindrical potential. These states contain an orbital momentum of the familiar meaning. There is now an additional set of arrows superposed on those shown in Fig.12. That set consists of arrows depicting $\boldsymbol{v}(\boldsymbol{r}) = \frac{\hbar}{m_0}\,\nabla\varphi(\boldsymbol{r})$ at the various points distributed according to $|\psi(\boldsymbol{r})|^2$. Clearly, a linear super-

position of those arrows is only possible as long as the velocities are within the non-relativistic regime. Otherwise the superposition is affected by spin-orbit coupling as a result of which $\varphi_\uparrow(\boldsymbol{r})$ and $\varphi_\downarrow(\boldsymbol{r})$ now become different. This point will be taken up again in Section 34. It will, further, be shown in Section 36 that the magnetic moment connected with the charged particle's "Zitterbewegung" has a fixed value, viz. the value of the Bohr magneton, and this is independent of the specific shape of the wavefunction. Different from the angular motion that has its roots in a classical orbital motion, the occurrence of spin does **not** presuppose spherical or cylindrical symmetry of the potential within which the particle moves. The potential must merely possess a center or an axis. There is an extra velocity field $\boldsymbol{v}_{spin}(\boldsymbol{r})$ associated with the particle-spin. This velocity field represents again an ensemble average over the individual quivering velocities in the respective elementary volumes about the points $\boldsymbol{r}$. As this extra velocity field must also be non-dissipative, it can be mapped onto a phase $\alpha(\boldsymbol{r})$ as the orbital velocity field $\boldsymbol{v}(\boldsymbol{r})$ could be mapped onto $\varphi(\boldsymbol{r})$. However, it should be kept in mind that the wavefunction $\psi(\boldsymbol{r})$ has been constructed such that $\varphi(\boldsymbol{r})$ represents its phase:

$$\psi(\boldsymbol{r}) = |\psi(\boldsymbol{r})| e^{i\,\varphi(\boldsymbol{r})}\,.$$

Only in this form Newton's modified second law (41) can be transformed - by using Eq.(75) - into the Schrödinger equation. Because of this rigid connection of $\varphi(\boldsymbol{r})$ with a velocity field $\boldsymbol{v}(\boldsymbol{r})$ that originates from the classical particle motion, an additional inclusion of $\alpha(\boldsymbol{r})$ into the phase of the wavefunction is not possible.
The circular spin motion is always in addition to the ordinary orbital motion. This is similar to the motion of a harmonic oscillator whose angular frequency is $\omega$. The energy $E_n$ in the $n$-th eigenstate is always in addition to its zero-point energy:

$$E_n = (n + \tfrac{1}{2})\hbar\,\omega\,.$$

It should be observed, however, that this simple addition only occurs when the axes of the two circular motions are collinear. In the non-relativistic limit there is no physical reason for collinearity because the two circular motions occur independently. However, in the relativistic case a new phenomenon, spin-orbit-coupling, comes into play which couples the two circular motions. This matter will not be pursued any further in the present exposition.
Since $\boldsymbol{v}_{spin}(\boldsymbol{r})$ possesses a velocity potential, this may - in analogy to the "ordinary" velocity field - be expressed

$$\boldsymbol{v}_{spin}(\boldsymbol{r}) = \frac{\hbar}{m_0}\nabla\alpha(\boldsymbol{r})\,.$$

It follows then that any path integral of it encircling the "spin axis" must yield a fixed value. As for the magnetic moment that is connected with the current $e\,\boldsymbol{v}_{spin}$ one is tempted to assume that it agrees with the Bohr

magneton. This assumption will prove to be consistent with the result one obtains from the Dirac equation.

## 28 Generalizing one-particle quantum mechanics by including particle spin

Several suggestions have already been made to incorporate particle spin into a theory that is akin to the ideas of the present article (s. e. g. Hestenes [72], Dankel [75], Dohrn et al. [76], Nelson [77]). We believe, however, that our approach is easier to envisage and hence appears to be most desirable in the spirit of v. Weizsäcker's statement [74] "... What we are dissatisfied with is basically not that the old perceptions have failed but that they could not be superseded by something immediately comprehensible.".

The points associated with the two subset of arrows in Fig.1 define probability densities $\rho_\uparrow(\boldsymbol{r})$ and $\rho_\downarrow(\boldsymbol{r})$ with $\uparrow$ and $\downarrow$ referring to the respective direction of the spin moment. Both densities integrate to unity

$$\int \rho_{\uparrow(\downarrow)}(\boldsymbol{r})\, d^3r = 1\,. \tag{235}$$

If one turns on an infinitesimally small magnetic field in the $z$-direction, the two densities split up. The density whose associated particle performs a right-handed motion about the $z$-axis doubles at the expense of the other density which disappears. The reverse applies to the density connected with the left-handed circular motion. Accordingly, the two densities occur at different energies due to their different interaction with the magnetic field. (As presupposed, they differ only infinitesmally little.)
We first concentrate on $\rho_\uparrow(\boldsymbol{r})$ and note:

$$\rho(\boldsymbol{r}) = \rho_\uparrow(\boldsymbol{r})\,. \tag{236}$$

What happens if one turns the coordinate system by some angle? For reasons which will become clear later, we rename the original coordinate system into $(x', y', z')$ and, accordingly, denote the new one by $(x, y, z)$. The spin-up-density in the new $z$-direction can only be a fraction of the original one, which is now associated with the $z'$-axis. It will, therefore, be smaller than the original one which integrated to unity. On the other hand, after one has turned the coordinate system the total charge density which the new $\rho_\uparrow(\boldsymbol{r})$ is a part of, still integrates to unity. To satisfy the latter requirement one might think of forming

$$\rho(\boldsymbol{r}) = |a|^2\, \rho_\uparrow(\boldsymbol{r}) + |b|^2\, \rho_\downarrow(\boldsymbol{r}) \tag{237}$$

where $\rho_\downarrow(\boldsymbol{r})$ represents the spin-down density for the new $z$-direction, and $a$ and $b$ denote coefficients whose modulus squares sum up to unity

$$|a|^2 + |b|^2 = 1\,. \tag{238}$$

It is not possible, however, to partition the wave function analogously: $\psi(\boldsymbol{r}) = a\,\psi_\uparrow(\boldsymbol{r}) + b\,\psi_\downarrow(\boldsymbol{r})$ because $\psi^*(\boldsymbol{r})\psi(\boldsymbol{r})$ would contain cross-terms which prevents $\psi^*(\boldsymbol{r})\psi(\boldsymbol{r})$ from integrating to unity. However, if one introduces a two-component spinor of the form

$$\underline{\psi}(\boldsymbol{r}) = \begin{pmatrix} a\,\psi_\uparrow(\boldsymbol{r}) \\ b\,\psi_\downarrow(\boldsymbol{r}) \end{pmatrix} = a\,\psi_\uparrow(\boldsymbol{r}) \begin{pmatrix} 1 \\ 0 \end{pmatrix} + b\,\psi_\downarrow(\boldsymbol{r}) \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{239}$$

and its adjoint $\underline{\psi}^\dagger(\boldsymbol{r}) = \left(a^*\psi_\uparrow^*(\boldsymbol{r}),\, b^*\psi_\downarrow^*(\boldsymbol{r})\right)$ where

$$\int |\psi_{\uparrow(\downarrow)}(\boldsymbol{r})|^2\, d^3r = 1\,, \tag{240}$$

one obtains as intended

$$\underline{\psi}^\dagger(\boldsymbol{r})\underline{\psi}(\boldsymbol{r}) = |a|^2\,|\psi_\uparrow(\boldsymbol{r})|^2 + |b|^2\,|\psi_\downarrow(\boldsymbol{r})|^2 = \rho(\boldsymbol{r})$$

and

$$\int \underline{\psi}^\dagger(\boldsymbol{r})\underline{\psi}(\boldsymbol{r})\, d^3r = 1\,. \tag{241}$$

The spinors $\underline{\psi}_{\uparrow(\downarrow)}(\boldsymbol{r})$ will be referred to as spin-up and spin-down components from now on.

As in the classical theory of electricity the circular motion of a charged particle is connected with a magnetic moment. This applies as well to the spin motion under discussion. The absolut value of this moment turns out to be identical with the Bohr magneton $\mu_B = \frac{e\hbar}{2m_0}$ as can be derived from the Dirac equation[6] (see Section 36). For the time being it is considered to be known. The above discussion started with a pure spin-up-state in the $z'$-direction. The necessity for forming its equivalent representation in a rotated cooordinate system by combining $\underline{\psi}_\uparrow(\boldsymbol{r})$ and $\underline{\psi}_\downarrow(\boldsymbol{r})$ leads to unexpected consequences. This becomes apparent if one applies a magnetic field in the $z$-direction. The energy densities of the interaction with the magnetic field for "up"- and "down"-spin may be cast as

$$-\mu_B B_z\,|a|^2\,\psi_\uparrow^*(\boldsymbol{r})\,\psi_\uparrow(\boldsymbol{r}) \quad \text{and} \quad +\mu_B B_z\,|b|^2\,\psi_\downarrow^*(\boldsymbol{r})\,\psi_\downarrow(\boldsymbol{r})\,.$$

from which the total interaction density results as

$$u_{magn.}(\boldsymbol{r}) = -\underline{\psi}^\dagger(\boldsymbol{r})\,\mu_B \underline{\underline{B}}\,\underline{\psi}(\boldsymbol{r}) \tag{242}$$

where we have introduced a matrix

$$\underline{\underline{B}} = \begin{pmatrix} B_z & 0 \\ 0 & -B_z \end{pmatrix}. \tag{243}$$

[6] As already mentioned earlier in connection with Eq.(234) quantum electrodynamics yields a small correction to this value.

Likewise, we may cast the non spin-dependent energy density of the electron as

$$\underline{\psi}^{\dagger}(\boldsymbol{r})\,\widehat{H}\,\underline{\psi}(\boldsymbol{r})$$

where

$$\widehat{H}=\widehat{H}_0+V(\boldsymbol{r})\quad\text{and}\quad\widehat{H}_0=\frac{(\widehat{\boldsymbol{p}}-e\boldsymbol{A}(\boldsymbol{r}))^2}{2\,m_0}\,, \tag{244}$$

and with $V(\boldsymbol{r})$ denoting some potential in which the electron moves.

# 29 The time-dependent non-relativistic Pauli equation

The basic two constituents of our approach, viz. $|\psi(\boldsymbol{r},t)|^2$ and $\nabla\varphi(\boldsymbol{r},t)$ remain unaffected by our incorporation of spin. Hence, it is in line with the conceptual idea of our approach to assume that the two theorems of Ehrenfest stay unaffected as well. That means, according to Ehrenfest's Second Theorem

$$\begin{aligned}\langle\boldsymbol{v}\rangle=\frac{d}{dt}\,\langle\boldsymbol{r}\,\rangle=\int\Big[&\dot{\underline{\psi}}^{\dagger}(\boldsymbol{r},t)\,\boldsymbol{r}\,\underline{\psi}(\boldsymbol{r},t)\\&+\underline{\psi}^{\dagger}(\boldsymbol{r},t)\,\boldsymbol{r}\,\dot{\underline{\psi}}(\boldsymbol{r},t)\Big]\,d^3r\,,\end{aligned} \tag{245}$$

and we have alternatively from Eq.(114)

$$\langle\boldsymbol{v}\rangle=\frac{1}{m_0}\int\underline{\psi}^{\dagger}(\boldsymbol{r},t)\widehat{\boldsymbol{P}}\,\underline{\psi}(\boldsymbol{r},t)\,, \tag{246}$$

which holds without modification also for the spinors we have introduced. Exploiting the relation

$$[\widehat{H}_0\,\boldsymbol{r}-\boldsymbol{r}\,\widehat{H}_0]\,\underline{\psi}(\boldsymbol{r},t)=-i\,\frac{\hbar}{m_0}\,\widehat{\boldsymbol{P}}\,\underline{\psi}(\boldsymbol{r},t)\,,$$

which follows from simply applying the chain rule, we may combine Eqs.(245) and (246) to obtain

$$\begin{aligned}\int\left(\left[\widehat{H}_0+i\hbar\,\frac{\partial}{\partial t}\right]\underline{\psi}^{\dagger}(\boldsymbol{r},t)\right)\,\boldsymbol{r}\,\underline{\psi}(\boldsymbol{r},t)\,d^3r\,-\\\int\underline{\psi}^{\dagger}(\boldsymbol{r},t)\,\boldsymbol{r}\,\left[\widehat{H}_0-i\,\hbar\frac{\partial}{\partial t}\right]\,\underline{\psi}(\boldsymbol{r},t)\,d^3r=0\,.\end{aligned} \tag{247}$$

This equation holds for any $t$ if $\underline{\psi}(\boldsymbol{r},t)$ satisfies

$$\left[\widehat{H}_0-i\,\hbar\frac{\partial}{\partial t}\right]\,\underline{\psi}(\boldsymbol{r},t)=-\underline{\underline{D}}\,\underline{\psi}(\boldsymbol{r})-F(\boldsymbol{r},t)\,\underline{\psi}(\boldsymbol{r},t)\,, \tag{248}$$

and correspondingly

$$\left[\widehat{H}_0 + i\,\hbar\frac{\partial}{\partial t}\right]\,\underline{\psi}^\dagger(\boldsymbol{r},t) = -\underline{\psi}^\dagger\,(\boldsymbol{r})\,\underline{\underline{D}} - \underline{\psi}^\dagger(\boldsymbol{r})\,F(\boldsymbol{r},t)\,,$$

where $F(\boldsymbol{r},t)$ is some integrable real-valued function and $\underline{\underline{D}}$ denotes some unitary 2×2-matrix that will be specified later to meet requirements of Ehrenfest's first theorem.
The expectation value of the force exercised on an electron which moves in a potential $V(\boldsymbol{r})$ and simultaneously - via its magnetic moment - feels a force in a spatially varying magnetic field $\boldsymbol{B}(z,t) = B_z(z,t)\,\boldsymbol{e}_z$ may be cast as

$$\langle \boldsymbol{F}\rangle = -\int \underline{\psi}^\dagger(\boldsymbol{r},t)\,\left[\nabla\{V(\boldsymbol{r}) + \mu_B\,\underline{\underline{B}}\}\right]\,\underline{\psi}(\boldsymbol{r},t)\,d^3r - \langle e\dot{\boldsymbol{A}}(\boldsymbol{r},t)\rangle\,. \quad (249)$$

The appearance of the induction-derived force $-\langle e\dot{\boldsymbol{A}}(\boldsymbol{r},t)\rangle$ is a consequence of Eq.(111).
We perform an integration by parts on the first integral and obtain

$$\langle \boldsymbol{F}\rangle = \int \left[\nabla\underline{\psi}^\dagger(\boldsymbol{r},t)\right]\,\{V(\boldsymbol{r}) + \mu_B\,\underline{\underline{B}}\}\,\underline{\psi}(\boldsymbol{r},t)\,d^3r +$$
$$\int \underline{\psi}^\dagger(\boldsymbol{r},t)\,\{V(\boldsymbol{r}) + \mu_B\,\underline{\underline{B}}\}\,\nabla\underline{\psi}(\boldsymbol{r},t)\,d^3r - \langle e\dot{\boldsymbol{A}}(\boldsymbol{r},t)\rangle\,. \quad (250)$$

From Eq.(114) we have

$$\frac{d}{dt}\,\langle \boldsymbol{p}\rangle = \frac{d}{dt}\int \underline{\psi}^\dagger(\boldsymbol{r},t)\,[-i\hbar\nabla - e\,\boldsymbol{A}(\boldsymbol{r},t)]\,\underline{\psi}(\boldsymbol{r},t)\,d^3r$$

which we rewrite

$$\frac{d}{dt}\,\langle \boldsymbol{p}\rangle = \int\left(-i\hbar\frac{\partial}{\partial t}\,\underline{\psi}^\dagger\right)\nabla\underline{\psi}\,d^3r + \underbrace{\int \underline{\psi}^\dagger\,\nabla\left(-i\hbar\frac{\partial}{\partial t}\,\underline{\psi}\right)\,d^3r}_{=-\int\nabla\underline{\psi}^\dagger\left(-i\hbar\frac{\partial}{\partial t}\underline{\psi}\right)\,d^3r} - \int \underline{\psi}^\dagger\,\underline{\psi}\,e\,\dot{\boldsymbol{A}}\,d^3r\,.$$

On forming $\langle \boldsymbol{F}\rangle - \langle \dot{\boldsymbol{p}}\rangle = 0$ (Ehrenfest's First Theorem) we obtain

$$\int\left(\nabla\underline{\psi}^\dagger\right)\,\left\{V + \mu_B\,\underline{\underline{B}} - i\hbar\frac{\partial}{\partial t}\right\}\,\underline{\psi}\,d^3r +$$
$$\int\left[\left(+i\hbar\frac{\partial}{\partial t}\underline{\psi}^\dagger\right)\nabla\underline{\psi} + \underline{\psi}^\dagger\{V + \mu_B\,\underline{\underline{B}}\}\,\nabla\underline{\psi}\right]\,d^3r = 0\,. \quad (251)$$

If we here eliminate the time-derivatives using Eqs.(248) and equate $\underline{\underline{D}}$ with $\mu_B\,\underline{\underline{B}}$ this equation takes the form:

$$-\int\left[(\nabla\underline{\psi}^\dagger)\,\widehat{H}_0\,\underline{\psi} + (\widehat{H}_0\,\underline{\psi}^\dagger)\nabla\underline{\psi}\right]\,d^3r +$$
$$\int\left[(\nabla\underline{\psi}^\dagger(\boldsymbol{r},t))\,\underline{\psi}(\boldsymbol{r},t) + \underline{\psi}^\dagger(\boldsymbol{r},t)\,\nabla\underline{\psi}(\boldsymbol{r},t)\right]\times\{V(\boldsymbol{r}) - F(\boldsymbol{r},t)\}\,d^3r = 0\,.$$

We temporarily assume that $\boldsymbol{A}(\boldsymbol{r},t) \equiv 0$. One recognizes then that the first integral vanishes. Thus

$$\int \nabla\rho(\boldsymbol{r},t)\{V(\boldsymbol{r}) - F(\boldsymbol{r},t)\}\, d^3r = 0 \quad \forall\, t\,. \tag{252}$$

We first consider the possibility that the expression in curly brackets does not vanish, but the integral does. As we have emphasized in defining probability densities $\rho(\boldsymbol{r},t)$ and average velocities $\boldsymbol{v}(\boldsymbol{r},t)$ through Eqs.(22) and (23), non-stationary states require a certain sample-time $T$ of the particle under study to allow its time-derived probability density $\rho(\boldsymbol{r},t)$ to become quasi-stationary. Hence, if we introduce at $t = t_0$ a small perturbational potential $V(\boldsymbol{r}) \to V(\boldsymbol{r}) + \delta v(\boldsymbol{r},t)$ where $t_0 \leq t \ll T$, the probability density $\rho(\boldsymbol{r},t)$, and thus its gradient remain practically unaffected, but the bracketed expression is now definitely different. We are hence led to conclude that Eq.(252) can only be satisfied if $F(\boldsymbol{r},t) \equiv V(\boldsymbol{r})$ holds for any time. That means - because of Eq.(248) - that the spinor function $\underline{\psi}(\boldsymbol{r},t)$ solves

$$\left[\widehat{H}_0 + V(\boldsymbol{r}) + \mu_B\, \underline{\underline{B}}\right]\, \underline{\psi}(\boldsymbol{r},t) \;= i\,\hbar \frac{\partial}{\partial t}\, \underline{\psi}(\boldsymbol{r},t) \tag{253}$$

as Eq.(248) holds also for $\boldsymbol{A}(\boldsymbol{r},t) \neq 0$. Eq.(253) constitutes the time-dependent non-relativistic Pauli equation.

