Unconventional Approach to Orbital-Free Density Functional Theory Derived from a Model of Extended Electrons

Werner A. Hofer

Abstract An equation proposed by Levy, Perdew and Sahni (Phys. Rev. A 30:2745, 1984) is an orbital-free formulation of density functional theory. However, this equation describes a bosonic system. Here, we analyze on a very fundamental level, how this equation could be extended to yield a formulation for a general fermionic distribution of charge and spin. This analysis starts at the level of single electrons and with the question, how spin actually comes into a charge distribution in a non-relativistic model. To this end we present a space-time model of extended electrons, which is formulated in terms of geometric algebra. Wave properties of the electron are referred to mass density oscillations. We provide a comprehensive and non-statistical interpretation of wavefunctions, referring them to mass density components and internal field components. It is shown that these wavefunctions comply with the Schrödinger equation, for the free electron as well as for the electron in electrostatic and vector potentials. Spin-properties of the electron are referred to intrinsic field components and it is established that a measurement of spin in an external field yields exactly two possible results. However, it is also established that the spin of free electrons is isotropic, and that spin-dynamics of single electrons can be described by a modified Landau-Lifshitz equation. The model agrees with the results of standard theory concerning the hydrogen atom. Finally, we analyze many-electron systems and derive a set of coupled equations suitable to characterize the system without any reference to single electron states. The model is expected to have the greatest impact in condensed matter theory, where it allows to describe an $N$-electron system by a many-electron wavefunction $\Psi$ of four, instead of $3N$ variables. The many-body aspect of a system is in this case encoded in a bivector potential.

Keywords Electron structure · Condensed matter physics · Electronic structure calculations · Density functional theory · Orbital free density functional theory
1 Introduction

Electronic structure simulations today underpin many models constructed to account for experimental data. Most of these simulations are based on an implementation of density functional theory (DFT). DFT itself is theoretically justified by the Hohenberg-Kohn theorems [1], even though a model based on the electron density was suggested much earlier by Thomas and Fermi [2–4]. A combination of Thomas-Fermi model and Hohenberg-Kohn DFT leads to the following description of a many-electron system [5],

$$\frac{\delta E[\rho]}{\delta \rho(r)} = \frac{\delta T[\rho]}{\delta \rho(r)} + v_H[\rho](r) + v_{ne}[\rho](r) + v_{xc}[\rho](r) = \mu.$$  (1)

Here, $T[\rho]$ is the kinetic energy functional, depending on the density of electron charge $\rho$, $v_H$ the Hartree potential or the electron-electron repulsion, $v_{ne}$ the electron-nuclei attraction, and $v_{xc}$ the exchange correlation potential. $\mu$ is the Lagrange multiplier due to the condition of charge conservation, or the chemical potential.

While this equation is generally valid, a transferable and fully general kinetic energy functional based on the density has so far remained elusive. It is known that the functional for the homogeneous electron gas is described exactly by the Thomas-Fermi kinetic energy functional (TF), or [2–4, 6]

$$T_{TF}[\rho] = C_{TF} \langle \rho^{5/3}(r) \rangle.$$  (2)

For hydrogen atoms, it is described exactly by the von Weizsäcker functional ($vW$), or [7]

$$T_{vW}[\rho] = \frac{1}{8} \langle \frac{|\nabla \rho(r)|^2}{\rho(r)} \rangle.$$  (3)

In present implementations of orbital-free DFT one either interpolates between the TF and $vW$ functionals for more general density distributions [6, 8], or one bases the whole calculation or parts of it on the Kohn-Sham (KS) method of DFT [5, 9]. The reason, one tries to avoid the KS method as much as possible is that the computational effort in this case scales with the cube of $N$, the number of electrons, which limits the number of atoms which can be included in the simulation to a few thousand. However, most of the technologically interesting materials e.g. in the semiconductor industry are very low doped; one dopant per millions of atoms of the host matrix. In this case current methods are unable to reliably simulate the material.

In a paper in 1984 Levy, Perdew and Sahni [10] showed that one should be able to describe the general density of a system by:

$$\left[ -\frac{1}{2} \nabla^2 + v_{ext} + v_{eff} - \mu \right] \rho^{1/2} = 0.$$  (4)

Here, $v_{ext}$ is the external ionic potential, $v_{eff}$ is the electron-electron repulsion combined with the exchange-correlation potential, and $\mu$ is again the chemical potential, which can be interpreted as a generalized and constant energy density. The problem, which was left unsolved, is that the equation seems to describe a bosonic system. Subsequently, Norman March and others extended the equation to account for
the fermionic nature of electrons. They introduced a Pauli potential, which describes Pauli repulsion between individual electrons in a system [11–13].

This was the starting point of our analysis of orbital free DFT some years ago. The appeal of the equation is that it has the same general form as the Schrödinger equation and that it only includes the density, thus is an orbital-free formulation of DFT. But it is necessary to extend the equation and to generalize it, so that it can be used for arbitrary fermionic systems. This, as will be shown, can be accomplished in a consistent manner. While previous approaches focussed on the extension of the effective potential [11], within the present framework we extend the square root of the density to incorporate electron spin. The analysis necessary to accomplish this task is very fundamental, since it has to start with the question, how spin actually comes into a density distribution in the non-relativistic limit. Such a fundamental analysis has to include not only the structure of electrons, but also its interactions with electromagnetic fields to establish, that the model is fully consistent with the standard results. The structure of the paper is as follows.

In Sect. 2 we review existing electron models in view of their suitability for the tasks at hand and give four postulates, which we think capture the requirements for a comprehensive electron model. We also introduce the wavefunction $\psi$ of single electrons as a multivector of three dimensional geometric algebra.

In Sect. 3 we give a short overview over geometric algebra necessary for the presentation. As condensed matter theorists will most likely not be acquainted with geometric algebra, we think this section is necessary for an understanding of the concepts.

In Sect. 4 we present a motivation why potential components of electrons in motion are necessary to attain wave properties of moving electrons. These electromagnetic energy components differ from the classical components previously introduced by Lorentz and Abraham.

In Sect. 5 we present a consistent and local model of a single-electron’s density and spin components in geometric algebra as well as a relation between these components and the wavefunction of the electron.

In Sect. 6 we determine the interactions of the electron with external static fields and show how the density and spin components change upon interaction.