# 30 The Cayley-Klein parameters and Pauli spin matrices

We want to adapt Eq.(253) to a situation where the direction of the magnetic field no longer coincides with the $z$-axis of the coordinate system. This can be achieved by exploiting a surprising alternative to the standard form of rotating the coordinate system by applying orthogonal 3×3 matrices. The idea goes back to Felix Klein (see e. g. H. Goldstein [78]) and is related to earlier work of Cayley. He considers the rotation of the coordinate system $(x, y, z \to x', y', z')$ to be performed in three steps described by the Euler angles $\phi, \theta$ and $\psi$ shown in Fig.13.
Instead of representing the position vector $\boldsymbol{r}$ by a column matrix he uses a 2×2-matrix $\underline{\underline{P}}(\boldsymbol{r})$ of the form

$$\underline{\underline{P}}(x,y,z) := \begin{pmatrix} z & x - i\,y \\ x + i\,y & -z \end{pmatrix}. \tag{254}$$

In place of the standard 3×3-rotation matrix one now has a 2×2-unimodular matrix

$$\underline{\underline{Q}}(\theta,\phi,\psi) \;=\; \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix} \tag{255}$$

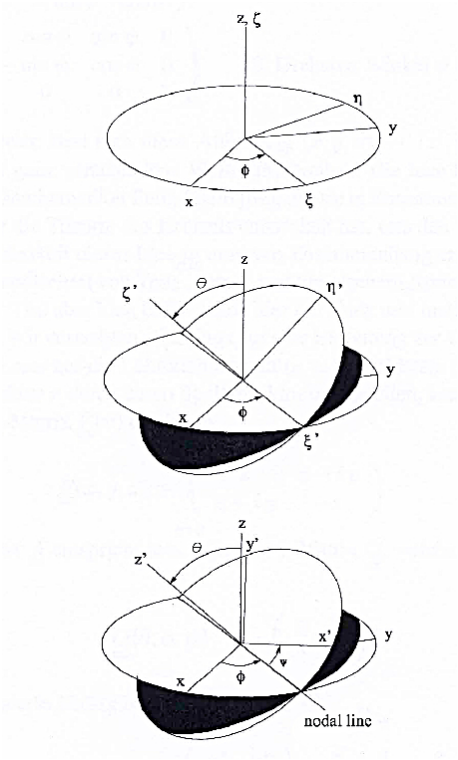


Figure 13: Euler angles

whose elements - the so-called Cayley-Klein parameters - are connected with the Euler angles through

$$\begin{aligned} \alpha &= e^{\frac{i}{2}(\psi+\phi)} \cos\frac{\theta}{2} \\ \beta &= ie^{\frac{i}{2}(\psi-\phi)} \sin\frac{\theta}{2} \\ \gamma &= ie^{-\frac{i}{2}(\psi-\phi)} \sin\frac{\theta}{2} \\ \delta &= e^{-\frac{i}{2}(\psi+\phi)} \cos\frac{\theta}{2}\,. \end{aligned} \tag{256}$$

After the three steps of the rotation have been performed the original position vector $\boldsymbol{r} = (x, y, z)$ is now associated with the new coordinates $x', y', z'$ that may be obtained from the transform

$$\underline{\underline{Q}}\,\underline{\underline{P}}\,\underline{\underline{Q}}^{+} = \underline{\underline{P}}'(x', y', z') = \begin{pmatrix} z' & x' - i\,y' \\ x' + i\,y' & -z' \end{pmatrix} \tag{257}$$

where $\underline{\underline{Q}}^{+}$ denotes the adjoint of $\underline{\underline{Q}}$, and we have

$$\underline{\underline{Q}}^{+}\,\underline{\underline{Q}} = \underline{\underline{Q}}\,\underline{\underline{Q}}^{+} = \underline{\underline{1}} \tag{258}$$

The matrix $\underline{\underline{B}}$ had been defined in Eq.(243) as

$$\underline{\underline{B}} = \begin{pmatrix} B_z & 0 \\ 0 & -B_z \end{pmatrix} = B_z \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} . \tag{259}$$

In Klein's representation the point $\boldsymbol{r} = (0, 0, z)$ attains the analogous form

$$\underline{\underline{P}}(\boldsymbol{r}) = z \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} .$$

Hence, $\underline{\underline{B}}$ has to be required to transform under coordinate rotation as $\underline{\underline{P}}$:

$$\underline{\underline{B}}' = \underline{\underline{Q}}\,\underline{\underline{B}}\,\underline{\underline{Q}}^{+} . \tag{260}$$

For a general orientation the magnetic field $\underline{\underline{B}}$ has the form analogous to $\underline{\underline{P}}$ in Eq.(254), viz.

$$\underline{\underline{B}} = \begin{pmatrix} B_z & B_x - i\,B_y \\ B_x + i\,B_y & -B_z \end{pmatrix} . \tag{261}$$

This matrix can be decomposed

$$\underline{\underline{B}} = B_x\,\underline{\underline{\sigma}}_x + B_y\,\underline{\underline{\sigma}}_y + B_z\,\underline{\underline{\sigma}}_z , \tag{262}$$

where the three matrices on the right-hand side are just the Pauli spin matrices

$$\underline{\underline{\sigma}}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \underline{\underline{\sigma}}_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \underline{\underline{\sigma}}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} . \tag{263}$$

They are commonly lumped together in the form of a vector

$$\vec{\sigma} = \underline{\underline{\sigma}}_x\,\boldsymbol{e}_x + \underline{\underline{\sigma}}_y\,\boldsymbol{e}_y + \underline{\underline{\sigma}}_z\,\boldsymbol{e}_z . \tag{264}$$

The matrix $\underline{\underline{B}}$ in Eq.(262) may therefore be cast as

$$\underline{\underline{B}} = \vec{\sigma} \cdot \boldsymbol{B} . \tag{265}$$

The Pauli equation (253) then attains the familiar form

$$\left[\widehat{H}_0 + V(\boldsymbol{r}) + \mu_B\,\vec{\sigma} \cdot \boldsymbol{B}\right] \underline{\psi}(\boldsymbol{r}, t) = i\hbar\,\frac{\partial}{\partial t}\,\underline{\psi}(\boldsymbol{r}, t) . \tag{266}$$

Actually, the spinor in this equation should be marked by a prime because it has changed under the transform as well. We have dropped the prime for simplicity. Since the density of the magnetic interaction energy is, of course, invariant under rotation of the coordinate system

$$u_{magn.}(\boldsymbol{r}) = u'_{magn.}(\boldsymbol{r}') ,$$

it can be shown then that the new $\psi'$ is connected to the original $\psi$ through

$$\underline{\psi}' \;=\; \underline{\underline{Q}}\,\underline{\psi} \tag{267}$$

and correspondingly

$$\underline{\psi}'^{\dagger} \;=\; \left(\underline{\underline{Q}}\,\underline{\psi}\right)^{\dagger} = \underline{\psi}^{\dagger}\,\underline{\underline{Q}}^{+}\,.$$

This becomes obvious from forming

$$\underline{\psi}'^{\dagger}\,\underline{\underline{B}}'\,\underline{\psi}'\;(=:\,u'_{mag}(\boldsymbol{r}',t)) = \underline{\psi}^{\dagger}\,\underline{\underline{Q}}^{+}\,\underline{\underline{B}}'\,\underline{\underline{Q}}\,\underline{\psi}\,.$$

If we insert Eq.(260) on the right-hand side we obtain

$$\underline{\psi}^{\dagger}\,\underline{\underline{Q}}^{+}\,\underline{\underline{B}}'\,\underline{\underline{Q}}\,\underline{\psi} = \underline{\psi}^{\dagger}\,\underbrace{\underline{\underline{Q}}^{+}\,\underline{\underline{Q}}}_{=\underline{\underline{1}}}\,\underline{\underline{B}}\,\underbrace{\underline{\underline{Q}}^{+}\,\underline{\underline{Q}}}_{=\underline{\underline{1}}}\,\underline{\psi} = u_{mag}(\boldsymbol{r},t)\,.$$

Because of

$$\underline{\psi}'^{\dagger}\,\underline{\psi}' = \underline{\psi}^{\dagger}\,\underline{\underline{Q}}^{+}\,\underline{\underline{Q}}\,\underline{\psi} = \underline{\psi}^{\dagger}\,\underline{\psi} = \rho(\boldsymbol{r},t)$$

the probability density is also invariant under rotation of the coordinate system which is consistent with our idea of a spin-defining motion decomposition at the beginning of our considerations. Moreover, if the state of the particle in the original coordinate system has the form

$$\psi_{\uparrow}(\boldsymbol{r})\,\begin{pmatrix}1\\0\end{pmatrix} \quad \text{or} \quad \psi_{\downarrow}(\boldsymbol{r})\,\begin{pmatrix}0\\1\end{pmatrix}\,, \tag{268}$$

it becomes after coordinate rotation

$$\underline{\psi}'_{\uparrow}(\boldsymbol{r}) = \psi_{\uparrow}(\boldsymbol{r})\,\underline{\underline{Q}}(\boldsymbol{r})\,\begin{pmatrix}1\\0\end{pmatrix} = \psi_{\uparrow}(\boldsymbol{r})\left[\alpha(\boldsymbol{r})\,\begin{pmatrix}1\\0\end{pmatrix} - \beta^{*}(\boldsymbol{r})\,\begin{pmatrix}0\\1\end{pmatrix}\right]$$

or

$$\underline{\psi}'_{\downarrow}(\boldsymbol{r}) = \psi_{\downarrow}(\boldsymbol{r})\,\underline{\underline{Q}}(\boldsymbol{r})\,\begin{pmatrix}0\\1\end{pmatrix} = \psi_{\downarrow}(\boldsymbol{r})\left[\beta(\boldsymbol{r})\,\begin{pmatrix}0\\1\end{pmatrix} + \alpha^{*}(\boldsymbol{r})\,\begin{pmatrix}1\\0\end{pmatrix}\right]\,,$$

where $\alpha(\boldsymbol{r})$ and $\beta(\boldsymbol{r})$ are the Cayley-Klein parameters describing the rotation which we have allowed here to be different at different positions $\boldsymbol{r}$.
The spin orientation with respect to the direction of a magnetic field is already uniquely defined by the two angles $\theta$ and $\phi$. Hence one is at liberty to choose $\psi$ at will without loss of generality. It is convenient to set $\psi = -\pi/2$. We consider the projection of the unit vector $\boldsymbol{e}'_z$ onto the original $x/y$-plane where it makes an angle $\varphi$ with the $x$-axis. This angle and the Euler-angle $\phi$ are interrelated

$$\phi = \varphi + \frac{\pi}{2}\,.$$

If one inserts this relation into Eqs.(255) and (256), $\underline{\underline{Q}}$ takes the familiar form

$$\underline{\underline{Q}}(\boldsymbol{r}) = \begin{pmatrix} \exp[\frac{i}{2}\varphi(\boldsymbol{r})]\,\cos\frac{\theta(\boldsymbol{r})}{2} & \exp[-\frac{i}{2}\varphi(\boldsymbol{r})]\,\sin\frac{\theta(\boldsymbol{r})}{2} \\ -\exp[\frac{i}{2}\varphi(\boldsymbol{r})]\,\sin\frac{\theta(\boldsymbol{r})}{2} & \exp[-\frac{i}{2}\varphi(\boldsymbol{r})]\,\cos\frac{\theta(\boldsymbol{r})}{2} \end{pmatrix} . \tag{269}$$

The above considerations on the magnetic interaction energy starting with the expression (242) carry over to the spin momentum

$$\langle S_z \rangle = \frac{\hbar}{2} \int \left[ |a|^2 \, |\psi_\uparrow(\boldsymbol{r})|^2 - |b|^2 \, |\psi_\downarrow(\boldsymbol{r})|^2 \right] \, d^3r \, . \tag{270}$$

The symbol $S_z$ refers to the effective spin moment in the $z$-direction with respect to which the functions $\psi_{\uparrow(\downarrow)}(\boldsymbol{r})$ have been defined. By analogy with (259) this expression can be compactified by introducing

$$\underline{\underline{S}}_z = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{271}$$

so that

$$\langle S_z \rangle = \int \underline{\psi}^+(\boldsymbol{r}) \, \underline{\underline{S}}_z \, \underline{\psi}(\boldsymbol{r}) \, d^3r \, . \tag{272}$$

In anticipation of Section 31 we have already introduced the prefactor $\frac{\hbar}{2}$. In case that the functions $\psi_{\uparrow(\downarrow)}(\boldsymbol{r})$ refer to a $z'$-direction that belongs to a rotated coordinate system $x', y', z'$, we have in analogy to Eq.(260)

$$\underline{\underline{S}}_{z'} = \underline{\underline{Q}} \, \underline{\underline{S}}_z \, \underline{\underline{Q}}^+ \, .$$

If we use the analogous relations pertaining to Eqs.(261) up to (265) we may cast $\underline{\underline{S}}_{z'}$ as

$$\underline{\underline{S}}_{z'} = \frac{\hbar}{2} \left[ \hat{\alpha}_x \, \underline{\underline{\sigma}}_x + \hat{\alpha}_y \, \underline{\underline{\sigma}}_y + \hat{\alpha}_z \, \underline{\underline{\sigma}}_z \right] \tag{273}$$

with $\hat{\alpha}_x, \hat{\alpha}_y, \hat{\alpha}_z$ denoting the component of the unit vector $\boldsymbol{e}_{z'}$ in the $z'$-direction

$$\begin{aligned} \hat{\alpha}_x &= \cos\varphi \, \sin\theta \\ \hat{\alpha}_y &= \sin\varphi \, \sin\theta \\ \hat{\alpha}_z &= \cos\theta \, . \end{aligned}$$

It is convenient to introduce a vector $\vec{S}$ (commonly referred to as "spin operator"), which is analogous to $\vec{\sigma}$, by setting

$$\vec{S} = \frac{\hbar}{2} \, \vec{\sigma} \, . \tag{274}$$

Eq.(273) may then be cast

$$\underline{\underline{S}}_{z'} = \boldsymbol{e}_{z'} \cdot \vec{S}\,,$$

and hence we have

$$\langle S_{z'} \rangle = \int \underline{\psi}^{+}(\boldsymbol{r})\, \underline{\underline{S}}_{z'}\, \underline{\psi}(\boldsymbol{r})\, d^3r = \boldsymbol{e}_{z'} \cdot \langle \vec{S} \rangle$$

where

$$\langle \vec{S} \rangle = \int \underline{\psi}^{+}(\boldsymbol{r})\, \vec{S}\, \underline{\psi}(\boldsymbol{r})\, d^3r\,. \tag{275}$$

If $\underline{\psi}(\boldsymbol{r},t)$ has the form (268), Eq.(275) yields $\langle \vec{S} \rangle = \pm\frac{\hbar}{2}\,\boldsymbol{e}_z$. On the other hand, if $\underline{\psi}(\boldsymbol{r},t)$ possesses two non-vanishing components, there will always be a coordinate system that is rotated with respect to the present one, in which $\langle \vec{S} \rangle$ becomes $\pm\frac{\hbar}{2}\,\boldsymbol{e}_{z'}$. One only has to turn the pertinent $z'$-axis in the plane spanned by the original direction of $\langle \vec{S} \rangle$ and the original $z$-axis until $\boldsymbol{e}_{z'}$ is parallel or anti-parallel to $\langle \vec{S} \rangle$.

## 31 Spin precession in a magnetic field

Commonly one assumes the magnetic field and the spin direction to be collinear. As an example for a non-collinear situation we consider an electron that is bound within an atom where it is initially exposed to a magnetic field along some direction. We omit here discussing the details of its spin alignment due to some minute time dependent perturbations and simply assume that it has eventually attained a stationary spinor state in which its spin momentum points parallel or anti-parallel to the direction of the magnetic field. If one now changes non-adiabatically the direction (and in general inevitably also the magnitude) of the magnetic field, the spin momentum can - without an appropriate external torque - not adjust to the new field direction, and hence the previously existing collinearity no longer obtains. As we shall show by discussing the pertinent solution to the time-dependent Pauli equation (266), the spin momentum now precesses about the new direction of the magnetic field in a completely classical way.
We equate the initial direction of the magnetic field with the $z'$-axis of a "primed" coordinate system in which the spin-aligned state of the electron has the form

$$\underline{\psi}'(\boldsymbol{r}') = \psi_0'(\boldsymbol{r}') \begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{276}$$

where $\psi_0'(\boldsymbol{r}')$ is the energetically lowest lying solution to the Schrödinger equation of the one-particle system under study. We denote this solution by

$\psi_0(\boldsymbol{r})$ in the unprimed coordinate system in which the new magnetic field lies along the $z$-direction and in which the spinor (276) can be cast as

$$\underline{\psi}(\boldsymbol{r}) = \underline{\underline{Q}}^{+}\,\underline{\psi}'(\boldsymbol{r}') = \underbrace{\psi_0(\boldsymbol{r})\,e^{-i\frac{\varphi}{2}}\,\cos\frac{\theta}{2}\begin{pmatrix}1\\0\end{pmatrix}}_{=\underline{\psi}_{0\uparrow}(\boldsymbol{r})} + \underbrace{\psi_0(\boldsymbol{r})\,e^{i\frac{\varphi}{2}}\,\sin\frac{\theta}{2}\begin{pmatrix}0\\1\end{pmatrix}}_{=\underline{\psi}_{0\downarrow}(\boldsymbol{r})}, \quad (277)$$

where $\theta, \varphi, \psi(=0)$ are the Euler angles that refer to the interrelation $(x', y', z') \rightarrow (x, y, z)$). Hence we have

$$\underline{\psi}(\boldsymbol{r}) = \underline{\psi}_{0\uparrow}(\boldsymbol{r}) + \underline{\psi}_{0\downarrow}(\boldsymbol{r})\,. \quad (278)$$

Note that the unit spinors in Eq.(277) are now referenced to the new $z$-axis! We now consider the Pauli equation (266)

$$i\hbar\,\frac{\partial}{\partial t}\,\underline{\psi}(\boldsymbol{r},t) = \left[\widehat{H}_0 + V(\boldsymbol{r}) + \mu_B\,\underline{\underline{\sigma}}_z\,B_z\right]\underline{\psi}(\boldsymbol{r},t)$$

for the time-independent case and in the absence of a magnetic field in which case $\underline{\psi}_{0\uparrow(\downarrow)}(\boldsymbol{r})$ are independent degenerate solutions and $\psi_0(\boldsymbol{r})$ satisfies the associated Schrödinger equation

$$\widehat{H}_0(\boldsymbol{r})\,\psi_0(\boldsymbol{r}) = E_0\,\psi_0(\boldsymbol{r})\,.$$

For $B_z \neq 0$ the two spinors belong to different energies $E_{0\uparrow(\downarrow)} = E_0 \pm \mu_B\,B_z$ and their sum does not satisfy the time-independent Pauli equation any more. However

$$\underline{\psi}(\boldsymbol{r},t) = \underline{\psi}_{0\uparrow}(\boldsymbol{r})\,e^{-\frac{i}{\hbar}E_{0\uparrow}\,t} + \underline{\psi}_{0\downarrow}(\boldsymbol{r})\,e^{-\frac{i}{\hbar}E_{0\downarrow}\,t} \quad (279)$$

solves the above time-dependent Pauli equation if we disregard effects of second and higher order in the magnetic field which arise from the appearance of $\boldsymbol{A}(\boldsymbol{r})$ in $\widehat{H}_0$ (s. Eq.(244)). We now insert the definitions of $\underline{\psi}_{0\uparrow(\downarrow)}(\boldsymbol{r})$ defined in (277) and obtain

$$\underline{\psi}(\boldsymbol{r},t) = \psi_0(\boldsymbol{r})\,\left[e^{-i\frac{(\varphi-\omega_L\,t)}{2}}\,\cos\frac{\theta}{2}\begin{pmatrix}1\\0\end{pmatrix} + e^{i\frac{(\varphi-\omega_L\,t)}{2}}\,\sin\frac{\theta}{2}\begin{pmatrix}0\\1\end{pmatrix}\right]e^{-\frac{i}{\hbar}E_0\,t}. \quad (280)$$

Here we have made use of $E_{0\uparrow(\downarrow)} = E_0 \pm \mu_B\,B_z$ and introduced the frequency $\omega_L$ which is defined through

$$E_{0\uparrow} - E_{0\downarrow} = 2\,\mu_B B_z = \hbar\omega_L\,. \quad (281)$$

The spin-vector $\vec{S}$ had been defined as

$$\vec{S} = \frac{\hbar}{2}\,\vec{\sigma}\,, \quad (282)$$

where $\vec{\sigma}$ is short-hand for the three matrices

$$\underline{\underline{\sigma}}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \underline{\underline{\sigma}}_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \underline{\underline{\sigma}}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} .$$

We pause here for a moment and recall that the prefactor $\frac{\hbar}{2}$ has not yet been justified. But it is clear from its physical meaning and its physical dimension that the expectation value of $\vec{S}$ will definitely be proportional to $\hbar$. For that reason we rewrite Eq.(282) alternatively, introducing a scalar dimensionless factor $a$

$$\vec{S} = a\,\hbar\,\vec{\sigma}\,, \tag{283}$$

to which we shall come back below.
If one forms the expectation value of $\vec{S}$ using (280) one obtains

$$\begin{aligned} \langle \vec{S} \rangle &= \int \underline{\psi}^+(\boldsymbol{r},t)\,\vec{S}\,\underline{\psi}(\boldsymbol{r},t)\,d^3r = \\ &= \frac{\hbar}{2}\left[\cos(\varphi-\omega_L t)\,\sin\theta\,\boldsymbol{e}_x + \sin(\varphi-\omega_L t)\,\sin\theta\,\boldsymbol{e}_y + \cos\theta\,\boldsymbol{e}_z\right] . \end{aligned} \tag{284}$$

Thus, the vector $\langle \vec{S} \rangle$ of the spin momentum moves on a circular cone with an apex angle of $2\,\theta$ about the direction of the magnetic field and its projection onto the $x/y$-plane rotates at an angular frequency $\omega_L$, the "Larmor frequency", about the $z$-axis. According to Eq.(281) this frequency is given by

$$\omega_L = \frac{\mu_B B_z}{\hbar/2}\,. \tag{285}$$

The spin precession is completely analogous to that of a classical spinning

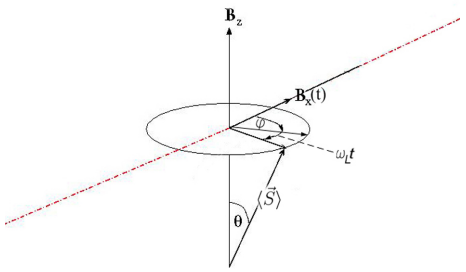


Figure 14: Quantum mechanical spin precession in a magnetic field

top which rotates about its symmetry axis at an angular frequency $\omega$ and

is exposed to the gravitational field of the earth. The precession frequency $\omega_P$ is in this case given by

$$\omega_P = \frac{F\, r_s}{L}\,,$$

where $L$ denotes the absolute value of the angular momentum, $F$ is the absolute value of the gravitational force acting on the top's center of mass, and $r_s$ is the distance of the center of mass from the point of support. In other words, $F\, r_s$ corresponds to $\mu_B B_z$ for the precessing spin momentum. If one would define $\vec{S}$ by Eq.(283) rather than by Eq.(282), one would have instead of Eq.(285)

$$\omega_L = \frac{\mu_B B_z}{a\hbar}$$

where $a\hbar$ has to be interpreted as the angular spin momentum because of the equivalence of classical and spin precession just revealed. Because of Eq.(281 )we have $\hbar\,\omega_L = 2\,\mu_B B_z$, and hence the above equation yields

$$a = \frac{1}{2} \quad \text{and therefore} \quad \vec{S} = \frac{\hbar}{2}\vec{\sigma}\,. \tag{286}$$

The completely classical behavior of a precessing spin moment in a magnetic field can also be made evident by the following consideration.
Using Eqs.(234) and (284) we may express the spin-derived magnetic moment $\vec{M}_{Spin}$ as

$$\vec{M}_{Spin} = \mu_B\, [\cos(\varphi - \omega_L t)\, \sin\theta\, \boldsymbol{e}_x + \sin(\varphi - \omega_L t)\, \sin\theta\, \boldsymbol{e}_y + \cos\theta\, \boldsymbol{e}_z]\,.$$

The time derivative of Eq.(284) can be written

$$\frac{d}{dt} < \vec{S} >= \mu_B\, B_z\, [\sin(\varphi - \omega_L t)\, \sin\theta\, \boldsymbol{e}_x - \cos(\varphi - \omega_L t)\, \sin\theta\, \boldsymbol{e}_y]\,, \tag{287}$$

where we have used $\omega_L = 2\mu\, B_z/\hbar$. We observe that $\boldsymbol{B} = B_z\, \boldsymbol{e}_z$ and

$$\boldsymbol{e}_x \times \boldsymbol{e}_z = -\boldsymbol{e}_y\,; \quad \boldsymbol{e}_y \times \boldsymbol{e}_z = \boldsymbol{e}_x\,; \quad \boldsymbol{e}_z \times \boldsymbol{e}_z = 0\,.$$

Hence, the right-hand side of Eq.(287) can be cast as

$$\mu_B\, B_z\, [\sin(\varphi - \omega_L t)\, \sin\theta\, \boldsymbol{e}_x - \cos(\varphi - \omega_L t)\, \sin\theta\, \boldsymbol{e}_y] = \vec{M}_{Spin} \times \boldsymbol{B}\,.$$

The result may be written

$$\frac{d}{dt} < \vec{S} >= \vec{M}_{Spin} \times \boldsymbol{B}\,. \tag{288}$$

This is identical with the classical equation of motion describing the temporal behavior of a spinning top that is acted upon by a torque $\vec{M}_{Spin} \times \boldsymbol{B}$. It corresponds to Ehrenfest's First Theorem, and it is this equation (288)

which governs the phenomena encountered in electron and nuclear spin resonance. (S. e. g. Slichter [79].) In applying magnetic resonance techniques one has to supplement Eq.(288) by perturbational terms that cause a change of the precession cone. An equation of this kind was put forward by Bloch [80] in 1945. If the atom is not exposed to a time-dependent perturbation the spin keeps precessing on the cone without changing its apex angle even when the strength of the magnetic field adiabatically increases or decreases. A change of the absolute value of $\boldsymbol{B}$ only changes the Larmor frequency $\omega_L$. However, as with the magnetic spin resonance, the apex angle changes continuously when one applies a small time-dependent magnet field across the strong stationary field $\boldsymbol{B} = B_z\,\boldsymbol{e}_z$ and when this smaller field oscillates at the angular frequency $\omega_L$. This will be outlined in the following section.

Spin precession in a magnetic field exhibits a peculiar feature that relates to the occurrence of the argument $\frac{\varphi}{2}$ in the exponential functions of Eq.(277). To see that we assume $\underline{\psi}(\boldsymbol{r})$ to represent a wavepacket of a free particle that traverses a homogeneous magnetic field in an orthogonal direction. When the wavepacket enters the magnetic field the spin component perpendicular to the field may point in the x-direction which is also the direction of flight. We then have

$$\varphi = 0 \quad \text{and hence} \quad e^{\pm i\,\frac{\varphi}{2}} = 1\,.$$

During the flight $\theta$ stays constant. When the wavepacket leaves the magnetic field after a full precession period we have

$$\varphi = 2\pi \quad \text{which means} \quad e^{\pm i\,\frac{\varphi}{2}} = -1\,.$$

Hence $\underline{\psi}(\boldsymbol{r})$ has changed its sign, or one may just as well say, its phase has been shifted by $\pi$. However, as can be seen from Eq.(284), $\langle\vec{S}\rangle$ points in the same direction as at the beginning of the precession. This phase shift is well detectable in double-beam experiments with spin-polarized neutrons (s. e. g. Rauch [81], Werner et al. [82]).

## 32 Magnetic spin resonance

A so-called magnetic spin resonance occurs when one applies a considerably smaller magnetic field, e. g. $B_x(t)$ in the $x$-direction. If this field oscillates at an angular frequency $\omega_L$ the precession cone widens or shrinks continuously depending on the relation between the phase of the oscillation and the position of the spin.
In the following we use a short-hand notation for the "precessing spinor" (280) :

$$\underline{\psi}(\boldsymbol{r},t) = \psi_0(\boldsymbol{r})\,\left[e^{-i\frac{(\varphi-\omega_L\,t)}{2}}\,c_\uparrow\,\underline{\chi}_\uparrow + e^{i\frac{(\varphi-\omega_L\,t)}{2}}\,c_\downarrow\,\underline{\chi}_\downarrow\right]e^{-\frac{i}{\hbar}E_0\,t} \tag{289}$$

where

$$|c_\uparrow|^2 + |c_\downarrow|^2 = 1 \quad \text{and} \quad \underline{\chi}_\uparrow = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \; ; \; \underline{\chi}_\uparrow^\dagger = (1\;0) \quad \underline{\chi}_\downarrow = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \; ; \; \underline{\chi}_\downarrow^\dagger = (0\;1)\,.$$

If $c_\uparrow$ and $c_\downarrow$ are time-independent constants the spinor (289) fulfills the time-dependent Pauli equation (266)

$$i\hbar \frac{\partial}{\partial t} \underline{\psi}(\boldsymbol{r}, t) = \left[ \widehat{H}_0 + V(\boldsymbol{r}) + \mu_B \underline{\underline{\sigma}}_z \, B_z \right] \underline{\psi}(\boldsymbol{r}, t)$$

in the presence of a magnetic field $B_z$ in the $z$-direction.
As will immediately become apparent, the perturbed Pauli equation

$$i\hbar \frac{\partial}{\partial t} \underline{\psi}(\boldsymbol{r}, t) = \left[ \widehat{H}_0 + V(\boldsymbol{r}) + \mu_B \underline{\underline{\sigma}}_z \, B_z + \mu_B \underline{\underline{\sigma}}_x \, B_x(t) \right] \underline{\psi}(\boldsymbol{r}, t) \qquad (290)$$

is satisfied if one allows the coefficients $c_\uparrow$ and $c_\downarrow$ in (289) to become time-dependent. Inserting (289) thus modified into Eq(290) one can cast the result as

$$\begin{aligned} & e^{-i\frac{(\varphi-\omega_L\,t)}{2}} \, i\hbar\,\dot{c}_\uparrow \, \underline{\chi}_\uparrow + e^{i\frac{(\varphi-\omega_L\,t)}{2}} \, i\hbar\,\dot{c}_\downarrow \, \underline{\chi}_\downarrow = \\ & \quad \mu_B \, B_x(t) \, e^{i\frac{(\varphi-\omega_L\,t)}{2}} \, c_\downarrow \, \underline{\chi}_\uparrow + \mu_B \, B_x(t) \, e^{-i\frac{(\varphi-\omega_L\,t)}{2}} \, c_\uparrow \, \underline{\chi}_\downarrow \,. \end{aligned}$$

Multiplying this equation by $c_\uparrow \, e^{i\frac{(\varphi-\omega_L\,t)}{2}} \, \underline{\chi}_\uparrow^\dagger$ from the left one obtains

$$i\hbar \, c_\uparrow \, \dot{c}_\uparrow = e^{i(\varphi-\omega_L\,t)} \, c_\uparrow \, c_\downarrow \, \mu_B \, B_x(t)\,.$$

Subtraction of the complex-conjugate of this equation yields

$$\frac{\partial}{\partial t} c_\uparrow^2 = c_\uparrow(t) \, c_\downarrow(t) \, \frac{2\mu_B}{\hbar} \, B_x(t) \, \sin(\varphi - \omega_L\,t)\,. \qquad (291)$$

Likewise, one gets

$$\frac{\partial}{\partial t} c_\downarrow^2 = -c_\downarrow(t) \, c_\uparrow(t) \, \frac{2\mu_B}{\hbar} \, B_x(t) \, \sin(\varphi - \omega_L\,t)\,,$$

thus

$$\frac{\partial}{\partial t} \left[ c_\uparrow^2 + c_\downarrow^2 \right] \equiv 0\,,$$

as has to be required.
If one observes

$$B_x(t) = B_{x\,0} \, \cos\omega_l\,t$$

and

$$\sin(\varphi - \omega_L\,t) = \sin\varphi \, \cos(\omega_L\,t) - \cos\varphi \, \sin(\omega_L\,t)$$

Eq.(291) takes the form

$$\frac{\partial}{\partial t}c_\uparrow^2 = c_\uparrow(t)\,c_\downarrow(t)\,\underbrace{\frac{2\mu_B}{\hbar}\,B_{x0}}_{=\omega_L\,q}\,\left[\sin\varphi\,\cos^2(\omega_L\,t) - \cos\varphi\,\cos(\omega_L\,t)\,\sin(\omega_L\,t)\right] \quad (292)$$

where

$$q \stackrel{def}{=} \frac{B_{x0}}{B_z}$$

has been introduced for brevity.
As $q = \frac{B_{x0}}{B_z}$ is presupposed to be very small compared to unity, the time average of this equation over one precession period does not sizably affect the time dependence of $c_\uparrow(t)$ and thus of $c_\downarrow(t)$ as well. Performing this averaging and omitting to denote the small effect on $c_{\uparrow(\downarrow)}(t)$ explicitly one obtains

$$\frac{\partial}{\partial t}c_\uparrow^2 = c_\uparrow(t)\,c_\downarrow(t)\,\omega_L\,\frac{q}{2}\,\sin\varphi\,.$$

Here $\varphi$ represents the azimuth position of $\langle\vec{S}\rangle$ when $B_x(t)$ has reached its maximum. In view of Eq.(280) we make an educated guess on the solution of this equation by setting

$$c_\uparrow(t) = \cos\frac{\theta(t)}{2}\,; \quad c_\downarrow(t) = \sin\frac{\theta(t)}{2} \;\hookrightarrow\; \quad c_\uparrow^2(t) + c_\downarrow^2(t) = 1$$
$$\frac{\partial}{\partial t}\cos^2\frac{\theta(t)}{2} = \cos\frac{\theta(t)}{2}\sin\frac{\theta(t)}{2}\,\dot{\theta}\,.$$

We thus arrive at

$$\dot{\theta} = \omega_L\,\frac{q}{2}\,\sin\varphi\,; \qquad \theta = [\omega_L\,\tfrac{q}{2}\,\sin\varphi]\,t\,.$$