In Sect. 7 we analyze the interaction of electrons and photons and show that the effect on the electron’s properties can be mimicked by a calculation including only momenta and energies of electrons and photons.

In Sect. 8 we show that the model is consistent with the standard model of hydrogen. However, we also present an extension of the standard model in the non-relativistic regime and including the spin of the electron.

In Sect. 9 we present the model of hydrogen molecules and extend (4) to an arbitrary density distribution and including the spin state of electrons.

Finally, in Sect. 10 we discuss the presented concepts in view of fundamental issues in quantum mechanics and the consistency of the model with existing experiments, in particular the experiments on fundamental quantum mechanics. We also present an outlook on future work to be undertaken to check on the method.

The guiding principle of this work is the ‘radical conservative—ism’ of Wheeler [14]: Insist on adhering to well-established physical laws (be conservative) but follow...
those laws into their most extreme domains (be radical), where unexpected insights into nature might be found. We do not attach any ontological claim to the model suggested. It is adopted purely for its usefulness, as it greatly simplifies the description of many-electron systems, in fact allowing for a coherent theoretical model from the level of single electrons to, in principle, macroscopic systems.

2 Single Electron Models

Generally, it has to be conceded that all attempts to ascribe a reality to the electron, which goes beyond a point particle with an intrinsic momentum and thus magnetic moment, have failed. The most convincing arguments against an internal structure and for a point-like electron come from single-electron diffraction and high-energy scattering experiments. In the first case, the point-like impacts of the single particles, gradually building up a diffraction pattern, are one of the great paradigms in quantum physics, which establish the existence of a guiding principle behind the statistical events [15]. Similarly, high-energy scattering experiments are routinely used to check the predictions of quantum field theory. So far, the agreement between experiment and theory is better than one part in a billion [16].

There have been attempts, most notably by de Broglie, Bohm, and Hestenes [17–23], to ascribe the observed duality of the electron, its wave-features and its discrete charge and mass without manifest volume, to a field-like construct. The pilot-wave theory, originally due to de Broglie, has even gained renewed interest in recent years, see for example the article by Antony Valentini in a recent Physics World issue [18]. However, it is not clear, how these models can be reconciled with the fundamental fields of interaction known in physics. These interactions are all subject to relativity and thus do not allow for action-at-a-distance. Ascribing a physical reality to the wavefunction of an electron itself, while still retaining the mechanical properties of a point particle, inevitably seems to lead to a pilot-wave or Bohm-type theory, where the potentials themselves become non-local [19, 20]. It thus only shifts the central problem, contained in the following question: “What actually is an electron, and which physical property describes its spin?” to the question: “What actually is a quantum potential and in which way does it relate to fundamental interactions?” In addition, it remains unclear, in these models, how spin enters the description of electrons, and how it interacts with magnetic fields. As this is the fundamental problem to be solved in the present context, one needs to go beyond the existing frameworks.

If one takes current experimental results at the atomic scale seriously, then one arrives most likely at the conclusion of Eigler [24]: “I don’t believe in this wave–particle duality … I think it’s mostly just the left-over baggage of having started off understanding the world in terms of particles and then being forced, because of the quantum revolution, to think of the world in terms of waves. Don’t even think about them as particles. Electrons are waves. And if you think of them in terms of waves, you will always end up with the right answer. Always”. A similar point of view, based on a mathematical analysis of quantum mechanical concepts, has recently been put forward by Nikolic [25], calling the wave–particle duality a “myth”. In addition, our most successful theory to describe solids, density functional theory (DFT), even
though it is based on second quantization, still ascribes a reality only to the density of electron charge and its field of interaction [1]. If this is the case, then a model of electrons could also be constructed, not from mechanics and an elementary mass or charge, but from a wave-like structure which interacts in the same way electrons do.

At this point one might observe that it is simply impossible to account for the electron’s spin within a classical model, i.e. a model where spin is represented by a vector in real-space. However, as Hestenes, and Doran and Lasenby have shown [26, 27], the algebra of electron spin, described by the Pauli matrices, is also obtained by a vector model within Geometric Algebra (maybe better known as Clifford Algebra), where it results from the general properties of rotations in three-dimensional space. Along the same lines of thought one also arrives at the result that the $\gamma$-matrices in the Dirac equation of the electron can be seen as expressions of the geometric algebra of four-dimensional space-time. From these facts it is possible to conclude that spin can actually be seen as a “classical” geometric property of the spacetime representation of the electron, which can be described by the even elements of a multivector in geometric algebra [27]. If we choose to represent the wavefunction in a manner which bears on these relations, then it can be written in the following form:

$$\psi = \alpha + \sum_{i \neq j} e_i \wedge e_j \beta_{ij} \quad \alpha, \beta_{ij} \in \mathbb{R}. \quad (5)$$

Here, the symbol $\wedge$ defines the “wedge-product" in geometric algebra between the vectors $e_{i,j}$ of the three-dimensional frame, which yields a “directed-plane” in space. Incidentally, in a frame of three dimensions this wedge product can be interpreted as the conventional cross-product $\times$ between two vectors times a “pseudoscalar”, which in turn can be seen as the imaginary unit, or $i$. In three dimensional space the imaginary component can be interpreted in three different ways: (i) It is either a “directed-plane”, which means it is due to the directions of two independent vectors, or (ii) it is a vector, since every directed-plane is dual to a vector, or (iii) it represents an angle and an axis of rotation [26, 27]. We choose the first interpretation in the following, because it allows for a straightforward interpretation of the observed oscillations of electron waves as charge density oscillations.

We shall start from some ideas developed more than ten years ago [28], and show that they can be extended to yield a model of electrons which is free of contradictions, in accordance with most fundamental results obtained in quantum mechanics, shows that a “wavefunction” of the electron exists which must comply with the Schrödinger equation, and which allows a representation of electron properties within geometric algebra. The clear difference to previous models, e.g. the ones by de Broglie [17], Hestenes [22] or Keller [29] is that (i) the relation between wavefunctions and physical variables like mass density or field amplitudes is made explicit, and (ii) that it is shown in a local and time dependent picture how external applied fields directly translate into a change of the wave-properties of the electron.

The clear disadvantage of the model is that it is unsuitable to describe single-electron diffraction [15]. In this respect, the interpretation of the electron as a point particle and the interpretation of the wavefunction as a probability measure seems indispensable.
However, the model does have conceptual advantages in that it allows for a direct and locally defined relationship between physical properties and (single-electron) wavefunctions. This gain, we think, makes it worthwhile to interpret electrons in this way. Moreover, it allows for a very efficient formulation of many-electron problems. There, it leads to the introduction of a conceptually new bivector potential. This potential is necessary to account for spin-properties in a correlated system. The description also remains remarkably simple and is thus potentially very useful in the development of numerical methods for the simulation of solid state and molecular systems.

The model of electrons rests on four distinct postulates:

1. The wave properties of electrons are a real physical property of electrons in motion.
2. Electrons in motion possess intrinsic electromagnetic potentials which are vector-like.
3. The magnetic moment of electrons is a consequence of the orientation of these electromagnetic potentials.
4. In equilibrium the energy density throughout the space occupied by a single electron is a constant.

It is a discerning feature of postulates that they cannot be derived from phenomena. The same applies to these postulates. However, their logical consequences have to be in line with experiments or a generally applicable theoretical framework. Moreover, they should make these consequences more transparent, i.e. they should lead to a gain in understanding. Finally they should enhance our ability to predict experimental results, i.e. they should lead to an extension of theoretical methods. We think, all this applies to our postulates, as we shall show presently.

3 A Short Introduction to Geometric Algebra

Most solid state physicists will not be familiar with geometric algebra. This short introduction is modeled on an introductory paper by Gull, Lasenby and Doran [30, 31], which in our view provides the easiest introduction to the topic. In a Gibbs vector algebra, built on Euclidean geometry, we have two separate products between vectors, an inner product $a \cdot b$, which is a scalar:

$$a \cdot b = \alpha \in \mathbb{R},$$

(6)

and an outer product $a \times b$, which is a vector:

$$a \times b = c \in \mathbb{R}^3.$$

(7)

In three dimensions the vector product is equal to the wedge product times the imaginary unit $i$, so that $a \times b = -ia \wedge b$. In geometric algebra the two products are combined in a Clifford product or the geometric product between vectors

$$ab = a \cdot b + a \wedge b.$$  

(8)
The geometric product contains thus two parts: a scalar, which is symmetric, i.e., it does not change its sign upon a change of the order of \( \mathbf{a} \) and \( \mathbf{b} \), and a bivector, which is antisymmetric:

\[
\mathbf{a} \cdot \mathbf{b} = \frac{1}{2} (\mathbf{ab} + \mathbf{ba}) = \mathbf{b} \cdot \mathbf{a},
\]

\[
\mathbf{a} \wedge \mathbf{b} = \frac{1}{2} (\mathbf{ab} - \mathbf{ba}) = -\mathbf{b} \wedge \mathbf{a}.
\]

The product of two parallel vectors is a scalar, while the product of two orthogonal vectors is a bivector, denoted by the wedge product. The general product usually contains both, a scalar and a bivector. The wedge product can be seen as a plane, more specifically a plane, the orientation of which is given by the order of the two vectors in the wedge product. In geometric algebra, this is called a directed plane.

It is important to realize that the geometric product, which adds a scalar and a bivector, will have properties of both, the scalar and the bivector. This is exactly like the relation between the real part and the imaginary part in a complex number. In two dimensions it can be shown that the wedge product carries the imaginary unit. The proof is simple. We assume two framevectors, \( \mathbf{e}_1 \) and \( \mathbf{e}_2 \), which are orthogonal. Then we get for the square of the wedge product:

\[
(e_1 \wedge e_2)^2 = e_1 e_2 e_1 e_2 = -e_1 e_1 e_2 e_2 = -1.
\]

This means that the wedge product carries an additional unit, the imaginary unit. A multivector, i.e., a sum of a scalar and a bivector in two dimensions can therefore be mapped onto the complex number space:

\[
z = x + ye_1 e_2 \equiv x + iy.
\]

At a deeper level this property is related to the fact that a wedge product is actually a rotator, or an element of geometric algebra which rotates vectors. This can be seen by acting with a wedge product on the frame vectors:

\[
(e_1 e_2) e_1 = -e_2 e_1 e_1 = -e_2,
\]

\[
(e_1 e_2) e_2 = e_1 e_2 e_2 = e_1.
\]

Rotations are in most undergraduate physics courses described by matrices. The possibility to describe rotations by geometric products suggests a deeper link between geometric products and matrices. In three dimensions a general multivector is described by a scalar, a vector, a bivector and a trivector. The geometric product between frame vectors has the following algebra:

\[
i = e_1 e_2 e_3,
\]

\[
e_1 e_2 = i e_3,
\]

\[
e_2 e_3 = i e_1,
\]

\[
e_3 e_1 = i e_2,
\]

\[
e_i e_i = 1.
\]
Here, $i$ is actually a pseudoscalar, or the highest geometric product (the product of three independent vectors) in three dimensional space. The algebra of three dimensional space is equivalent to the algebra of the Pauli matrices, given by [30, 31]:

$$e_i e_j = \delta_{ij} + i \epsilon_{ijk} e_k,$$

$$\hat{\sigma}_i \hat{\sigma}_j = I \delta_{ij} + i \epsilon_{ijk} \hat{\sigma}_k.$$  \hspace{1cm} (14)

The Pauli matrices $\hat{\sigma}_k$ in this case can be seen as matrix representations of the 3-dimensional geometric algebra. A similar relation between framevectors of a 4-dimensional geometric algebra and Dirac’s $\gamma$-matrices indicates that these matrices also can be seen as an expression of 4-dimensional spacetime [27].

From a general point of view it thus turns out that imaginary components are quite frequently an indication of a geometric basis behind our formulations in a given vector space. It will be seen that this allows for a natural distinction between density related and spin related components in the electron wavefunction.