That means that depending on $\sin\varphi$ the apex angle $2\,\theta$ widens or shrinks linearly in time and proportional to the amplitude of the perturbing magnetic field $B_x(t)$. This is exactly the behavior of a classical spinning top.
As opposed to the impression that is commonly invited by even the most recent literature, Eqs.(280, (288) and (292) constitute purely quantum mechanical results and they are in no way "semi-classical" or "macroscopical". The fact that from our derivation $\langle\vec{S}\rangle_z$ may lie anywhere between $+\frac{\hbar}{2}\vec{e}_z$ and $-\frac{\hbar}{2}\vec{e}_z$, seems to contradict the principle of "orientation quantization" according to which $\langle\vec{S}\rangle_z$ may only be equal to $\pm\frac{\hbar}{2}\vec{e}_z$. Clearly, if $\langle\vec{S}\rangle$ is not parallel or anti-parallel to $\boldsymbol{B}$ but rather precesses about the direction of the latter, the electron emits magnetic dipole radiation until its spin is aligned. But this is a weak electromagnetic interaction, and therefore the state of non-alignment may well be regarded as meta-stable in certain experimental situations. This is exploited in spin-echo experiments where one starts with an ensemble of (nuclear) spins which, in the beginning, are all aligned along the $z$-direction of the magnetic field. As discussed above, these spins

are then additionally exposed to a weaker oscillating magnetic field in the $x$-direction for a certain time $T$ such that $\dot{\theta}\,T = \frac{\pi}{2}$. As $T$ is long compared to the precession time, this way of applying an oscillating magnetic field is commonly referred to as subjecting the spin system to a "rectangular $\frac{\pi}{2}$ puls of frequency $\omega_L$". After the puls has been applied all spins precess in a plane perpendicular to the $B_z\,\boldsymbol{e}_z$ This is the situation alluded to above: The spins are no longer in one of their Zeeman eigenstates, but rather in a metastable state of an enormous life time if it were not for dissipative processes caused by the environment. Further, when the spin precesses in a plane perpendicular to the magnetic field, it has only absorbed the energy $\mu_B\,B_z$, that is $\frac{\hbar\omega_L}{2}$. That fraction is even less, when one cuts the oscillating magnetic field off some time earlier. For that reason, any attempt to bring spin resonance phenomena and the absorption of photons (coming from the oscillating magnet) in a meaningful physical relation is doomed to fail.
As for the spin-echo effect, one first realizes that the directions of the spins fan apart once they start precessing in that plane perpendicular to $B_z\,\boldsymbol{e}_z$. This is due to the unavoidable inhomogeneities of the magnetic field. If one now applies a rectangular $\pi$-puls the spins spiral down until they have reached anti-parallel orientation with respect to $B_z\,\boldsymbol{e}_z$ and, further, spiral up until they precess again in the plane perpendicular to $z$. But this time the "slow spins" are in front of the faster ones in the group of spins all of which are precessing in the same direction. Hence, after some time the faster ones have caught up and the group is closer together again which can be detected as an "echo" by an electromagnetic pick-up coil.

## 33 A theory of the Stern-Gerlach experiment

*"...Phenomena of this kind made physicists despair of finding any consistent space-time picture of what goes on the atomic and subatomic scale...many came to hold not only that it is difficult to find a coherent picture but that it is wrong to look for one..."*

John Bell [83]

Quite a few attempts have already been made on a theory of the Stern-Gerlach (SG-) experiment [84]. For a recent rather complete update of the pertinent literature see Home et al.[85]. But a coherent picture of the fundamental mechanism is still missing. Most physicists seem to favor the idea that the electronic state of the atom on entering the magnet constitutes a linear combination of spin states "up" and "down", and the modulus square of the associated coefficients defines the probability of the atom for either being pulled up or down, that is, parallel or anti-parallel to the magnetic field gradient. On detection of the atom in the "up"- or "down"-beam the atomic wave function collapses onto the respective component of the linear combination. From our point of view this is unjustifiably associating the

process of detection with some mystical influence of "observing", based on pure claim: the atomic beam would behave differently if it would not be detected. In the standard literature this experiment is even elevated to represent the prime example of measurement in quantum mechanics.
By contrast, we believe that the outcome of the experiment is completely determined by the time-dependent Pauli equation and is hence a result of a "quantum mechanics without observer".
Our approach implies a linear combination of spin states as well, that is, we describe the electronic 1s-state of the atom that we shall consider below by

$$\underline{\psi}_{atom}(\boldsymbol{r},t) = \psi_{1s}(\boldsymbol{r}-\boldsymbol{v}\,t)\left[a_\uparrow \begin{pmatrix}1\\0\end{pmatrix} + a_\downarrow \begin{pmatrix}0\\1\end{pmatrix}\right]$$

where $\boldsymbol{v}$ denotes the velocity of the atom, and the coefficients $a_\uparrow, a_\downarrow$ have the property $|a_\uparrow|^2+|a_\downarrow|^2=1$. The unit spinors are referenced to the direction of the field gradient $\frac{\partial B_z}{\partial z}\,\boldsymbol{e}_z$. Hence, the expectation value of the force acting on the atom in the SG-magnet is given by Eq.(249) if we neglect the induction derived term and assume electrostatic forces being absent

$$\langle \boldsymbol{F}_{atom}\rangle = \mu_B \int \underline{\psi}^\dagger_{atom}(\boldsymbol{r},t)\,\frac{\partial B_z}{\partial z}\,\underline{\psi}_{atom}(\boldsymbol{r},t)\,d^3r\,\boldsymbol{e}_z\,.$$

For simplicity we equate the field gradient to a constant so that $\langle \boldsymbol{F}_{atom}\rangle$ reduces to

$$\langle \boldsymbol{F}_{atom}\rangle = \mu_B\,\frac{\partial B_z}{\partial z}\,[|a_\uparrow|^2-|a_\downarrow|^2]\,\boldsymbol{e}_z\,.$$

It can obviously attain any value between $-\mu_B\,\frac{\partial B_z}{\partial z}\,\boldsymbol{e}_z$ and $+\mu_B\,\frac{\partial B_z}{\partial z}\,\boldsymbol{e}_z$ depending on the value of the coefficients when the atom enters the magnet. Therefore a splitting into two well separated beams cannot possibly occur as long as there is no particular mechanism which inhibits a random distribution. In the following we shall outline such a possible mechanism.
We assume that the reader is sufficiently familiar with the essential features of the experimental setup. To simplify the line of argument we content ourselves with considering the experiment by Wrede [86] who used a primary beam of hydrogen atoms in a setup that was practically identical with that of Stern and Gerlach. Hydrogen offers the advantage of reducing the spin-orientation problem to that of a single electron. The standpoint we take here is akin to that of Mott and Massey [87] who remark: *"From these arguments we must conclude that it is meaningless to assign to the free electron a magnetic moment. It is a property of the electron that when it is bound in an S state in an atom, the atom has a magnetic moment."*[7]
The hydrogen atoms effuse from some source where they are (almost unavoidably) exposed to the terrestrial magnetic field or at least to the weak

[7]However, we want to modify this debatable statement by saying that also free electrons display a magnetic moment when they are exposed to a magnetic field where their motion perpendicular to the field becomes confined to a circular area of a certain diameter.

fringe field of the SG-magnet. That field causes a weak Zeeman-splitting of the spin up and spin down level of the electronic 1s-state. Because of the weakness of the splitting the two Zeeman-levels are at the temperature of the source equally occupied, that is, 50% of the effusing atoms have their electronic spins oriented parallel to the weak external field, the spins of the remaining 50% atoms are anti-parallel. As the atoms approach the SG-magnet they feel in a co-moving coordinate system a magnetic field whose field strength increases continuously and will in general change its direction. We assume for simplicity that the spin orientation is transverse and that the atom moves along the $x$-axis of a laboratory-fixed coordinate system so that changes of the spin orientation will only take place in the $y/z$-plane parallel to the respective plane of the co-moving coordinate system. As soon as the field direction in the co-moving coordinate system departs by a small angle $\delta\theta$ from the original direction of $\vec{B} = B_z\,\boldsymbol{e}_z$ at the onset of the atom's trajectory, a small $y$-component $\vec{B_y} = B_z\,\sin\delta\theta\,\boldsymbol{e}_y$ of the field appears as a consequence of which the magnetic moment of the atom experiences a torque $-\mu_B\,B_z\,\sin\delta\theta\,\boldsymbol{e}_\varphi$, where $\boldsymbol{e}_\varphi$ denotes the unit vector in the direction of increasing azimuth angle $\varphi$ in the $x/y$-plane. This torque causes a change $\dot{\boldsymbol{L}}$ of the spin angular momentum

$$\dot{\boldsymbol{L}} = -\frac{\hbar}{2}\,\sin\delta\theta\,\omega_L\,\boldsymbol{e}_\varphi\,,$$

where we have used $2\mu_B\,B_z = \hbar\,\omega_L$ (Eq.(281)). Hence, the spin momentum starts precessing about the new direction of the magnetic field. We ignore the slight tilt of the co-moving new $x/y$-plane perpendicular the new field direction.
We envisage a short time span for which we assume the changes of $\theta$ to be small so that

$$\sin\delta\theta \approx \delta\theta = \dot{\theta}\,t\,, \tag{293}$$

where $t = 0$ coincides with the beginning of the rotation of the field. The following considerations exploit the typical experimental condition that the precession frequency $\omega_L$ is some orders of magnitude larger than the speed of the field rotation. (In the terrestrial magnetic field of magnitude $\approx 5{\cdot}10^{-5}\,T$ the precession frequency of the electronic spin is about $10^6\,s^{-1}$. At an atomic speed of $10^5\mathrm{cm\,s}^{-1}$, a distance of about 10 cm and a maximum rotation angle of $\pi/2$ one has $\dot{\theta}\ \approx 10^4\,\mathrm{s}^{-1}$.) As will become apparent from the following calculations we may limit ourselves to a short time span comprising only few precession periods during which the magnetic field rotates only by a small angle ($\theta \ll 2\pi$) so that one is justified in assuming $\dot{\theta}$ to be constant:

$$\dot{\theta} = const.$$

The unit vector $\boldsymbol{e}_\varphi$ may be decomposed

$$\boldsymbol{e}_\varphi = -\boldsymbol{e}_x\,\sin\varphi + \boldsymbol{e}_y\,\cos\varphi\,. \tag{294}$$

At $t = 0$ we have $\varphi(t = 0) = -\frac{\pi}{2}$, that is $\boldsymbol{e}_\varphi = \boldsymbol{e}_x$. Thus, it is advisable to replace $\varphi$ with $\varphi + \frac{\pi}{2}$, but we omit denoting the new azimuth angle differently. Hence we have $\varphi = 0$ for $t = 0$, and we obtain instead of Eq.(294)

$$\boldsymbol{e}_\varphi = \boldsymbol{e}_x \, \cos\varphi + \boldsymbol{e}_y \, \sin\varphi \, .$$

The spin precession that now occurs is anti-clockwise

$$\dot{\varphi} = -\omega_L \quad \text{that is} \quad \varphi = -\omega_L \, t \, .$$

Thus

$$\dot{\boldsymbol{L}} = \frac{\hbar}{2} \, \dot{\theta} \, \omega_L \, \left[ \boldsymbol{e}_x \, t \, \cos\omega_L \, t - \boldsymbol{e}_y \, t \, \sin\omega_L \, t \right] \, .$$

This results in a change of the angular momentum after one precession period $T = 2\pi/\omega_L$

$$\Delta\boldsymbol{L} = \frac{\hbar}{2} \, \dot{\theta} \, \left[ \omega_L \, \boldsymbol{e}_x \, \int_0^T t \, \cos\omega_L \, t \, dt - \, \boldsymbol{e}_y \, \omega_L \, \int_0^T t \, \sin\omega_L \, t \, dt \right] \, .$$

Hence, using

$$\int_0^{2\pi} \xi \, \sin\xi \, d\xi = -2\pi \quad \text{and} \quad \int_0^{2\pi} \xi \, \cos\xi \, d\xi = 0 \, ,$$

we may $\Delta\boldsymbol{L}(T)$ cast as

$$\Delta\boldsymbol{L}(T) = \frac{\hbar}{2} \, \underbrace{\dot{\theta} \, T}_{\equiv \Delta\theta} \, \boldsymbol{e}_y$$

that is in the spirit of our approximation (293)

$$\Delta\boldsymbol{L}(T) = \frac{\hbar}{2} \, \sin\Delta\theta \, \boldsymbol{e}_y \, .$$

The $y$-component of the magnetic field which equaled zero at the beginning of the rotation is now given by $\vec{B}_y = B_z \, \sin\Delta\theta \, \boldsymbol{e}_y$. That means: after one precession period $T$ the magnetic field and the atomic spin angular momentum have turned by the same angle $\Delta\theta$. The spin orientation follows the magnetic field - within the present approximation - without slip, that is adiabatically. (This is similar to the physics of a spinning artillery shell whose spin axis follows the course of the shell's bending trajectory leaving only a small precession angle.) Thus, the atoms enter the SG-magnet (almost) fully oriented with respect to the SG-magnetic field. This applies to the atoms with anti-parallel spin orientation accordingly. Hence, the two beams leaving the SG-magnet reflect merely the two kinds of atoms associated with the two Zeeman levels before they leave the reservoir.
It is worth mentioning that Leu [88] carried out Stern-Gerlach-type experiments using beams of Na-, K-, Zn-, Cd- and Tl-atoms instead of Ag-atoms.

The Zn- and Cd-atoms possess two s-valence electrons which results in a zero net spin momentum of the atoms and consequently one does not observe a beam splitting in the Stern-Gerlach magnet. On the other hand, Tl-atoms possess a 6p-valence electron that is subjected to spin-orbit coupling. This gives rise to a Landé factor $g = \frac{2}{3}$ as a result of which the effective magnetic moment is for $M_j = \frac{1}{2}$ given by

$$\mu_{eff} = \mu_B \, g \, M_j = \frac{1}{3} \, \mu_B \, .$$

This is, in fact, confirmed by the experiments.
If one were dealing with atoms that possess a total angular momenta $J = (l \pm \frac{1}{2}) \, \hbar$ associated with $2l + 2$ different magnetic quantum numbers $M_j$, one would have $2l + 2$ different states in the initial weak field and therefore as many different sorts of atoms entering the Stern-Gerlach magnet where they are deflected according to their magmetic moment. That means one would have $2l + 2$ different beams instead of 2.
Our explanation of the SG-experiment is much in the spirit of Stern's conjecture that the spin of an atom follows adiabatically the directional change of the magnetic field within a co-moving coordinate system from the starting point where the atomic spin has originally been aligned. In cooperation with Phipps [89] he devised an experiment where one of the beams at the exit of a first SG-magnet was focused into a linear array of three successive magnets whose weaker, essentially homogeneous fields pointed in three different directions perpendicular to the atomic trajectory. The difference between these directions was 120°. If the spin of the selected beam was pointing up after leaving the first SG-magnet and assuming that the spin would adiabatically adjust to the local magnetic field on its passage through the three magnets, it was thus to be expected that it would be finally back to its previous "up"-orientation. To test this the beam was sent into a second SG-magnet identically oriented as the first. There was only one beam coming out of this magnet indicating that the spin was pointing again in the same direction as on entering the three "turn magnets". In other words: even after a turn of 360° no slip between spin orientation and the direction of the magnetic field had occurred. We mention here only in passing that our result on the Phipps-Stern experiment agrees with that of Rosen and Zener [90] published already in 1932. Different from our more summary analysis these authors attempt to stay close to explicitly solving the time-dependent Pauli equation.
Surprisingly, the interpretation of the SG-experiment as demonstrating a coherent splitting of the de Broglie-wave of the incoming atom into two beams has become the most popular view on which a host of considerations on "measurement" is based. Proponents of this view argue that the forked de Broglie-wave collapses onto one of the two detector sites when either the "up" or "down"-detector of the SG-setup has monitored the atom

("performed the measurement on it"). Papers on the so-called "Humpty-Dumpty-problem" (s. e. g. Englert et al. [91]) deal explicitly with a possible reconstruction of the original single wave by appropriately merging the two coherent beams within some space reached later. We believe that such thought experiments are without substance. As we have clearly demonstrated, the SG-magnet does not cause a splitting of the incoming matter wave. The SG-situation is distinctly different from that in neutron spin-flip experiments by Rauch and coworkers [92] where a transverse spin polarized beam of neutrons hits a plate of a Si single crystal such that each matter wave packet splits up into two widely separated beams of packets due to dynamical diffraction within the crystal. This diffraction process is spin-independent. The two beams are coherently merged then by dynamical diffraction at a second Si-plate.

Many authors give the impression as if it would be beyond all question that Stern-Gerlach experiments with charged free particles (like electrons) are just as feasible as with spin-carrying neutral atoms. Bohr had very early pointed out (s. Wheeler and Zurek [93]) that such experiments could not possibly succeed because "the Lorentz force would inevitably blur any Stern-Gerlach pattern". Nevertheless, the literature on EPRB- (Einstein-Podolsky-Rosen-Bohm) correlation with pairs of fermions in a singlet state (s. e. g. Einstein et al. [54], Bohm [55]) abounds with allusions to "measuring separately the $x/y/z$-spin components" of the particles by means of Stern-Gerlach magnets. (S. e. g. Wigner [98].) Even when one were dealing with neutral fermions what kind of mechanism should yield such information on those spin **components**? How would the time evolution of the respective solution to the time-dependent Pauli equation look like in this case?