### 4 Wave Properties and Electrons

In this section we review the original motivation to postulate the existence of field-like energy components for an electron in motion. We show that if one assumes that wave properties of electrons are similar to the wave properties of electromagnetic fields, then the total energy of an electron will be different from its kinetic energy. As stated in previous publications, this is the only possibility to account for wave properties in a physical picture [28]. The approach in quantum mechanics, where one assumes from the outset that the only energy component of an electron must be its kinetic energy, leads invariably to the conclusion that the wave properties of the electron cannot be real which requires then to interpret them as related to the probability density [32–34]. This has been pointed out some time ago. However, here we start from the picture of waves developed in electrodynamics, and shall extend this picture to encompass also electrons in motion. In electrodynamics, the relation between the wavelength $\lambda$ of an electromagnetic wave and its frequency in vacuum $\nu$ is given by the dispersion relation:

$$\lambda \nu = c.$$  \hspace{1cm} (15)

Here, $c$ is the velocity of a photon in vacuum. For photons we also must account for Planck’s relation between the energy $E$ and the frequency $\nu$ of a particle:

$$E = h \nu.$$  \hspace{1cm} (16)

Here, $h$ is the Planck constant, or $6.626 \times 10^{-34}$ Js. For electrons, we start with the de Broglie relation between wavelength and momentum of an electron. This relation was first verified by electron scattering experiments of Davisson and Germer in the 1920s [35] and is today checked routinely in many labs around the world performing low energy electron diffraction experiments. It states that:

$$\lambda = \frac{h}{mv_{el}}.$$  \hspace{1cm} (17)
$m$ in this case is the mass of the electron, or $9.1 \times 10^{-31}$ kg. To see, what happens, if we assume that the Planck and de Broglie relations are both valid for an electron, we now take the velocity $c$ in (15) to be the velocity of the electron $v_{el}$, and combine it with (16) and (17). Then we find that the energy of the electron should be twice its kinetic energy, since:

$$\lambda = \frac{v_{el}}{E} = \frac{h}{mv_{el}} = \frac{1}{v_{el}} \Rightarrow E = mv_{el}^2 = 2 \times E_{kin}.$$  

(18)

If we assume that an electron has wave properties which are similar to the wave properties of a photon, then we immediately arrive at the result that its energy is not its kinetic energy alone. It is, of course, not very plausible that its energy is double its kinetic energy, since this would require in every energy balance of electron acceleration or deceleration that a factor of two should mysteriously show up in the balance sheet. This has never been observed, so the conclusion is fairly safe that this cannot be strictly correct. However, it illustrates a general point which will be the basis of our electron model: wave properties related to physical properties of single electrons (not a statistical manifold of many electrons) are only possible if the electron possesses more than just its kinetic energy. But it is also clear that the energy of the electron must be on average its kinetic energy, because any other assertion requires too many additional assumptions to be reconciled with the energy principle.

5 Oscillating Electron Densities and Potentials

Concerning the electron, one could ask what property of an electron could actually be responsible for its wave features, if these are taken to be real. The obvious answer to this question, and one which will not seem strange to condensed matter theorists, is electron charge (or mass) density. In condensed matter these charge density waves are actually routinely observed, in particular in atomic scale experiments on metal surfaces.

It is therefore also quite natural to assume that the wave properties will be related to some form of density oscillation. Here, we assume that the number density varies in the interval $[0, 1]$, where 1 indicates the density maximum. In the simplest case, that of a free electron traveling at a constant velocity $v_{el}$ in z-direction, these oscillations are described by the plane wave:

$$\rho(z,t) = \frac{\rho_0}{2} \left[ 1 + \cos \left( \frac{4\pi}{\lambda} z - 4\pi vt \right) \right].$$  

(19)

The amplitude $\rho_0$ will be subject to constraints, for example the condition that the density integrated over a certain volume equals unity. This condition, however, need not concern us at this point and it will in fact be shown that all fundamental results necessary can be derived without this normalization condition. It is important, though, to check that the ansatz is compatible with the limit of inertia. For vanishing velocity we get, using (16) and (17):

$$\lim_{v_{el} \to 0} \rho = \rho_0,$$  

(20)

Springer
which is compatible with our basic assumption that the wave properties of electrons and their oscillating density are a direct consequence of their state of motion. An oscillating density of charge for a free electron is ruled out, if no external or internal potential energy components are present, since it violates the energy conservation principle. We thus have to introduce potentials to make up for the periodic variations. As the simplest case, these could be thought of as oscillating $E$ or $B$ fields. The reason for choosing vector fields rather than scalar ones lies in the one known additional property of an electron: electrons possess an intrinsic magnetic moment or a spin. Since such a property is incompatible with a scalar distribution of field properties, it has to be related in the simplest case at least to some kind of vector field. Whether this is sufficient, has to be established subsequently by an analysis of interactions of electrons with external electro-magnetic fields. The two additional fields we introduce are an electric $E$ and a magnetic $H$ field, which are thought transverse as in the case of photons, but with double the wavelength and consequently half the frequency of the density oscillations.

$$E = e_1 E_0 \cos \left( \frac{2\pi}{\lambda} z - 2\pi \nu t + \phi \right),$$

$$H = e_2 H_0 \cos \left( \frac{2\pi}{\lambda} z - 2\pi \nu t + \phi \right).$$

The helicity in this way can either be positive—it complies with the standard right-hand behaviour—or negative—it is the opposite. This feature introduces two possible groundstates of the free electron, which shall be later identified as its spin-up and spin-down state. The additional phase $\phi$ has been added to account for energy conservation of electrons at the local level.

Electromagnetic components to the electron’s mass are not a new concept. They have also been proposed by Abraham and Lorentz in their “classical” models of electrons [36, 37]. Compared to these classical models, the present one is different in two aspects: (i) The shape of the electron, e.g. a point or a sphere, is not imposed from the outset. Such a shape would show up in high-energy scattering events in the scattering cross sections. While this is true for protons or, more generally, for atomic nuclei, it has never been found for electrons. One reason could be that electrons actually do not possess a defined shape, but that their shape depends on the potential environment. (ii) The electromagnetic components are not constant, but depend on the state of motion of the electron. This is, as analyzed in previous sections, necessary to reconcile the assumption with the wave features of electrons.