## 34 The time-dependent Dirac equation

In extending the theory to relativistic systems we retain the following two fundamental assumptions which characterize the non-relativistic quantum mechanics we have been dealing with so far:

1. The universal existence of stochastic forces that necessitate an ensemble description of the one-particle system under study. The fundamental constituents of this approach are: $\rho(\boldsymbol{r}, t)$ for the occurrence of the particle at $\boldsymbol{r}$ and time $t$ and $\boldsymbol{p}(\boldsymbol{r}, t)$ for the associated ensemble average of the particle momentum

2. Lumping together the two real-valued functions $\rho(\boldsymbol{r}, t)$ und $\boldsymbol{p}(\boldsymbol{r}, t)$ in the form of a complex-valued function $\psi(\boldsymbol{r}, t)$

$$\psi(\boldsymbol{r}, t) = \sqrt{\rho(\boldsymbol{r}, t)}\; e^{i\,\varphi(\boldsymbol{r}, t)} \tag{295}$$

where

$$\boldsymbol{p}(\boldsymbol{r},t) = \hbar\,\nabla\varphi(\boldsymbol{r},t)\,. \tag{296}$$

From $\psi(\boldsymbol{r},t) = |\psi(\boldsymbol{r},t)|\,e^{i\,\varphi(\boldsymbol{r},t)}$ one then obtains the momentum current density

$$\boldsymbol{j}_p(\boldsymbol{r},t) = \rho(\boldsymbol{r},t)\,\boldsymbol{p}(\boldsymbol{r},t) = \frac{1}{2}\,[\psi^*(\boldsymbol{r},t)\,\hat{\boldsymbol{p}}\,\psi(\boldsymbol{r},t) - \psi(\boldsymbol{r},t)\,\hat{\boldsymbol{p}}\,\psi^*(\boldsymbol{r},t)] \tag{297}$$

where

$$\hat{\boldsymbol{p}} \stackrel{\text{def}}{=} -i\,\hbar\,\nabla.$$

Eq.(296) implies that $\boldsymbol{p}(\boldsymbol{r},t)$ is irrotational, that is, the stochastic forces do not cause friction.
From Eq.(325) follows for the expectation value of the particle momentum

$$<\boldsymbol{p}(t)>=\int \boldsymbol{j}_p(\boldsymbol{r},t)\,d^3r = \int \psi^*(\boldsymbol{r},t)\,\hat{\boldsymbol{p}}\,\psi(\boldsymbol{r},t)\,d^3r\,. \tag{298}$$

If one replaces $\psi(\boldsymbol{r},t)$ with its Fourier integral

$$\psi(\boldsymbol{r},t) = (2\pi)^{-\frac{3}{2}}\int C(\boldsymbol{k},t)\,e^{i\,\boldsymbol{k}\cdot\boldsymbol{r}}\,d^3k\,,$$

one obtains on insertion into Eq.(326)

$$<\boldsymbol{p}(t)>=\int \psi^*(\boldsymbol{r},t)\,\hat{\boldsymbol{p}}\,\psi(\boldsymbol{r},t)\,d^3r = \int C^*(\boldsymbol{k},t)\,\hbar\,\boldsymbol{k}\,C(\boldsymbol{k},t)\,d^3k\,, \tag{299}$$

and analogously

$$\int \psi^*(\boldsymbol{r},t)\frac{\hat{\boldsymbol{p}}^2}{2\,m_0}\,\psi(\boldsymbol{r},t)\,d^3r = \int C^*(\boldsymbol{k},t)\,\frac{\hbar^2\,\boldsymbol{k}^2}{2\,m_0}\,C(\boldsymbol{k},t)\,d^3k\,. \tag{300}$$

Newton's modified second law (41) which we have derived for the non-relativistic case, contains an additional "quantum force" $\boldsymbol{F}_{QP} = -\nabla V_{QP}$ whose expectation value equals zero. As a result one arrives at Ehrenfest's two theorems.

$$<\boldsymbol{v}>=\frac{d}{dt}\;<\boldsymbol{r}>=<\nabla_{\boldsymbol{p}}E(\boldsymbol{p})> \tag{301}$$

and

$$\frac{d}{dt}<\boldsymbol{p}>=<\boldsymbol{F}>=<-\nabla V>\;. \tag{302}$$

The salient point here is that these two equations apply to the non-relativistic case, and we require them to persist unaffected in the relativistic case if the particle is assumed - as before - to perform a dissipationless motion under

stochastic extra forces.

Conversely, one can derive the time-dependent Schrödinger equation just by starting from Eqs.(329) and(330) and going along the same line of argument used in our derivation of the time-dependent Pauli equation in Section 29. In the following we shall refer to the latter. However, instead of

$$E(\boldsymbol{p}) = \frac{\boldsymbol{p}^2}{2m_0} + m_0\,c^2 + V(\boldsymbol{r})$$

we now have

$$E(\boldsymbol{p}) = \underbrace{\sqrt{\boldsymbol{p}^2\,c^2 + m_0^2\,c^4}}_{=E_{kin}+m_0\,c^2} + V(\boldsymbol{r}) \tag{303}$$

with $c$ denoting the velocity of light in vacuo.
Hence $< \nabla_{\boldsymbol{p}} E(\boldsymbol{p}) >=< \boldsymbol{v} >$ in Eq.(329) has to be dealt with differently in the relativistic case. Following Dirac [94] we construct a Fourier-transform $\underline{\underline{H}}_0(\boldsymbol{k})$ that corresponds to the sought-for energy-operator $\hat{\underline{\underline{H}}}_0$ just as $\hbar^2\,k^2/2\,m_0$ in Eq.(327) relates to the expression $\frac{\hat{\boldsymbol{p}}^2}{2\,m_0}$. If one rewrites $E_{kin}(\boldsymbol{k}) + m_0\,c^2$ in Eq.(303) in the form

$$E_{kin}(\boldsymbol{k}) + m_0\,c^2 = \hbar\,c\,\sqrt{\textstyle\sum_{\mu=0}^{3} k_\mu^2} \quad \text{where} \quad p_\mu = \hbar\,k_\mu$$

and $$k_0 = \tfrac{m_0\,c}{\hbar}$$

and replaces the right-hand side with a 4×4-matrix $\underline{\underline{H}}_0(\boldsymbol{k})$ defined by

$$\underline{\underline{H}}_0(\boldsymbol{k}) = \hbar\,c\,\sum_{\mu=0}^{3} \underline{\underline{\alpha}}_\mu\,k_\mu\,,$$

where $\underline{\underline{\alpha}}_\mu$ denotes constant dimensionless 4×4 matrices, $\underline{\underline{H}}_0(\boldsymbol{k})$ must obviously possess the property

$$\begin{aligned}
\underline{\underline{H}}_0^2(\boldsymbol{k}) &= \hbar^2\,c^2\,\sum_{\mu=0}^{3}\sum_{\mu'=0}^{3} k_\mu\,k_{\mu'}\,\delta_{\mu\mu'}\,\underline{\underline{1}} \\
&= \frac{\hbar^2\,c^2}{2}\,\sum_{\mu=0}^{3}\sum_{\mu'=0}^{3} k_\mu\,k_{\mu'}\,\left[\underline{\underline{\alpha}}_\mu\,\underline{\underline{\alpha}}_{\mu'} + \underline{\underline{\alpha}}_{\mu'}\,\underline{\underline{\alpha}}_\mu\right]\,.
\end{aligned}$$

That means that the matrices $\underline{\underline{\alpha}}_\mu$ have to comply with the requirement

$$\frac{1}{2}\,\left[\underline{\underline{\alpha}}_\mu\,\underline{\underline{\alpha}}_{\mu'} + \underline{\underline{\alpha}}_{\mu'}\,\underline{\underline{\alpha}}_\mu\right] = \delta_{\mu\mu'}\,\underline{\underline{1}}\,.$$

As can be verified by just performing the multiplications, the matrices $\underline{\underline{\alpha}}_\mu$ meet this requirement if they have the form

$$\underline{\underline{\alpha}}_0 = \begin{pmatrix} \underline{\underline{1}} & \underline{\underline{0}} \\ \underline{\underline{0}} & -\underline{\underline{1}} \end{pmatrix} \quad \text{and} \quad \underline{\underline{\alpha}}_\mu = \begin{pmatrix} \underline{\underline{0}} & \underline{\underline{\sigma}}_\mu \\ \underline{\underline{\sigma}}_\mu & \underline{\underline{0}} \end{pmatrix} \text{ for } \mu = 1,2,3\,.$$

Here $\underline{\underline{\sigma}}_\mu$ denotes 2×2-matrices which are identical with the Pauli matrices (263). Similar to the latter one can lump the 4×4-matrices $\underline{\underline{\alpha}}_\mu$ together by forming a vector $\underline{\alpha}$ so that $\underline{\underline{H}}_0(\boldsymbol{k})$ may be cast as

$$\underline{\underline{H}}_0(\boldsymbol{k}) = c\,\underline{\alpha}\cdot\hbar\boldsymbol{k} + \underline{\underline{\alpha}}_0\, m_0\, c^2\,. \tag{304}$$

The feasibility of the above line of thought requires a consistent extension of the hitherto discussed spinor function to a bispinor function

$$\underline{\psi}(\boldsymbol{r},t) = \begin{pmatrix} \psi^1_\uparrow(\boldsymbol{r},t) \\ \psi^1_\downarrow(\boldsymbol{r},t) \\ \psi^2_\uparrow(\boldsymbol{r},t) \\ \psi^2_\downarrow(\boldsymbol{r},t) \end{pmatrix} \quad \text{and} \quad \underline{\psi}^\dagger(\boldsymbol{r},t) = \big(\psi^1_\uparrow(\boldsymbol{r},t), \psi^1_\downarrow(\boldsymbol{r},t), \psi^2_\uparrow(\boldsymbol{r},t), \psi^2_\downarrow(\boldsymbol{r},t)\big)$$

where

$$\psi^{(j)}_{\uparrow(\downarrow)}(\boldsymbol{r},t) = |\psi^{(j)}_{\uparrow(\downarrow)}(\boldsymbol{r},t)|\, e^{i\varphi^{(j)}_{\uparrow(\downarrow)}(\boldsymbol{r},t)}\,, \quad j=1,2\,.$$

The associated phases $\varphi^{(j)}_{\uparrow(\downarrow)}(\boldsymbol{r},t)$ represent as in Eq.(296) potentials of ensemble averages of momenta which means

$$\boldsymbol{p}(\boldsymbol{r},t) = \sum_{\substack{j=1,2 \\ (\uparrow,\downarrow)}} \frac{|\psi^{(j)}_{\uparrow(\downarrow)}(\boldsymbol{r},t)|^2}{\rho(\boldsymbol{r},t)} \boldsymbol{p}^{(j)}_{\uparrow(\downarrow)}(\boldsymbol{r},t)$$
$$\text{where} \quad \boldsymbol{p}^{(j)}_{\uparrow(\downarrow)}(\boldsymbol{r},t) = \hbar\,\nabla\,\varphi^{(j)}_{\uparrow(\downarrow)}(\boldsymbol{r},t)\,.$$

The quantities $\boldsymbol{p}^{(j)}_{\uparrow(\downarrow)}$ are now different for "spin up" and "spin down" if the particle in question moves in a spatially varying potential. Only in the strictly non-relativistic case the spin generating component of the quivering motion and the orbital motion remain unaffected on superposition. In this case we have $\psi_{\uparrow(\downarrow)}(\boldsymbol{r},t) = |\psi_{\uparrow(\downarrow)}(\boldsymbol{r},t)|\, e^{i\,\varphi(\boldsymbol{r},t)}$.
If one performs a Fourier transform one obtains completely analogous to Eq.(327) also in the relativistic case

$$< \boldsymbol{p}(t) >= \int \underline{C}^\dagger(\boldsymbol{k},t)\,\hbar\,\boldsymbol{k}\,\underline{C}(\boldsymbol{k},t)\,d^3k\,. \tag{305}$$

Correspondingly one gets

$$\int \underline{C}^\dagger(\boldsymbol{k},t)\,\underline{\underline{H}}_0(\boldsymbol{k})\,\underline{C}(\boldsymbol{k},t)\,d^3k = \int \underline{\psi}^\dagger(\boldsymbol{r},t)\,\underbrace{[c\,\underline{\alpha}\cdot\hat{\boldsymbol{p}} + \underline{\underline{\alpha}}_0\, m_0\, c^2]}_{\stackrel{\text{def}}{=}\underline{\underline{\hat{H}}}_0}\,\underline{\psi}(\boldsymbol{r},t)\,d^3r\,.$$

We now form $< \boldsymbol{v} >$ according to

$$< \boldsymbol{v} >=< \nabla_{\boldsymbol{p}} E(\boldsymbol{p}) >= \int \underline{C}^\dagger(\boldsymbol{k},t)\,[\hbar^{-1}\,\nabla_{\boldsymbol{k}}\underline{\underline{H}}_0(\boldsymbol{k})]\,\underline{C}(\boldsymbol{k},t)\,d^3k\,. \tag{306}$$

If we substitute $\underline{C}(\boldsymbol{k})$ for its Fourier transform we obtain from Eq.(305)

$$< \boldsymbol{p}(t) >= \int \underline{\psi}^{\dagger}(\boldsymbol{r},t)\, \hat{\boldsymbol{p}}\, \underline{\psi}(\boldsymbol{r},t)\, d^3r\,.$$

and from Eq.(306)

$$< \boldsymbol{v}(t) >= \int \underline{\psi}^{\dagger}(\boldsymbol{r},t)\, c\, \underline{\alpha}\, \underline{\psi}(\boldsymbol{r},t)\, d^3r\,.$$

Exploiting the identity

$$\underline{\underline{\hat{H}}}_0\, \boldsymbol{r} - \boldsymbol{r}\, \underline{\underline{\hat{H}}}_0 = -i\, c\, \hbar\, \underline{\alpha}\,,$$

and going through the same set of arguments as with deriving the Pauli equation, we arrive at the time-dependent Dirac equation

$$[\underline{\underline{\hat{H}}}_0 + V(\boldsymbol{r})]\, \underline{\psi}(\boldsymbol{r},t) = i\, \hbar\, \frac{\partial}{\partial t}\, \underline{\psi}(\boldsymbol{r},t)\,. \tag{307}$$

The derivation can be extended by including electromagnetic fields, again completely analogous to the derivation of the Pauli equation. In so doing one recovers Eq.(307) with

$$\underline{\underline{\hat{H}}}^{0}_{Dirac} \stackrel{def}{=} c\, \underline{\alpha} \cdot (\hat{\boldsymbol{p}} - e\boldsymbol{A}(\boldsymbol{r},t)) + \underline{\underline{\alpha}}_0\, m_0\, c^2 \quad \text{standing in place of} \quad \underline{\underline{\hat{H}}}_0\,. \tag{308}$$

The ensuing two sections follow largely the conventional line of thought and are merely for the sake of completeness.

## 35 Covariant form of the Dirac equation

One can rewrite the Dirac equation in a particularly compact form by introducing Dirac's fundamental matrices

$$\underline{\underline{\gamma}}_0,\, \vec{\gamma} = (\underline{\underline{\gamma}}_1, \underline{\underline{\gamma}}_2, \underline{\underline{\gamma}}_3)$$

which are defined

$$\underline{\underline{\gamma}}_0 = \underline{\underline{\alpha}}_0 \quad \text{and} \quad \vec{\gamma} = \underline{\underline{\alpha}}_0\, \vec{\alpha}\,.$$

These 4 matrices may be lumped together to yield formally a 4-dimensional vector

$$\vec{\hat{\gamma}} = (\underline{\underline{\gamma}}_0, \vec{\gamma})\,.$$

One rewrites Eqs.(307), (308) in the form

$$\left[-i\hbar\frac{\partial}{\partial t} + c\,(\vec{\alpha} \cdot (\hat{\boldsymbol{p}} - e\boldsymbol{A}(\boldsymbol{r},t)) + V(\boldsymbol{r}) + \underline{\underline{\alpha}}_0\, m_0 c^2\right] \underline{\psi}(\boldsymbol{r},t) \tag{309}$$

If this equation is multiplied from the left by $-\frac{1}{c}\,\underline{\underline{\alpha}}^0$ and if one observes that

$$\underline{\underline{\alpha}}_0^2 = \underline{\underline{\gamma}}_0^2 = \underline{\underline{1}}\,,$$

one gets

$$\left[ i\,\hbar\,\underline{\underline{\alpha}}_0\,\partial_0 - \underline{\underline{\alpha}}_0 \sum_{n=1}^{3} \underline{\underline{\alpha}}_n \left( -i\hbar \frac{\partial}{\partial x_n} - eA_n(\boldsymbol{r},t) \right) - m_0\,c - \underline{\underline{\alpha}}_0\,\frac{V(\boldsymbol{r})}{c} \right] \underline{\psi}(\boldsymbol{r},t) = 0\,. \tag{310}$$

Here we have introduced the abbrevations $\partial_n$ for $n = 0, 1, 2, 3$, by setting

$$\frac{\partial}{\partial t} = c\,\frac{\partial}{\partial c\,t} \stackrel{def}{=} c\,\frac{\partial}{\partial x_0} = c\,\partial_0 \quad \text{and} \quad \frac{\partial}{\partial x_n} \stackrel{def}{=} \partial_n \quad \text{for} \quad n = 1, 2, 3\,.$$

In the following we make use of a particular short-hand notation introduced by Feynman for a four-vector $\boldsymbol{b} = (b_0, b_1, b_2, b_3)$:

$$\underline{\underline{\hat{\boldsymbol{b}}}} \stackrel{def}{=} \sum_{n=0}^{3} \underline{\underline{\gamma}}_n\, b_n = \underline{\underline{\gamma}}_0\, b_0 - \sum_{n=1}^{3} \underline{\underline{\gamma}}_n\, b_n\,.$$

Recalling the definition of the fundamental matrices we have for the first terms on the left-hand side of Eq.(310)

$$i\hbar\,\underline{\underline{\alpha}}_0\,\partial_0 - \underline{\underline{\alpha}}_0 \underbrace{\sum_{n=1}^{3} \underline{\underline{\alpha}}_n \left( -i\hbar \frac{\partial}{\partial x_n} \right)}_{=\vec{\alpha}\cdot\hat{\boldsymbol{p}}} = \underline{\underline{\gamma}}_0\, i\hbar\partial_0 - \vec{\gamma}\cdot\hat{\boldsymbol{p}}\,.$$

If we equate $\boldsymbol{b}$ with $i\hbar(\partial_0, \partial_1, \partial_2, \partial_3)$, this may be cast as

$$\underline{\underline{\gamma}}_0\, i\hbar\partial_0 - \vec{\gamma}\cdot\hat{\boldsymbol{p}} = \sum_{n=0}^{3} \underline{\underline{\gamma}}_n \left( i\,\hbar \frac{\partial}{\partial x_n} \right) \stackrel{def}{=} \underline{\underline{\hat{\boldsymbol{p}}}}\,.$$

By analogy equating $\boldsymbol{b}$ with the four-vector $(\frac{\phi}{c}, A_1, A_2, A_3)$ one obtains

$$\underline{\underline{\hat{\boldsymbol{A}}}} \stackrel{def}{=} \sum_{n=0}^{3} \underline{\underline{\gamma}}_n\, \boldsymbol{A}_n = \underline{\underline{\gamma}}_0\, \frac{\phi}{c} - \vec{\gamma}\cdot\boldsymbol{A}$$

where the particle's potential energy $V(\boldsymbol{r})$ has been replaced with $e\phi$. The time-dependent Dirac equation (310) thus takes the compact form

$$\left[ \underline{\underline{\hat{\boldsymbol{p}}}} - e\,\underline{\underline{\hat{\boldsymbol{A}}}} - m_0\,c \right] \underline{\psi}(\boldsymbol{r},t) = 0\,.$$

which is Lorentz-covariant.

## 36 Recovering Bohr's magneton

Although the salient point of deriving the Dirac equation seems to differ from that of its non-relativistic counterpart, the Pauli equation, merely by the energy/momentum relation, the outcome yields unexpected quantitative information on the particle's magnetic moment.
One starts from the time-independent version of Eq.(309) which may be cast

$$\Big(E - \underline{\underline{\alpha}}_0\, m_0c^2 - V(\boldsymbol{r})\Big)\, \underline{\psi}(\boldsymbol{r}) - c\,(\vec{\alpha}\cdot(\hat{\boldsymbol{p}} - e\boldsymbol{A}(\boldsymbol{r}))\, \underline{\psi}(\boldsymbol{r}) = 0\,. \tag{311}$$

This bispinor equation may be decomposed into two spinor eqations equations by lumping together the first two and, alternatively, the following two components of the bispinor equation

$$\big(E' - V(\boldsymbol{r})\big) \begin{pmatrix} \psi^1_\uparrow(\boldsymbol{r}) \\ \psi^1_\downarrow(\boldsymbol{r}) \end{pmatrix} = c\,\vec{\sigma}\cdot\hat{\boldsymbol{P}} \begin{pmatrix} \psi^2_\uparrow(\boldsymbol{r}) \\ \psi^2_\downarrow(\boldsymbol{r}) \end{pmatrix} \tag{312}$$

and

$$\big(E' + 2m_0c^2 - V(\boldsymbol{r})\big) \begin{pmatrix} \psi^2_\uparrow(\boldsymbol{r}) \\ \psi^2_\downarrow(\boldsymbol{r}) \end{pmatrix} = c\,\vec{\sigma}\cdot\hat{\boldsymbol{P}} \begin{pmatrix} \psi^1_\uparrow(\boldsymbol{r}) \\ \psi^1_\downarrow(\boldsymbol{r}) \end{pmatrix}, \tag{313}$$

where $\vec{\sigma}$ represents the three Pauli matrices. Further, $E'$ stands for $E - m_0c^2$, and $\hat{\boldsymbol{P}}$ for $\hat{\boldsymbol{P}} = \hat{\boldsymbol{p}} - eA(\boldsymbol{r})$ which had already been introduced earlier.
The following discussion confines itself to an approxmation that applies to a particle with kinetic energy well below twice its rest energy $m_0c^2$, that is

$$2m_0c^2 \approx 2m_0c^2 + \underbrace{E' - V(\boldsymbol{r})}_{=E_{kin}} = 2m_0c^2(1+\tfrac{\beta}{4}^2)\,;\quad \tfrac{\beta}{4}^2 \ll 1 \;\text{ where }\; \tfrac{\beta}{4}^2 = \frac{E_{kin}}{2m_0c^2}\,.$$

In the non-relativistic limit when $E_{kin} \approx \frac{m_0}{2}v^2$ the quantity $\beta$ becomes $\frac{v}{c}$. The expression $\frac{\beta}{4}^2$ will be neglected in the following.
Hence, within this approximation one obtains from Eq.(313)

$$\begin{pmatrix} \psi^2_\uparrow(\boldsymbol{r}) \\ \psi^2_\downarrow(\boldsymbol{r}) \end{pmatrix} = \frac{1}{2m_0c}\,\vec{\sigma}\cdot\hat{\boldsymbol{P}} \begin{pmatrix} \psi^1_\uparrow(\boldsymbol{r}) \\ \psi^1_\downarrow(\boldsymbol{r}) \end{pmatrix}.$$

If this is inserted into Eq.(312) one gets

$$\big(E' - V(\boldsymbol{r})\big) \begin{pmatrix} \psi^1_\uparrow(\boldsymbol{r}) \\ \psi^1_\downarrow(\boldsymbol{r}) \end{pmatrix} = \frac{1}{2m_0} \Big(\vec{\sigma}\cdot\hat{\boldsymbol{P}}\Big)\Big(\vec{\sigma}\cdot\hat{\boldsymbol{P}}\Big) \begin{pmatrix} \psi^1_\uparrow(\boldsymbol{r}) \\ \psi^1_\downarrow(\boldsymbol{r}) \end{pmatrix}. \tag{314}$$

The prefactor $\Big(\vec{\sigma}\cdot\hat{\boldsymbol{P}}\Big)\Big(\vec{\sigma}\cdot\hat{\boldsymbol{P}}\Big)$ on the right-hand side contains the sought-for information on the particle's magnetic moment, but its discussion requires

particular care. In further analyzing this expression one has to resort to a sophisticated identity:

$$(\vec{\sigma}\cdot\vec{a})\,(\vec{\sigma}\cdot\vec{b}) = \underline{\underline{1}}\,(\vec{a}\cdot\vec{b}) + i\,\vec{\sigma}(\vec{a}\times\vec{b}) \tag{315}$$

which applies to any two vectors $\vec{a}$ and $\vec{b}$. It can be verified by just performing the multiplications. A less laborious verification consists in choosing an appropriate coordinate system for the two vectors such that the $x/z$-plane of this system coincides with the plane spanned by these two vectors. Further, one chooses $\vec{a}$ parallel to the $z$-axis. The vector $\vec{b}$ cannot have a $y$-component then. Hence

$$\vec{a} = a_z\,\boldsymbol{e}_z\,; \quad \vec{b} = b_x\,\boldsymbol{e}_x + b_z\,\boldsymbol{e}_z\,.$$

One obtains then by performing the multiplications

$$(\vec{\sigma}\cdot\vec{a})\,(\vec{\sigma}\cdot\vec{b}) = \underline{\underline{\sigma}}_z\,a_z(\underline{\underline{\sigma}}_z\,b_z + \underline{\underline{\sigma}}_x\,b_x) = \underline{\underline{1}}\,a_z b_z + i\underline{\underline{\sigma}}_y\ \underbrace{a_z b_x}_{=(\vec{a}\times\vec{b})_y}$$

$$= \underline{\underline{1}}(\vec{a}\cdot\vec{b}) + i\,\vec{\sigma}(\vec{a}\times\vec{b})\,.$$

$$\underline{\underline{\sigma}}_z\,\underline{\underline{\sigma}}_x = i\underline{\underline{\sigma}}_y$$

which can be verified by performing the multiplication.
If one equates the vectors $\vec{a}$ and $\vec{b}$ with $\hat{\boldsymbol{P}}$, Eq.(315) attains the form

$$(\vec{\sigma}\cdot\hat{\boldsymbol{P}})(\vec{\sigma}\cdot\hat{\boldsymbol{P}}) = \underline{\underline{1}}\hat{\boldsymbol{P}}^2 + i\,\vec{\sigma}(\hat{\boldsymbol{P}}\times\hat{\boldsymbol{P}})\,. \tag{316}$$

In the following one has to observe that all operators in the equations are meant to apply on a spinor $\underline{\psi}(\boldsymbol{r})$ on the right, but it is left out for simplicity. However, its presence has to be paid attention to when one applies the chain rule.
The second term on the right-hand side of the equation above represents the most interesting constituent:

$$(\hat{\boldsymbol{P}}\times\hat{\boldsymbol{P}}) = (\hat{\boldsymbol{p}} - e\boldsymbol{A})\times(\hat{\boldsymbol{p}} - e\boldsymbol{A}) = \underbrace{\hat{\boldsymbol{p}}\times\hat{\boldsymbol{p}}}_{=0} - e\boldsymbol{A}\times\hat{\boldsymbol{p}} - e\hat{\boldsymbol{p}}\times\boldsymbol{A} + e^2\,\underbrace{\boldsymbol{A}\times\boldsymbol{A}}_{=0}$$

On invoking the chain rule

$$-e\hat{\boldsymbol{p}}\times\boldsymbol{A} = e\boldsymbol{A}\times\hat{\boldsymbol{p}} - e\boldsymbol{A}\times\hat{\boldsymbol{p}}\,,$$

and observing that

$$-e(\hat{\boldsymbol{p}}\times\boldsymbol{A}) = ie\hbar(\underbrace{\nabla\times\boldsymbol{A}}_{=curl\boldsymbol{A}=\boldsymbol{B}})$$

Eq.(316) can be recast

$$\tfrac{1}{2m_0}\left(\vec{\sigma}\cdot\hat{\boldsymbol{P}}\right)(\vec{\sigma}\cdot\hat{\boldsymbol{P}}) = \underline{\underline{1}}\,\frac{\hat{\boldsymbol{P}}^2}{2m_0} - \underbrace{\frac{e\hbar}{2m_0}}_{\stackrel{def}{=}\mu_B}\vec{\sigma}\cdot\boldsymbol{B}\,.$$

Inserting this result into Eq.(314) one recovers the time-independent version of the Pauli equation (266)

$$\left[\frac{\hat{\boldsymbol{P}}^2}{2m_0} + V(\boldsymbol{r}) - \mu_B \vec{\sigma}\cdot\boldsymbol{B}\right]\underline{\psi}(\boldsymbol{r}) = E'\,\underline{\psi}(\boldsymbol{r}) \quad \text{where} \quad \underline{\psi}(\boldsymbol{r}) = \begin{pmatrix} \psi^1_\uparrow(\boldsymbol{r}) \\ \psi^1_\downarrow(\boldsymbol{r}) \end{pmatrix}.$$

# 37 Spatial particle correlation beyond the limit of entanglement. Spooky action at a distance

As discussed in Section 24 the electrons of two hydrogen atoms will respond independently to local perturbations once the inter-atomic distance has become macroscopically large. The electronic wave function factorizes then and becomes the product of two one-particle wave functions. One would therefore expect two free fermions that have moved sufficiently far away in opposite directions with their spins being transverse and anti-parallel, to display the same features. If they were still described by an anti-symmetric wave function the particle properties would remain non-locally intertwined in that each of the particles would appear at distant detectors with only half of the total probability. Therefore a realistic description can only be ensured by a product of two one-particle wave functions, wavepackets moving in opposite directions, one for spin up and the other one for spin down or vice versa, the choice randomly distributed among the pairs generated in succession. Consequently, there will be a complete loss of the "common-cause"-spin correlation of the particles when they hit differently oriented spin detectors. The latter scatter the incoming fermion depending on the angle which the fermion's spin direction encloses with the scattering plane. To be as concrete as possible we refer in this section to the fundamental experiment by Lamehi-Rachti and Mittig [95] who were able to generate pairs of protons of about 8 MeV with spins paired anti-parallel and moving apart such that the proton's velocities in the center of mass system have the same absolute value but opposite directions. The spin orientation was analyzed by letting each of the protons impinge on a device akin to a Mott detector familiar from polarized electron detection. The incoming proton is scattered at some carbon atom of a carbon foil. Each Mott-type detector is associated with two particle detectors whose axes point to the scattering center and enclose an angle $\pm\alpha$ with the flight direction of the incoming proton. Together with that direction these axes form the scattering plane. The differential cross section of the carbon scatterer for a proton with spin up perpendicular to the scattering plane is given by

$$\sigma(\alpha,\beta) = (|f(\alpha)|^2 + |g(\alpha)|^2)\,[1 - S(\alpha)\sin\beta] \tag{317}$$

where $S(\alpha)$ represents the Sherman function for carbon/proton scattering, $\beta$ stands for the azimuthal angle in the plane perpendicular to the proton flight

direction and $f(\alpha)$ and $g(\alpha)$ denote the scattering and spin-flip amplitude. The latter is associated with spin-orbit coupling [8] which determines also the magnitude of $S(\alpha)$. In view of the objective of this article, we wish to emphasize at this point that Eq.(317) is a consequence of solving the relativistic Pauli equation, and the experimentally verifiable results that will be discussed below, are another objective consequence which is definitely not affected by the process of particle detection (the "measurement").
In accordance with the notation familiar from EPRB-experiments we denote the Mott-type analyzer at the end of the left proton track by A and that at the end of the right track by B. Furthermore, the detector on the right side of the scattering plane will be characterized by a "+"-sign, that on the left side by a "-"-sign. The two particle detectors of each Mott-type analyzer are located at $\beta = \mp\pi/2$, and $\alpha$ was set $\approx 50°$. Hence the difference between the respective differential cross sections (the "left-right asymmetry") is given by $\Delta\sigma = \sigma^+ - \sigma^- = (|f|^2 + |g|^2)\, 2S$. If the spin of the incoming proton encloses an angle $\Delta$ with the normal of the scattering plane, the sin-factor in Eq.(317) becomes $\sin(\Delta \mp \pi/2) = \mp \cos\Delta$ with $\beta = \mp\pi/2$ denoting the positions of the two particle detectors as before. Thus one has $\Delta\sigma = (|f|^2 + |g|^2)\, 2S\, \cos\Delta$. In order to capture the general case, we introduce an orthogonal Cartesian coordinate system whose $x/y$-plane is spanned by the two proton tracks before they enter the Mott-type analyzers. The axis of alignment of the proton spins encloses in general an angle $\varphi$ with the $z$-axis thus introduced. The pertinent orientation angles of the scattering planes with respect to that $z$-axis are denoted by $\theta$ and $\phi$ for the normals of the A and B-plane, respectively. That means: $\Delta_A = \theta - \varphi$ and $\Delta_B = \phi - \varphi$. To make contact to the familiar notation, we define a quantity $P^{\pm}_{A(B)}$ through

$$\frac{\sigma^{\pm}_{A(B)}}{2\,[|f|^2 + |g|^2]} = P^{\pm}_{A(B)} = S\,[\tfrac{1}{2\,S} \pm \tfrac{1}{2}\,\cos\Delta_{A(B)}] \tag{318}$$

which has the property

$$P^{+}_{A(B)} + P^{-}_{A(B)} = 1\,.$$

Obviously, $P^{\pm}_{A(B)}$ is proportional to the count rate of the respective detector, and $\frac{1}{S}\,(P^{+}_{A(B)} - P^{-}_{A(B)}) = \cos\Delta_{A(B)}$ describes the degree of spin orientation of the incoming proton with respect to the normal of the associated scattering plane. If the spin of the proton impinging on the analyzer at A is parallel to that normal, that is perpendicular to the associated scattering plane, we have $\Delta_A = 0$ and hence $\frac{1}{S}\,(P^{+}_{A} - P^{-}_{A}) = 1$. The joint probability of finding the proton pair with one of the protons at A and orientation angle $\Delta_A = \theta - \varphi$ and the other proton at B with orientation angle $\Delta_B = \phi - \varphi - \pi$

[8] Although spin-orbit coupling represents a constituent of the relativistic Pauli approximation to the Dirac equation, we consider it here as given.

is given by

$$P_{joint} = (P_A^+ - P_A^-)\,(P_B^+ - P_B^-) = P^{++} + P^{--} - P^{+-} - P^{-+} \qquad (319)$$

where $P^{\pm\pm} = P_A^{\pm}\,P_B^{\pm}$ and $P^{\pm\mp} = P_A^{\pm}\,P_B^{\mp}$. Because of the definition (318) we have

$$P^{++} + P^{--} + P^{+-} + P^{-+} = 1\,.$$

To make sure that the count rates refer definitely to proton pairs, the counts associated with $P^{\pm\pm}$ and $P^{\pm\mp}$ are filtered by coincidence electronics.
Since for principal reasons one has in general $S < 0$ (in the case under study $S \approx 0.7$), $P^+ - P^- = S\,\cos\Delta$ can never become unity even when the particle enters the analyzer with its spin perpendicular to the scattering plane, that is when $\Delta = 0$. It is therefore suggestive to introduce an $S$-independent joint count rate $\hat{P}_{joint} = \frac{1}{S^2}\,P_{joint}$ which, on combining Eqs.(318) and (319), takes the form

$$\hat{P}_{joint}(\theta,\phi,\varphi) = -\cos(\theta-\varphi)\,\cos(\phi-\varphi)\,. \qquad (320)$$