Energy conservation requires that the energy density at every single point of the electron is a constant. The energy density of the field components at a given point is:

$$E_{\text{field}} = \frac{1}{2} \varepsilon_0 E^2 + \frac{1}{2\mu_0} H^2$$

$$= \left( \frac{1}{2} \varepsilon_0 E_0^2 + \frac{1}{2\mu_0} H_0^2 \right) \cos^2 \left( \frac{2\pi}{\lambda} z - 2\pi \nu t + \phi \right).$$

The simplest solution to the constant energy density problem, which is also the simplest solution for the wave propagation of an electron is a phase shift of the fields by
\pi/2, so that
\[ \phi = \frac{\pi}{2} \Rightarrow E_{\text{field}} = \left( \frac{1}{2} \varepsilon_0 E_0^2 + \frac{1}{2} \mu_0 H_0^2 \right) \sin^2 \left( \frac{2\pi}{\lambda} z - 2\pi \nu t \right). \] (23)

At this stage the introduction of fields with the given frequencies and wavelengths becomes clear, because we can eliminate periodic components of the total energy density with the help of the relation for the cosine at half angles:
\[ 2 \cos^2(x) = 1 + \cos(2x). \] (24)

The kinetic energy density is then, in a first step:
\[ E_{\text{kin}} = \frac{1}{4} \rho_0 v_{\text{el}}^2 \left[ 1 + 2 \cos^2 \left( \frac{2\pi}{\lambda} z - 2\pi \nu t \right) - 1 \right]. \] (25)

And with the following ansatz for the amplitudes of the fields:
\[ \left( \frac{1}{2} \varepsilon_0 E_0^2 + \frac{1}{2} \mu_0 H_0^2 \right) = \frac{1}{2} \rho_0 v_{\text{el}}^2. \] (26)

We get for the total energy density:
\[ E_{\text{tot}} = \frac{1}{4} \rho_0 v_{\text{el}}^2 + \frac{1}{4} \rho_0 v_{\text{el}}^2 \left[ 2 \cos^2 \left( \frac{2\pi}{\lambda} z - 2\pi \nu t \right) + 2 \sin^2 \left( \frac{2\pi}{\lambda} z - 2\pi \nu t \right) - 1 \right] \]
\[ = \frac{1}{2} \rho_0 v_{\text{el}}^2. \] (27)

In contrast to the statement in (18), the model leads to the result that the total energy is equal to the kinetic energy of the electron, as also assumed in quantum mechanics. At a fundamental level, this is due to one feature of the ansatz: the wavelengths of field components and mass density components are different. The electron’s energy density is determined by its mass density at the groundstate, i.e. \( v_{\text{el}} \to 0 \), even though the electron wave is a physically real—i.e. with a physical property, the density, periodic in space and time—feature. The relation between the frequency \( \nu \) and the wavelength \( \lambda \) of this wave is the same as for a de Broglie wave, i.e., the group velocity is equal to:
\[ v_g = \frac{d \omega}{dk} = \frac{d (m v_{\text{el}}^2 / 2 \hbar)}{d (m v_{\text{el}} / \hbar)} = v_{\text{el}}. \] (28)

At this point the model captures at least four fundamental properties of the electron in the conventional model. These properties are:

- The wavelength of the electron wave is inverse proportional to its momentum (de Broglie).
- The frequency of the electron wave is proportional to its kinetic energy (Planck).
- The total energy of the electron is just the kinetic energy of its rest mass at every point of wave propagation (Energy conservation).
The total density of a free electron including the fields is a constant and equal to the inertial electron density (quantum mechanical plane wave).

So far all variables introduced, the density as well as the fields are thought to be physical quantities, i.e. they should be in principle measurable. But the ansatz also leads to the conclusion that a wavefunction, if defined on the basis of this model and in line with the required properties, cannot be a physical quantity. This is shown in the following section.

5.1 Stability of Free Electrons

Before, we have to consider an additional problem, which becomes imminent, as soon as the electron is considered to be a structure with a finite extension in space and not a point-particle without structure: the problem of Coulomb repulsion. In DFT this problem arises due to the requirement that one electron does not interact with itself. Exchange and correlation potentials thus have to be corrected for this constraint [38]. The situation is different in classical electrodynamics, where the electron, as a point particle, would carry infinite electrostatic energy (see p. 751 of [39]). This has been the starting point of early attempts by Abraham and Lorentz to circumvent the problem by stating that the electron’s mass was purely electromagnetic [36, 37]. The electron radius, its classical radius, is then about 2.8 fm. However, this is still orders of magnitude larger than the largest possible radius inferred from high-energy scattering experiments. In relativistic quantum electrodynamics the problem of electron self-energy is removed by renormalization [40].

In the present context the problem is rather trivially solved (with, of course, the remaining problem of electron self-interference, see the discussion), by defining a cohesive static potential \( \phi_{coh} \), depending on the electron density. Electron charge densities are typically one electron per sphere with a Wigner-Seitz radius \( r_s \) of about two atomic units, as found in solids. We start from a spherical charge distribution of density \( \rho_0 \), with a radius of \( r_s \). Then the repulsion energy is given by the following integral (we use atomic units in the following derivation):

\[
W = \rho_0^2 \int_0^{r_s} dr \frac{4\pi r^3}{3} r^4 \frac{1}{r^2} = \left( \frac{4\pi}{3} r_s^3 \rho_0 \right) \left( \frac{4\pi}{3} r_s^3 \rho_0 \right) \frac{3}{5 r_s} = \frac{3}{5 r_s}.
\]  

(29)

The potential associated with this repulsion, the Hartree potential, is thus:

\[
V_H = V_H(r_s) = \frac{3}{5} r_s^{-1}.
\]

(30)

For electrons in metals the typical value for \( r_s \) is about two Bohr radii. There is no reason to assume that the density for a free electron will be substantially different. Thus the additional cohesive potential for a free electron should be:

\[
V_{coh} = -\frac{3}{5 r_s} \approx (r_s = 2 \text{ au}) \approx -8.16 \text{ eV}.
\]

(31)
For a free electron the sum of both potentials must be zero. The repulsive and attractive fields are \((\Omega_1\text{ is the volume of the Wigner-Seitz cell):}\)

\[
\frac{W_{coh}}{\Omega} = -\rho_0 \phi_{coh} = -\rho_0 \left(\frac{4\pi}{3} r_s^3 \rho_0\right) \frac{3}{5r_s},
\]

\[
\phi_{coh} = -\frac{3}{5r_s}, \quad \phi_H = \frac{3}{5r_s},
\]

\[
\phi_{el,0} = \phi_{coh} + \phi_H = 0.
\]

(32)

Summarizing the results of this analysis we find that a model of free electrons, which refers wave properties to oscillating charge densities and electromagnetic potentials, can be in line with conventional experimental and theoretical models because the total energy of the electron is in both cases equal to the kinetic energy of the electron, and complies with the fundamental Planck and de Broglie relations. The repulsive Hartree potential within a single electron is corrected by a cohesive potential, which depends on the density of electron charge. The total electrostatic potential in this case vanishes, as required by all conventional theoretical models of single electrons. For the following derivations we use atomic units, where \(e = m = c = \hbar = 1\).

5.2 Why Wavefunctions are not Physical Objects

The requirements for a wavefunction \(\psi\) or a spinor in the context of the Dirac theory are that the wavefunction can be written as a complex number (vector for spinors), that a duality operation \(\psi \rightarrow \psi^\dagger\) exists, and that the product of \(\psi\) and \(\psi^\dagger\) is positive and equal to the number density of the electron. In atomic units the number density is equal to the mass density and also, multiplied with the square of the velocity of light in vacuum, the energy density. In the following analysis this eases the notation considerably, while it would have to be complemented by suitable constants if performed in the SI system of units. Given the two separate energy contributions in our model, we can readily identify the real part of the wavefunction as the square root of the number density, or \(\rho^{1/2}\). The imaginary part is more difficult to pin down. The requirement here is that it must be related to the magnetic properties of the electron, or its “spin”. The simplest ansatz is due to geometric algebra and the geometric product between vectors. Following our model we assume that the velocity vector of the electron is parallel to \(e_3\). For ease of notation we introduce here a Poynting-like vector, where the electromagnetic energy flux is given by (in atomic units \(c = 1\)):

\[
S = \mathcal{E} \mathcal{H} = e_1 e_2 E_0 H_0 \sin^2 \left(\frac{2\pi}{\lambda} z - 2\pi vt\right).
\]

(33)

Then the energy density of field components is given by the following scalar:

\[
S = i e_3 S,
\]

(34)

\[
S = E_0 H_0 \sin^2 \left(\frac{2\pi}{\lambda} z - 2\pi vt\right),
\]

(35)

\[
S = S_0 \sin^2 \left(\frac{2\pi}{\lambda} z - 2\pi vt\right), \quad S_0 \equiv E_0 H_0.
\]

(36)
If we require that the real part of the wavefunction does not change under a transformation from positive to negative helicity, and that the imaginary part is antisymmetric, then we can write the wavefunction in the following way:

$$\psi = \rho^{1/2} + S^{1/2}e_1e_2 = \rho^{1/2} + iS^{1/2}e_3. \quad (37)$$

The wavefunction in this case is a multivector composed of a scalar (the “real” component) and a bivector (the “imaginary” component). The duality operation changes the helicity of the electron; so exchanging the direction of $E$ and $H$ we obtain:

$$\psi^\dagger = \rho^{1/2} + S^{1/2}e_2e_1 = \rho^{1/2} - iS^{1/2}e_3. \quad (38)$$

For the product of $\psi$ and $\psi^\dagger$ we get consequently:

$$\psi^\dagger\psi = \psi\psi^\dagger = \rho + S. \quad (39)$$

And if we set, as before:

$$\rho = \rho_0 \cos^2 \left( \frac{2\pi}{\lambda} z - 2\pi \nu t \right),$$
$$S = S_0 \sin^2 \left( \frac{2\pi}{\lambda} z - 2\pi \nu t \right), \quad S_0 = \rho_0. \quad (40)$$

Then we obtain the result that the product $\psi^\dagger\psi$ corresponds to the inertial number density of the electron:

$$\psi^\dagger\psi = \rho + S = \rho_0 = \text{constant} \quad (41)$$

which is the standard result in quantum mechanics and also in density functional theory. However, within the present framework wavefunctions also have a physical content, contrary to their role in the standard model where only their square has a meaning, that of a probability density. One could pin down the difference by saying that even though the wavefunction is certainly not a physical object of the same reality as an electromagnetic field vector or a scalar potential, it contains physically real objects like fields and mass (or charge) densities—or rather the roots thereof.

The multivector $\psi$ does not comply with the time-dependent Schrödinger equation, because the single time derivative of $\psi$ will yield the sum of a vector and an imaginary number (the “odd” elements of a multivector in three dimensions). In our view this bears on the fact that the model developed so far is not covariant. For applications in DFT this is not relevant, as the LPS (4) is based on the time-independent Schrödinger equation. In order to compare the extended model of the electron to standard theory, we therefore define the Schrödinger wavefunction $\psi_S$ as a complex number, retaining the direction perpendicular to the field vectors $e_3$ as a hidden variable:

$$\psi_S = \rho_0^{1/2} \left[ \cos \left( \frac{2\pi}{\lambda} z - 2\pi \nu t \right) + i \sin \left( \frac{2\pi}{\lambda} z - 2\pi \nu t \right) \right]$$
$$= \rho_0^{1/2} \exp i \left( \frac{2\pi}{\lambda} z - 2\pi \nu t \right). \quad (42)$$
The kinetic energy operator or the time differential acting on $\psi_S$ then returns the energy eigenvalue of the free electron:

$$-\frac{1}{2} \nabla^2 \psi_S = -i^2 \frac{4\pi^2}{\lambda^2} \psi_S = \frac{1}{2} v_{el}^2 \psi_S = E \psi_S,$$

$$i \frac{\partial}{\partial t} \psi_S = -i^2 \omega \psi_S = \omega \psi_S = E \psi_S.$$  \hspace{1cm} (43)

It is interesting to note that the current density $\mathbf{J}$, as defined from the continuity equation and the time-dependent Schrödinger equation will be a function without local density variations. From the continuity equation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{J} = \frac{\partial}{\partial t} \psi_S^\dagger \psi_S + \nabla \cdot \mathbf{J} = 0,$$  \hspace{1cm} (44)

we obtain the following result for $\mathbf{J}$:

$$\mathbf{J} = \frac{1}{2i} \left( \psi_S^\dagger \nabla \psi_S - \psi_S \nabla \psi_S^\dagger \right),$$

$$\mathbf{J} = \frac{2i}{2i} \left[ (\rho)^{1/2} \nabla S^{1/2} - S^{1/2} \nabla (\rho)^{1/2} \right]$$

$$= \rho_0 \left[ \cos \left( \frac{2\pi}{\lambda} z - 2\pi vt \right) \frac{\partial}{\partial z} \sin \left( \frac{2\pi}{\lambda} z - 2\pi vt \right) + \sin \left( \frac{2\pi}{\lambda} z - 2\pi vt \right) \frac{\partial}{\partial z} \cos \left( \frac{2\pi}{\lambda} z - 2\pi vt \right) \right] \mathbf{e}_3$$

$$= \rho_0 v_{el} \left[ \sin^2 \left( \frac{2\pi}{\lambda} z - 2\pi vt \right) + \cos^2 \left( \frac{2\pi}{\lambda} z - 2\pi vt \right) \right] \mathbf{e}_3 = \rho_0 v_{el} \mathbf{e}_3$$

which is equal to the momentum density of the inertial electron mass. It thus gives a consistent picture of the electron as an entity without any inner structure.