In practice the experiments have been carried out with the scattering plane of the B-analyzer lying in the $x/y$-plane, which means $\phi = 0$. Since all proton pairs are prepared 100% polarized, that is with their spins aligned parallel and antiparallel with respect to the $z$-axis, we have also $\varphi = 0$ so that Eq.(320) simplifies to

$$\hat{P}_{joint} = -\cos\theta\,, \qquad (321)$$

and this is in agreement with the experimental results.
We emphasize again that this equation has been obtained by assuming a factorization of the two-proton wave function which means that the motion of the "A"-proton is controlled only by the potentials specifying the "A"-analyzer. There is no influence of the potentials that belong to "'B". Analogous statements apply to the "B"-proton. Hence, for each pair of protons there is no correlation between their respective "A" and "B"- scattering processes. However, it has been the objective of the experiments, as the authors expressly state, to demonstrate that there is such a correlation. Yet in order to prove that point, the experiments should have allowed a preparation of proton pairs with an axis of spin alignment that encloses an angle $\varphi$ with the $z$-axis as originally assumed above. According to the established terminology that angle has to be regarded as a "hidden variable". The values of $\varphi$ associated with the various pairs should have random character. One can form then a new expression from $\hat{P}_{joint}(\theta,\phi,\varphi)$ by averaging over $\varphi$:

$$\hat{P}_{av}(\theta,\phi) = \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \rho(\varphi)\,\hat{P}_{joint}(\theta,\phi,\varphi)\,d\varphi\,. \qquad (322)$$

where $\rho(\varphi)$ denotes a weight function normalized to unity. Clearly, in the experiment the averaging occurs automatically and unavoidably.
If one assumes a uniform distribution of $\varphi$ over the interval $\pi$, that is $\rho(\varphi) = \frac{1}{\pi}$, and inserts here $\hat{P}_{joint}(\theta, \phi, \varphi)$ from Eq.(320), one obtains

$$\hat{P}_{av}(\theta, \phi) = -\tfrac{1}{2}\,\cos(\theta - \phi)\,, \tag{323}$$

where

$$\cos(\theta - \varphi)\,\cos(\phi - \varphi) = \tfrac{1}{2}\,\cos(\theta - \phi) + \tfrac{1}{2}\,\cos(\theta + \phi - 2\varphi)$$

has been used. Hence, for $\phi = 0$ as specified in the experiment, Eq.(323) yields

$$\hat{P}_{av}(\theta, \phi) = -\tfrac{1}{2}\,\cos\theta$$

which differs from (321) by a factor of $\frac{1}{2}$.
At this point it is instructive to contemplate the change that would occur if there would be a non-local correlation between the two analyzers in the following sense:
If the "B"-proton has been specified by the "B"-analyzer as polarized perpendicular to the associated scattering plane, that is if $\varphi = \phi$, and if this property is by some "spooky action at a distance" transferred to the "A"-proton, $\varphi$ attains the same value for the "A"-proton. The measurement on the "A"-proton would then become "contextual": it would depend on the result obtained for the "B"-proton. Consequently, the detection rate (320) would take the form

$$\hat{P}_{joint} = -\cos(\theta - \phi) = -\cos(\vec{a}, \vec{b}) = -\vec{a} \cdot \vec{b}\,. \tag{324}$$

where we have introduced the quantities $\vec{a}$ and $\vec{b}$ as normal vectors for the "A"- and "B"-scattering plane, respectively, which enclose angles $\theta$ and $\phi$ with the $z$-axis. For the situation specified by the experiment (viz. $\phi = 0$), this result becomes identical with (321). Thus, a distinction between the two mechanisms is not possible within the given limitations. One might argue that a derivation based on a "spooky-action-at-a-distance"-hypothesis has to be rejected anyway. But the same hypothesis works perfectly for the analogous experiment with pairs of linearly polarized photons where that particular limitation does not exist. (S. Aspect et al. [96].)
By referring to the expectation value

$$\langle \Psi | \vec{\sigma}_A \cdot \vec{a} \otimes \vec{\sigma}_B \cdot \vec{b} | \Psi \rangle = -\cos(\vec{a}, \vec{b})$$

where $\Psi$ denotes the anti-symmetric singlet-state two-proton wave function and $\vec{\sigma}_{A/B}$ the spin operators, Eq.(324) is commonly discussed as "the quantum mechanical prediction" for the experiment in question. Considering all the details of our analysis it is hard to see how this expectation value can

have anything to do with the experiment except that it happens to yield the same $-\cos(\vec{a},\vec{b})$.
We shortly return to the idea pursued by Lamehi-Rachti and Mittig in their paper. In order to exclude the possibility that their result might accidentally coincide with the prediction of a hidden parameter model, they resort to Bell's theorem [97]. It refers to quantities of the type $\hat{P}_{av}(\vec{a},\vec{b})$ in Eq.(322) which - according to Eq.(323) - becomes equal to $-\frac{1}{2}\cos(\vec{a},\vec{b})$ if $\varphi$ is uniformly distributed. In general the weight function $\rho(\varphi)$ will be unknown, and hence a complete lack of correlation between the "A"- and "B"-scattering processes, as implied by our treatment, will not show up simply as a numerical correction factor of the "correlated result". Bell [97] could show that in performing an EPRB-type experiment one is definitely dealing with a non-classical (i. e. non-local) particle correlation if - irrespective of the form of the weight function and irrespective of the kind of hidden variable - the following inequality is violated:

$$|\hat{P}_{av}(\vec{a},\vec{b}) - \hat{P}_{av}(\vec{a},\vec{b}')| \leq 2\,|\hat{P}_{av}(\vec{a}',\vec{b}') + \hat{P}_{av}(\vec{a}',\vec{b})|\,,$$

where $\vec{a},\vec{a}',\vec{b},\vec{b}'$ denote different analyzer settings. In fact, the authors succeeded in verifying this violation, but it appears to us, because of the limitations discussed above, that this result is absolutely not convincing.

## 38 Concluding remarks

In summarizing the essence of quantum mechanics Wigner states in a fundamental article [98] under the headline "What is the state vector?": *"We recognize ....that the state vector is only a shorthand expression of that part of information concerning the past of the system which is relevant for predicting (as far as possible) the future behavior thereof."*
In our view the most impressive success of quantum mechanics in understanding the stability, composition and properties of the building blocks of nature consists in predicting the systematic order in the periodic table, the phenomenon of chemical valency and the groundstate properties of molecules and solids. The state vector of these systems, the groundstate wave function $\Psi(\boldsymbol{r}_1,\boldsymbol{r}_2,\ldots\boldsymbol{r}_N)$, is a function of the particle coordinates $\boldsymbol{r}_1,\boldsymbol{r}_2,\ldots\boldsymbol{r}_N$ in terms of which their Coulomb interaction enters the calculation of the system's total energy. But for every experimentalist there is no doubt that these coordinates are fundamentally inaccessible to measurement, and hence cannot possibly be regarded as "information gained from measurements". As is amply demonstrated by modern ab initio-calculations, the wave function allows one to determine the total energy as a function of nuclear positions, bond angles, vibrational frequencies, lattice constants, elastic moduli, phonon spectra, saturation magnetizations, electric conductivities etc.. These quantities are in common-sensible terms true observables whereas the

particle coordinates remain definitely hidden parameters. As we have repeatedly explained, this applies to the eigenvalues of Hermitian operators as well, thus putting a serious question mark behind "Kochen-Specker"-type [99] and "no-go" theorems (s. e. g.[46]) which are all based on the exasperatingly artificial assumption that "measurements" yield eigenvalues or "probabilities for eigenvalues". Occasionally a certain awareness of this puzzling inconsistency surfaces as in the revealing statement of Wigner's [37] that we have already alluded to in Section 17.

It is deplorable to notice the impropriety with which certain advocates of the Copenhagen school of thought dismiss supporters of Nelson's attempt to develop a "quantum mechanics without observer" as "stranded enthusiasts"(s. Streater [16]), and ironically base their criticism on the old, actually absurd, arguments how indeterminacy enters the theory through measurement and how commuting "observables" correlate with the result of simultaneous measurements. All this has been iterated umpteen times although it is well known to every experimentalist that exactly these "measurements" are inexecutable altogether. With the same insensitivity to reality castigators of the proponents of Nelson's approach think it fully justified to equate the physics of photon-correlation experiments with analogous, but actually extremely scarce experiments with massive particles. In the optical experiments the correlated photons are guided by an electromagnetic wave which - in vacuo - propagates at the velocity of light and obeys the laws of classical electrodynamics when it hits optical objects. In analogous experiments with massive particles the guiding wave is defined by an ensemble whose propagation in real-space is to a large extent dictated by Newtonian mechanics. This becomes particularly evident in our derivation.
We believe we have presented ample evidence that quantum mechanics is in detail derivable from classical mechanics plus a modified physical vacuum by allowing the latter to undergo energy fluctuations. Their action on massive particles is calibrated by Planck's constant, and despite their presence the conservation of energy (and with free particles: the conservation of particle momentum) is ensured on average. We hope that the present article can contribute to an unbiased reassessment of present-day quantum mechanics concerning these two questions:

- Which elements of the old doctrine are obsolete and dispensable?
- Does "measurement" really play a particular role in quantum mechanics or is its alleged importance simply a misunderstanding?

# 39 Appendix A: Brownian motion and the Navier-Stokes equation

As Brownian motion is evidently fundamental to the entire concept of the present exposition we think it necessary to give a short account on its theory. According to Section 5 we describe the effect of the vacuum on the $j$-th particle of the ensemble by a stochastic force

$$\boldsymbol{F}^B_{sj}(t) = \boldsymbol{F}^B_{rj}(t) - \frac{m_0}{\tau}\,\boldsymbol{v}_j(t) \tag{325}$$

where $\boldsymbol{v}_j$ is the particle's velocity and $\boldsymbol{F}^B_r = (F_{r1}, F_{r2}, F_{r3})$ denotes a random force with a Gaussian distribution

$$P(F^B_{rk}) = \frac{1}{\sqrt{\pi}\,F_{r0}}\,e^{-(F^B_{rk}/F_{r0})^2} \quad (k = 1, 2, 3)\,.$$

The quantity $F_{r0}$ is defined

$$F_{r0} = \frac{1}{\tau_{coll.}}\,\sqrt{m_0\,k_B\,T} \tag{326}$$

where it has been assumed that the "vacuum" can be associated with an effective temperature $T$. The quantity $k_B$ denotes the Boltzmann constant, and $\tau_{coll.}$ describes a mean time of momentum transfer. Hence Eq.(326) can alternatively be cast as

$$\frac{\overline{\Delta p_k^2}}{2\,m_0} = \frac{1}{2}\,k_B\,T \;\longrightarrow \frac{\overline{\Delta \boldsymbol{p}^2}}{2\,m_0} = \frac{3}{2}\,k_B\,T \tag{327}$$

where $\overline{\Delta p_k^2}$ is the mean square of the momentum transfer in the $x_k$-direction.

At this point we want to emphasize that the ensuing considerations which provide a description of Brownian motion do not by necessity presuppose an embedding medium which is gas-like and thermal. The only requirement is that the embedding acts on the particle under study with stochastic forces whose components underly a normal distribution.

To avoid gaps in the understanding of our considerations we restate some essential steps in the derivation of Einstein's law [29] on the mean square displacement of the particle.

We assume the particle motion in the ensemble, specifically the motion of the $j$-th particle, to be controlled by Langevin's equation [100]

$$m_0\,\ddot{\sigma}_{j\,k} + \frac{m_0}{\tau}\dot{\sigma}_{j\,k} = F_{j\,k} + F^B_{rj\,k}(t) \tag{328}$$

where $\underline{\sigma}_j = (\sigma_1, \sigma_2, \sigma_3)$ describes the shift of the particle's position and

$$\boldsymbol{F}_j = -\nabla V(\boldsymbol{r}_j) \tag{329}$$

is the external classical force acting on the particle, $V(\boldsymbol{r})$ the associated potential. The shift $\underline{\sigma}_j$ may be subdivided into a portion $\underline{\sigma}_{rj}$ that is caused by the random force, and a portion $\underline{\sigma}_c$ that occurs when the random force is absent. The subscript "c" stands for "convection". Hence, these shifts obey equations

$$\ddot{\sigma}_{rj\,k} + \frac{1}{\tau}\dot{\sigma}_{rj\,k} = f_{rj\,k} \tag{330}$$

and

$$\ddot{\sigma}_{cj\,k} + \frac{1}{\tau}\dot{\sigma}_{cj\,k} = f_{j\,k} \tag{331}$$

where

$$f^B_{rj\,k} = \frac{1}{m_0} F^B_{rj\,k}\,; \quad f_{j\,k} = \frac{1}{m_0} F_{j\,k}$$

Obviously, the sum of Eqs.(330) and (331) yields Eq.(328).
Muliplication of Eq.(330) by $\sigma_{rj\,l}$ gives

$$\frac{d}{dt}\left(\sigma_{rj\,l}\;\dot{\sigma}_{rj\,k}\right) - \dot{\sigma}_{rj\,l}\;\dot{\sigma}_{rj\,k} = -\frac{1}{\tau}\,\sigma_{rj\,l}\;\dot{\sigma}_{rj\,k} + \sigma_{rj\,l}\,f^B_{rj\,k} \tag{332}$$

where we have observed that

$$\frac{d}{dt}\left(\sigma_{rj\,l}\;\dot{\sigma}_{rj\,k}\right) = \sigma_{rj\,l}\;\ddot{\sigma}_{rj\,k} + \dot{\sigma}_{rj\,l}\;\sigma_{rj\,k}\;.$$

We now form the ensemble average of Eq.(332) by analogy with Eq.(21) in Section 4. As there is no correlation between $\sigma_{rj\,l}$ and $f^B_{rj\,k}$ including $l = k$, we have

$$\frac{1}{n(\boldsymbol{r},t)}\;\sum_{j}^{n(\boldsymbol{r},t)}\sigma_{rj\,l}\,f^B_{rj\,k} = 0\;.$$

The sum runs over the products $\sigma_{rj\,l}\,f^B_{rj\,k}$ that belong to the $n(\boldsymbol{r},t)$ different particles in the elementary volume about $\boldsymbol{r}$ at time $t$.
There is also no correlation between $\dot{\sigma}_{rj\,l}$ and $\dot{\sigma}_{rj\,k}$ for $l \neq k$, and hence

$$\frac{1}{n(\boldsymbol{r},t)}\;\sum_{j}^{n(\boldsymbol{r},t)}\dot{\sigma}_{rj\,l}\,\dot{\sigma}_{rj\,k} = \delta_{l\,k}\left[\dot{\sigma}_{rk}(\boldsymbol{r},t)\right]^2\;.$$

Because of Eq.(327) we thus have

$$\left[\dot{\sigma}_{rk}(\boldsymbol{r},t)\right]^2 = \frac{k_B\,T}{m_0}\,. \tag{333}$$

As a result, the ensemble average of Eq.(332) takes the form

$$\frac{\partial}{\partial t}(\sigma_{r\,l}\;\dot{\sigma}_{r\,k}) + \frac{1}{\tau}\,(\sigma_{r\,l}\;\dot{\sigma}_{r\,k}) = \delta_{l\,k}\;\frac{k_B\,T}{m_0}\;. \tag{334}$$

The solution of this equation can be cast as

$$\sigma_{r\,l}\;\dot{\sigma}_{r\,k} = \delta_{l\,k}\;\frac{k_B\,T\,\tau}{m_0}\left[1 - C\,e^{-\frac{(t-t_0)}{\tau}}\right]$$

where $C$ is some constant. Without loss of generality $\underline{\sigma}_r$ may be defined such that $\underline{\sigma}_r(\boldsymbol{r}, t_0) = 0$. In that case C becomes equal to one.
For a time interval

$$\Delta t = t - t_0 \gg \tau \tag{335}$$

the second term in the above equation may be neglected, and we arrive at

$$\sigma_{r\,l}\;\dot{\sigma}_{r\,k} = \delta_{l\,k}\,\nu \tag{336}$$

where

$$\nu = \frac{k_B\,T\,\tau}{m_0} \tag{337}$$

denotes the kinematic viscosity which the particle experiences in the embedding medium.
We observe that

$$\sigma_{r\,k}\;\dot{\sigma}_{r\,k} = \frac{1}{2}\,\frac{\partial}{\partial t}\,\sigma^2_{r\,k}$$

and integrate Eq.(336) over the time interval $[t_0, t_0 + \Delta t]$. The result may be written

$$\sigma_{r\,l}\;\sigma_{r\,k} = \delta_{l\,k}\,2\nu\,\Delta t \tag{338}$$

where we have set $\sigma^2_{r\,k}(\boldsymbol{r}, t_0) = 0$ in agreement with our assumption on $\underline{\sigma}_r(\boldsymbol{r}, t_0)$ above.
Eq.(338) represents Einstein's famous law on the time dependence of the mean square diplacement of a particle driven by a random force with a Gaussian distribution in a viscous medium.
The total displacement of the particle, $\underline{\sigma}_j$, is given by $\underline{\sigma}_{rj} + \underline{\sigma}_{cj}$. When we form the ensemble average of $\sigma_{j\,l}\,\sigma_{j\,k}$ and exploit the fact that $\sigma_{cj\,l}$ and $\sigma_{rj\,k}$ are definitely uncorrelated, we may write the result

$$\sigma_l\,\sigma_k = \frac{1}{n(\boldsymbol{r}, t)}\;\sum_{j=1}^{n(\boldsymbol{r},t)}\,(\sigma_{cj\,l} + \sigma_{rj\,l})\;(\sigma_{cj\,k} + \sigma_{rj\,k}) = \sigma_{cl}\,\sigma_{ck} + \sigma_{r\,l}\,\sigma_{r\,k}\,. \tag{339}$$

Below we shall be concerned with time-dependencies within intervals $\Delta t$ that are small but still large enough to comply with the requirement (335). Without loss of generality we may also set $\sigma_{c\,k}(\boldsymbol{r}, t_0) = 0$ and then expand $\sigma_{c\,k}(\boldsymbol{r}, t_0 + \Delta t)$ only to linear order in $\Delta t$:

$$\sigma_{c\,k}(\boldsymbol{r}, t_0) = \dot{\sigma}_{c\,k}(\boldsymbol{r}, t_0)\,\Delta t\,. \tag{340}$$

As $\sigma_{c\,l}$ and $\sigma_{c\,k}$ are uncorrelated for $l \neq k$, Eq.(339) may be given the form

$$\sigma_l\,\sigma_k = \delta_{l\,k}\left(2\nu\,\Delta t + \dot{\sigma}^2_{c\,k}\,\Delta t^2\right) \tag{341}$$

where Eqs.(338) and (340) have been used. This result may be cast in a form that will prove particularly suited for the ensuing considerations.
Let $P^M(\boldsymbol{r}, \underline{\sigma}, t, \Delta t)\,d^3\sigma$ be the (*transition*)-probability of finding a particle after a time span of $\Delta t$ in the elementary volume $d^3\sigma$ about a position $\boldsymbol{r} + \underline{\sigma}$ if it was definitely at $\boldsymbol{r}$ and time $t$. If one sums over all displacements $\underline{\sigma}$ which the particle may undergo, one obtains certainty for a displacement. Hence, the probability density $P^M(\boldsymbol{r}, \underline{\sigma}, t, \Delta t)$ is normalized:

$$\int P^M(\boldsymbol{r}, \underline{\sigma}, t, \Delta t)\,d^3\sigma = 1\,. \tag{342}$$