To summarize the findings of this analysis we may say that even though this model electron is an entirely physical object, all of whose properties are described by standard physical quantities, we can only describe it as a scalar complex number, i.e. a wavefunction, if this wavefunction itself does not have a direct physical meaning.

### 6 Electrons in Static External Fields

While quantum mechanics, as shown in the previous section, describes an electron by a complex number, a wavefunction, which is not strictly speaking a physical object, it does so consistently by assigning a current density to the propagation of the electron’s inertial mass. Then, of course, an external electric or magnetic field cannot affect the density distribution of the electron in a physically transparent manner. Within the present context, where all components of an electron in motion are actually physical objects, we have to develop an understanding, at a very fundamental level, what actually takes place if an electron is accelerated. Let us assume that this is
due to an external potential $\phi$. From a physical point of view, four discrete processes are bound to happen:

1. The electron velocity will change.
2. The electron’s density distribution will change.
3. The electromagnetic field components will change.
4. The intensity of the external field $\phi$ will be diminished due to energy transfer.

The way to account for all four processes is captured in the following equation:

$$f = -\nabla \phi = \rho_0 \frac{d v_{el}}{dt}. \quad (46)$$

The sink in the scalar field $\phi$ here accounts for the transfer of energy from the external field to the electron. It is easy to prove that the internal variations of the mass density or the field $S$ do not change this equation. We know from the preceding derivations that

$$\rho + S = \rho_0 = \text{constant}. \quad (47)$$

Then it follows that:

$$\dot{S} + \dot{\rho} = 0 \quad \rightarrow \quad \frac{d}{dt} \langle \psi_S^\dagger \psi_S \rangle v = \rho_0 \frac{d v_{el}}{dt}. \quad (48)$$

Therefore (46) is valid without restrictions. Again, as for the current density, we find that the density variations are hidden in the combined effect on density and field contributions. Interestingly, this is only the case because the time derivative of the density variations is of equal magnitude but opposite sign as the derivative of the field variations.

6.1 The Problem of Frequency

At this point it is unclear, what the frequency of an electron wave after acceleration in an external potential will be. We cannot use the conventional reasoning in quantum mechanics that the total energy is reflected by the frequency, while the wavelength is connected to the kinetic energy. This reasoning, which is one of the heuristic arguments to introduce the Schrödinger equation, is only justified on the basis of classical mechanics. In particular, it is still unclear, how an external potential actually influences the frequency of an electron wave. However, a closer look at the fundamental experimental results leading to the development of quantum mechanics reveals that the change of frequency with the intensity of electrostatic fields is already implicitly contained in Einstein’s work on photoelectron emission. There, the kinetic energy of a metal electron and its frequency are related to the frequency of the incident photon and the intensity of the metal potential $\phi_m$ via:

$$\frac{v_{el}^2}{2} = \omega_{el} = \omega_{ph} - \phi_m. \quad (49)$$

Generalizing this result, it can be said that the frequency $\omega_{el}$ of an electron in an electrostatic field, compared to the frequency $\omega_{el}^0$ of a free electron, shifts due to the
existence of an electrostatic potential with:

$$\omega_{el}(\phi_m) = \omega^0_{el} - \phi_m.$$  (50)

Then the density components and the field components of the electron in an external potential $\phi$ will comply with:

$$\psi_S = \rho^{1/2} + i S^{1/2},$$

$$\rho^{1/2} = \rho^0_{1/2} \cos \left[ \frac{2\pi}{\lambda} z - (\omega^0_{0} - \phi_m)t \right],$$

$$S^{1/2} = \rho^0_{1/2} \sin \left[ \frac{2\pi}{\lambda} z - (\omega^0_{0} - \phi_m)t \right],$$

$$\psi_S = \rho^0_{1/2} \exp i \left[ \frac{2\pi}{\lambda} z - (\omega^0_{0} - \phi_m)t \right].$$  (51)

It should be clearly understood at this point that the frequency transferred to the electron is not the original frequency of the photon, but that this frequency is diminished, within the metal, due to the effect of the metal’s electrostatic field. This diminished frequency is the frequency which the photon could actually transfer to the electron. The free electron, which is then measured, has this diminished frequency and a wavelength, which corresponds to this frequency: a mechanism of enforcing a wavelength, which we shall analyze in some details further down when we present a detailed model of photon-electron interactions. At this point it becomes clear that this wavefunction, corrected for a change of frequency due to electrostatic potentials compared to the wavefunction of a free electron, complies with the general Schrödinger equation for electrons in a potential $V = -\phi_m$:

$$-\frac{1}{2} \nabla^2 \psi_S = \frac{\omega^2_{el}}{2} \psi_S = \omega^0 \psi_S,$$

$$i \frac{\partial}{\partial t} \psi_S = (\omega^0_{0} - \phi_m) \psi_S,$$

$$i \frac{\partial \psi_S}{\partial t} = \left[ -\frac{1}{2} \nabla^2 + V \right] \psi_S.$$  (52)

Again, it should be kept in mind that while the wavefunction itself is not a physical object, but a multivector in geometric algebra, its components, the real part and the bivector or imaginary part, are related to real physical properties. Here, we have assumed one direction of motion of the electron. It is, however, clear that the same general relation must apply to a general direction of motion. Equation (52) is therefore generally valid.

Considering, for example, an electron in a one-dimensional well $V$ of length $L$, we find the usual result that $k = 2\pi/L \cdot n$. In this case a superposition of left and right
traveling waves corresponds to:

\[
\begin{align*}
\psi^+ &= \rho^{1/2} + i e_3 S^{1/2}, \\
\psi^- &= \rho^{1/2} - i e_3 S^{1/2}, \\
\psi &= \frac{1}{2} (\psi^+ + \psi^-) = \rho^{1/2}, \\
\psi^2 &= \rho.
\end{align*}
\] (53)

The density distribution measured, e.g. in Mike Crommie’s quantum corral experiments [41], is then the real electron density and not the probability density.