The superscript "M" stands for "Markov process".(S. remarks in Section 16.)
Using these properties we obtain

$$\frac{1}{n(\boldsymbol{r}, t)}\sum_{j=1}^{n(\boldsymbol{r},t)}\sigma_{j\,l}(t + \Delta t)\,\sigma_{j\,k}(t + \Delta t) =$$

$$\sigma_l(\boldsymbol{r}, t + \Delta t)\,\sigma_k(\boldsymbol{r}, t + \Delta t) = \int \sigma_l\,\sigma_k\,P^M(\boldsymbol{r}, t, \Delta t)\,d^3\sigma\,,$$

and hence Eq.(341) can be cast as

$$\int \sigma_l\,\sigma_k\,P^M(\boldsymbol{r}, \underline{\sigma}, t, \Delta t)\,d^3\sigma = \delta_{l\,k}\left(2\nu\,\Delta t + \dot{\sigma}^2_{c\,k}\,\Delta t^2\right)\,. \tag{343}$$

Here $\nu = \eta/m_0\,n_0$ denotes, as already stated, the "kinematic viscosity" of the embedding system, $\eta$ represents the common "dynamical viscosity" and $n_0$ is the particle density of the embedding system. The kinematic viscosity $\nu$ happens to agree with the coefficient of diffusion $D$.
As follows immediately from the definition of $P^M(\boldsymbol{r}, \underline{\sigma}, t, \Delta t)$, the following equation holds

$$\rho(\boldsymbol{r}, t + \Delta t) = \int \rho(\boldsymbol{r} - \underline{\sigma}, t)P^M(\boldsymbol{r} - \underline{\sigma}, \underline{\sigma}, t, \Delta t)d^3\sigma \tag{344}$$

which is known as the Smoluchowski equation [101]. Here $\rho(\boldsymbol{r}, t+\Delta t)$ denotes the probability density of finding the particle within the elementary cube

about $\boldsymbol{r}$ at time $t + \Delta t$. This density is normalized to unity within the fundamental volume $V$.
We approximate the $\sigma$-dependence of the function

$$G(\boldsymbol{r} - \underline{\sigma}, \underline{\sigma}, t, \Delta t) = \rho(\boldsymbol{r} - \underline{\sigma}, t)\, P^M(\boldsymbol{r} - \underline{\sigma}, \underline{\sigma}, t, \Delta t)$$

by a Taylor polynomial of second degree

$$G(\boldsymbol{r} - \underline{\sigma}, \underline{\sigma}, t, \Delta t) = G(\boldsymbol{r}, \underline{\sigma}, t, \Delta t) - \sum_{k=1}^{3} \sigma_k \frac{\partial}{\partial x_k} G(\boldsymbol{r}, \underline{\sigma}, t, \Delta t) + \\ + \frac{1}{2} \sum_{l,k} \sigma_l\, \sigma_k\, \frac{\partial^2}{\partial x_l\, \partial x_k}\, G(\boldsymbol{r}, \underline{\sigma}, t, \Delta t)$$

and insert this expression under the integral in Eq.(**??**). We thus obtain

$$\rho(\boldsymbol{r}, t + \Delta t) = \rho(\boldsymbol{r}, t) - \sum_{k=1}^{3} \frac{\partial}{\partial x_k} \left[ \rho(\boldsymbol{r}, t) \int \sigma_k\, P^M(\boldsymbol{r}, \underline{\sigma}, t, \Delta t)\, d^3\sigma \right] + \\ + \frac{1}{2} \sum_{l,k} \frac{\partial^2}{\partial x_l\, \partial x_k} \left[ \rho(\boldsymbol{r}, t) \int \sigma_l\, \sigma_k\, P^M(\boldsymbol{r}, \underline{\sigma}, t, \Delta t)\, d^3\sigma \right] \quad (345)$$

where we have used the normalization (342).
Because of

$$\sigma_k = \sigma_{r\,k} + \sigma_{c\,k}$$

and

$$\int \sigma_{r\,k}\, P^M(\boldsymbol{r}, \underline{\sigma}, t, \Delta t)\, d^3\sigma = 0\,,$$

the first integral on the rhs yields

$$\int \sigma_{c\,k}\, P^M(\boldsymbol{r}, \underline{\sigma}, t, \Delta t)\, d^3\sigma = v_{c\,k}(\boldsymbol{r}, \bar{t})\, \Delta t$$

where $\boldsymbol{v}_c$ is the convective velocity associated with $\underline{\sigma}_c$, and $\bar{t}$ is a suitably chosen time from the interval $[t, t + \Delta t]$.
The third expression on the rhs of Eq.(345) contains the integral (343). Dividing by $\Delta t$ we obtain in the limit $\Delta t \to 0$

$$\frac{\partial\, \rho}{\partial\, t} + \nabla \cdot (\rho\, \boldsymbol{v}_c) - \nu \Delta \rho = 0\,. \quad (346)$$

This represents the so-called Fokker-Planck equation [102] which is a special case of Kolmogorov's second differential equation [103] derived considerably later. For $\boldsymbol{v}_c = 0$ Eq.(346) reduces to the equation of diffusion

$$\frac{\partial\, \rho}{\partial\, t} = \nu\, \Delta\, \rho\,.$$

In deriving Eq.(346) one should keep in mind that it is actually inadmissible to let $\Delta t$ go to zero because it conflicts with the coarse graining requirement (335). Eq.(346) and everything that follows should therefore be taken with caution. It is exactly this point which will prove crucial in combining the behavior of the A-and the B-system to accomplish a modification of particle motion by reversible scattering.
Apart from Eq.(346) the temporal changes of $\rho(\boldsymbol{r},t)$ must also obey the continuity equation

$$\frac{\partial\,\rho}{\partial\,t}+\nabla\cdot\boldsymbol{j}=0 \tag{347}$$

which preserves the number of particles of the ensemble.
We define a diffusive (or "osmotic") current density by

$$\boldsymbol{j}_d=\boldsymbol{j}-\boldsymbol{j}_c \tag{348}$$

connected with an osmotic velocity $\boldsymbol{u}$

$$\boldsymbol{j}_d=\rho\,\boldsymbol{u} \tag{349}$$

in analogy to

$$\boldsymbol{j}=\rho\,\boldsymbol{v}\,. \tag{350}$$

Eqs.(346) and (347) are simultaneously satisfied if

$$\boldsymbol{j}_d=-\nu\,\nabla\rho \tag{351}$$

which is Fick's law.
From Eqs.(346) to (351) we thus obtain

$$\boldsymbol{v}=\boldsymbol{v}_c+\boldsymbol{u} \tag{352}$$

which is just Eq.(24) used in advance in Section 5. Furthermore, we have

$$\boldsymbol{u}(\boldsymbol{r},t)=-\nu\,\frac{1}{\rho(\boldsymbol{r},t)}\,\nabla\rho(\boldsymbol{r},t)\quad\textbf{"osmotic velocity"}\,. \tag{353}$$

Replacing $\rho(\boldsymbol{r},t)$ in Eq.(344) with $\rho\,v_{c\,k}$, one obtains

$$\frac{\partial\rho\,v_{c\,k}}{\partial t}|_{scatter}=-\nabla\cdot(\rho\,v_{c\,k}\,\boldsymbol{v}_c)+\nu\,\Delta(\rho\,v_{c\,k})\,,$$

There is an additional (local) change in time of the momentum current density effected by the external force

$$\frac{\partial\rho\,v_{c\,k}}{\partial t}|_{force}=\hat{f}_k(\boldsymbol{r})\equiv\frac{1}{m_0}\,\rho(\boldsymbol{r})\,F_k(\boldsymbol{r})\,.$$

Summing up we thus have

$$\frac{\partial \rho\, v_{ck}}{\partial t} = \frac{\partial \rho\, v_{ck}}{\partial t}|_{scatter} + \frac{\partial \rho\, v_{ck}}{\partial t}|_{force}\,.$$

Adding the right-hand sides of the equations for $\frac{\partial \rho\, v_{ck}}{\partial t}|_{scatter}$ and $\frac{\partial \rho\, v_{ck}}{\partial t}|_{force}$ we obtain

$$v_{ck}\,\frac{\partial \rho}{\partial t} + \rho\,\frac{\partial v_{ck}}{\partial t} = \underbrace{-v_{ck}\,\left(\frac{\partial \rho\, v_{cx}}{\partial x} + \frac{\partial \rho\, v_{cy}}{\partial y} + \frac{\partial \rho\, v_{cz}}{\partial z}\right)}_{=-v_{ck}\,\nabla\cdot\underbrace{\rho\,\boldsymbol{v}_c}_{=\boldsymbol{j}_c}} -$$
$$\underbrace{\left(\rho\, v_{cx}\,\frac{\partial}{\partial x}\,v_{ck} + \rho\, v_{cy}\,\frac{\partial}{\partial y}\,v_{ck} + \rho\, v_{cz}\,\frac{\partial}{\partial z}\,v_{ck}\right)}_{=-\rho\,\boldsymbol{v}_c\cdot\nabla v_{ck}} +$$
$$\nu\,\Delta(\rho\, v_{ck}) + \frac{1}{m_0}\,\rho\, F_k\,.$$

Further, one has

$$\nu\,\Delta(\rho\, v_{ck}) = \nabla\cdot(\nabla\nu\,\rho\, v_{ck}) = \nabla\cdot(v_{ck}\,\nu\,\nabla\rho) + \nabla\cdot\,(\nu\,\rho\,\nabla v_{ck})$$

where

$$\nabla\cdot(v_{ck}\,\nu\,\nabla\rho) = v_{ck}(\nu\,\Delta\rho) + \underbrace{\nu\,\nabla\rho}_{=-\rho\,\boldsymbol{u}}\cdot\nabla v_{ck}$$

and

$$\nabla\cdot(\nu\,\rho\,\nabla\, v_{ck}) = \nu\,\rho\,\Delta v_{ck} + \nabla\, v_{ck}\cdot\underbrace{\nu\,\nabla\,\rho}_{=-\rho\,\boldsymbol{u}}\,.$$

One can now reorder the various expressions by collecting those which contain $v_{ck}$ as a factor and another group which has the factor $\rho$ in common:

$$v_{ck}\,\underbrace{\left[\frac{\partial \rho}{\partial t} + \nabla\cdot\boldsymbol{j}_c - \nu\,\Delta\rho\right]}_{=0\hookrightarrow Fokker-Planck-Eq.} +$$
$$\underbrace{\rho\left[\frac{\partial v_{ck}}{\partial t} + (\boldsymbol{v}_c\cdot\nabla)v_{ck} + 2\,\boldsymbol{u}\cdot\nabla v_{ck} - \nu\,\Delta v_{ck} - \frac{1}{m_0}F_k\right]}_{=0\hookrightarrow Eq.(354)} = 0\,.$$

Thus we have

$$\frac{\partial \boldsymbol{v}_c}{\partial t} + (\boldsymbol{v}_c + 2\,\boldsymbol{u})\cdot\nabla\boldsymbol{v}_c - \nu\,\Delta\boldsymbol{v}_c = \frac{1}{m_0}\,\boldsymbol{F}(\boldsymbol{r})\,. \tag{354}$$

Substituting here $\boldsymbol{v}_c$ with $\boldsymbol{v}-\boldsymbol{u}$ we arrive at our Eq.(25):

$$\frac{\partial}{\partial t}\,(\boldsymbol{v}-\boldsymbol{u}) + [(\boldsymbol{v}+\boldsymbol{u})\nabla(\boldsymbol{v}-\boldsymbol{u})] - \nu\,\Delta(\boldsymbol{v}-\boldsymbol{u}) = \tfrac{1}{m_0}\,\boldsymbol{F}(\boldsymbol{r})\,.$$

In hydrodynamics $|\boldsymbol{u}|$ is usually neglected compared to $|\boldsymbol{v}|$ and $\frac{1}{m_0}\,\boldsymbol{F}(\boldsymbol{r})$ is given by the internal mass-referenced force $-\frac{1}{\hat{\rho}(\boldsymbol{r},t)}\,\nabla p\,(\boldsymbol{r},t)$ with $\hat{\rho}(\boldsymbol{r},\,t) = m_0\,\rho(\boldsymbol{r},t)$ denoting the massive density and $p\,(\boldsymbol{r},t)$ the pressure. Under these circumstances the above equation takes the familiar Navier-Stokes-form:

$$\hat{\rho}(\boldsymbol{r},t)\,\underbrace{\left(\frac{\partial\,\boldsymbol{v}}{\partial t}\;+\boldsymbol{v}\cdot\nabla\boldsymbol{v}\right)}_{\frac{d\boldsymbol{v}(\boldsymbol{r},t)}{dt}}-\mu\,\Delta\boldsymbol{v}+\nabla p\,(\boldsymbol{r},t)=0\quad\text{where}\quad\mu=\nu\,\hat{\rho}\,.$$

The derivation of this equation is due to Gebelein [19].

# 40 Appendix B: The origin of quantized electromagnetic fields

As already mentioned earlier, electromagnetic waves owe their occurrence generally to charged oscillating massive particles which obey the time-dependent Schrödingerequation (neglecting relativistic effects). Therefore, they come about in energy portions. We want to demonstrate this for the more general case of an $N$-electron system that represents the complete electronic portion of an atom, molecule or solid. Again, we suppress spin coordinates and assume the $N_n$ nuclei (or the nucleus ($N_n = 1$) being clamped at positions $\boldsymbol{R}_\alpha$. The associated Hamiltonian operator of the system reads

$$\hat{H}=\sum_{j=1}^{N}\left[\frac{(\hat{\boldsymbol{p}}_j-e\,\boldsymbol{A}(\boldsymbol{r}_j,t))^2}{2\,m_0}-\sum_{\alpha=1}^{N_n}\frac{Z_\alpha\,e^2}{4\pi\,\epsilon_0|\boldsymbol{r}_j-\boldsymbol{R}_\alpha|}\right]+\tfrac{1}{2}\sum_{\substack{j,\kappa\\ j\neq\kappa}}\frac{e^2}{4\pi\,\epsilon_0|\boldsymbol{r}_j-\boldsymbol{r}_\kappa|}$$

$$\text{where}\quad\hat{\boldsymbol{p}}_j=-i\hbar\nabla_j\,.$$

Here $e$ denotes the fundamental charge, $m_0$ the rest mass of the electron, and $Z_\alpha$ the atomic number.
For $\boldsymbol{A}(\boldsymbol{r},t)\equiv 0$ we assume the time-independent Schrödingerequation

$$\hat{H}\,\Psi(\boldsymbol{x}_1,\boldsymbol{x}_2,\ldots\boldsymbol{x}_N)=E\,\Psi(\boldsymbol{x}_1,\boldsymbol{x}_2,\ldots\boldsymbol{x}_N)$$

being solved for the groundstate $\Psi_0(\boldsymbol{x}_1,\boldsymbol{x}_2,\ldots\boldsymbol{x}_N)$ and for some excited state $\Psi_k(\boldsymbol{x}_1,\boldsymbol{x}_2,\ldots\boldsymbol{x}_N)$ with eigenvalues $E_0$ and $E_k$, respectively. To keep the argument simple we presuppose the excited state to be a real-valued function. A linear combination of the two solutions

$$\Psi(\boldsymbol{r}_1,\boldsymbol{r}_2,\ldots\boldsymbol{r}_N,t)=c_0\Psi_0(\boldsymbol{r}_1,\boldsymbol{r}_2,\ldots\boldsymbol{r}_N)e^{-i\frac{E_0}{\hbar}\,t}+c_k\Psi_k(\boldsymbol{r}_1,\boldsymbol{r}_2,\ldots\boldsymbol{r}_N)e^{-i\frac{E_k}{\hbar}\,t}$$

satisfies the associated time-dependent Schrödingerequation with constant coefficients $c_0$ and $c_k$ as long as $\boldsymbol{A}(\boldsymbol{r},t)$ remains zero. However, the linear

combination gives rise to an oscillating current density

$$\boldsymbol{j}(\boldsymbol{r},t) = \frac{e\,\hbar}{m_0}\,|c_k^*\,c_0|\,N[\int\ldots\int[\Psi_0(\boldsymbol{r},\boldsymbol{r}_2,\ldots\boldsymbol{r}_N)\nabla\,\Psi_k(\boldsymbol{r},\boldsymbol{r}_2,\ldots\boldsymbol{r}_N)d^3r_2\ldots d^3r_N - \int\ldots\int[\Psi_k(\boldsymbol{r},\boldsymbol{r}_2,\ldots\boldsymbol{r}_N)\nabla\,\Psi_0(\boldsymbol{r},\boldsymbol{r}_2,\ldots\boldsymbol{r}_N)\,d^3r_2\ldots d^3r_N]\sin(\omega\,t+\varphi)\,.$$

where

$$\omega = \frac{E_k - E_0}{\hbar} \quad \hookrightarrow \quad \hbar\omega = E_k - E_0\,. \tag{355}$$

Because of Eq.(154) this gives rise to an outgoing electromagnetic wave which causes a "radiation feedback" since $\boldsymbol{A}(\boldsymbol{r},t)$ now appears in the Hamiltonian as in the previous section. The coefficients $c_0$ and $c_k$ become time-dependent as shown in Fig.11 . That means, within a certain transition time $\tau$ the energy $E_k - E_0$ has left the system and has been transferred to the outgoing wave packet with angular frequency $\omega$. Because of Eq.(355) the energy of that wave packet now appears as "quantized".

# 41 Suggested Reading

There is already a rich literature on attempts that have been made at deriving non-relativistic quantum mechanics from a concept of dissipationless stochastic point mechanics. A precursor of the idea of correlating the probabilistic character of quantum mechanics with the action of a stochastic background field may be seen in the paper by Bohm and Vigier [104]. The present contribution draws on later work on this subject but avoids certain implications that have often been criticized during the past 30 years. See e.g. W. Weizel [105], E. Nelson [106], [107], Guerra and Morato, [108], M. Baublitz [109], L. de la Peña and A. H. Cetto [110], Petroni and Morato [111], T. C. Wallstrom [20] and numerous references therein. For a rather complete review see R.F. Streater [16]. An earlier review covering work up to 1986 is given in a book by Namsrai [112].) More recent contributions are due to Fritsche and Haugk [113] and Xiao-Song Wang [114]
Another approach that also relates to vacuum fluctuations, but draws on non-equilibrium thermodynamics has recently been put forward by Grössing [115]·[116].

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