6.2 Electron in a Magnetic Field

The acceleration of electrons in an external magnetic field is, conventionally, described by the Lorentz force equation:

\[
\rho_0 \frac{dv}{dt} = \rho_0 (E + v \times B).
\] (54)

In geometric algebra, the same relation is expressed in a Lorentz covariant manner and using the Faraday multivector \( F \) (see p. 157 of [27]):

\[
F = E + i B, \quad \dot{v} = F \cdot v.
\] (55)

We have shown in the previous sections dealing with electron acceleration that the electron’s momentum change is described by the product of the inertial electron density times the change of the electron velocity. This result is in accordance with the standard model, e.g. in density functional theory, where the electron does not possess an intrinsic and variable structure. Here, we only need to add that the same applies to the component of the Lorentz force which is perpendicular to the electron’s velocity. A separate verification is therefore not required.

The situation becomes more interesting, if we analyze the change of the electron’s intrinsic structure in a constrained trajectory. One can think, for example, of an electron contained in the potential well of a atomic nucleus, which has to follow the velocity vector of the nucleus. Then, the changes due to the external magnetic field must act on the electron’s intrinsic properties as well. The important question, in the context of quantum mechanics, is how an external field will affect the electron’s “spin”. However, we have not yet defined what the spin of an electron actually is in the present model. Following Doran and Lasenby [27] we could define the spin of an electron as:

\[
s = \frac{1}{2} \psi e_3 \psi^\dagger.
\] (56)
Since $\psi = \rho^{1/2} + e_1 e_2 S^{1/2}$ and $\psi^\dagger = \rho^{1/2} - e_1 e_2 S^{1/2}$ the spin in this case is perpendicular to the field plane:

$$\psi e_3 \psi^\dagger = \rho e_3 - (\rho S)^{1/2} e_3 e_1 e_2 + (\rho S)^{1/2} e_1 e_2 - S e_1 e_2 e_1 e_2$$

$$= (\rho + S) e_3 + (\rho S)^{1/2} (e_1 e_2 + e_2 e_1) e_3 = \rho_0 e_3,$$

(57)

$$s = \frac{1}{2} \rho_0 e_3.$$

The spin, defined in this manner, is a constant vector associated with the direction perpendicular to the $S$ plane. However, this is not compatible with the experimental results on Stern-Gerlach experiments [42], because an external magnetic field perpendicular to the electron’s trajectory would lead to a vanishing magnetic moment. Calculating the equivalent expression for the direction $e_2$, which is perpendicular to the direction of motion, we obtain:

$$\psi e_2 \psi^\dagger = \left(\rho^{1/2} + i e_3 S^{1/2}\right) e_2 \left(\rho^{1/2} - i e_3 S^{1/2}\right)$$

$$= \rho^{1/2} e_2 \rho^{1/2} - \rho^{1/2} e_2 i e_3 S^{1/2} + i e_3 S^{1/2} e_2 \rho^{1/2} - i e_3 S^{1/2} e_2 i e_3 S^{1/2}$$

$$= (\rho + S) e_2 + i (\rho S)^{1/2} (e_3 e_2 - e_2 e_3)$$

$$= \rho_0 \left[ e_2 + \sin\left(\frac{4\pi}{\lambda} z - 2\omega t\right) e_1 \right].$$

(58)

In the last lines we have used the anticommutation of frame vectors and the trigonometric relations for half angles. The directions $e_1$ and $e_2$, perpendicular to the direction of electron motion, yield equivalent results: a constant vector in one direction and an oscillating vector in the direction perpendicular to it. The spin vector, defined in the same manner as above, would then be:

$$s = \frac{1}{2} \psi e_2 \psi^\dagger = \frac{\rho_0}{2} \left[ e_2 + \sin\left(\frac{4\pi}{\lambda} z - 2\omega t\right) e_1 \right].$$

(59)

Here we slightly modify our electron model: we assume that the plane of electromagnetic fields is not perpendicular to the velocity vector, but that the velocity vector encloses an angle of $45^\circ$ with its projection in the plane. The spin vector for this electron can then be described by:

$$s^\pm = \frac{1}{2} \rho_0 \left[ \pm \frac{e_3 + e_2}{\sqrt{2}} \pm \frac{1}{\sqrt{2}} \sin\left(\frac{4\pi}{\lambda} z - 2\omega t\right) e_1 \right].$$

(60)

The spin average over one period $\tau = 1/\nu$ will then be:

$$\langle s^\pm \rangle = \frac{1}{\tau} \int_0^\tau s^\pm dt = \pm \frac{1}{2} \rho_0 \frac{e_3 + e_2}{\sqrt{2}}.$$

(61)

It should be clear, though, that the previous derivations remain valid also for this modification of the electromagnetic plane. The reason for this is that the scalar and bivector components are separately accounted for and every cross product will vanish
for a term $\psi^\dagger \psi$. The orientation of the bivector plane is a free variable in the description, the energy conservation principle restricts only the phase of the wave, but not the orientation of the plane. According to postulate 3 of the introduction the magnetic properties of the electron should be due to the orientation of the fields, which in the previous equation has been linked to the orientation of the spin vector. Then we may define a magnetic moment density of the electron by:

$$\vec{\mu} = \gamma \langle \mathbf{s} \rangle = \gamma \rho_0 \frac{\pm (\mathbf{e}_3 + \mathbf{e}_2)}{\sqrt{2}}.$$  \hspace{1cm} (62)

In an external magnetic field, aligned for example in the $\mathbf{e}_2$ direction, the magnetic moment density will interact with the field and lead to a variation of the static potential according to:

$$\phi_B = -\vec{\mu} \cdot \mathbf{B}_{\text{ext}} = -\vec{\mu} \cdot B_0 \mathbf{e}_2.$$  \hspace{1cm} (63)

This static potential will affect the frequency of the electron wave in the same way as an electrostatic potential. Writing, for efficiency, the wavefunction of the system in the magnetic field as:

$$\psi = \psi_0 e^{-i\omega_B t},$$  \hspace{1cm} (64)

where $\psi_0$ encapsulates all other degrees of freedom of the electron wave and it is assumed that we can completely separate the magnetic degrees of freedom in the wavefunction $\psi$. Then from the time-dependent Schrödinger equation we get immediately:

$$i \frac{\partial \psi}{\partial t} = \omega_B \psi = \pm \frac{\gamma B_0 \rho_0}{2 \sqrt{2}} \psi,$$

$$\omega_B = \pm \frac{\gamma B_0 \rho_0}{2 \sqrt{2}}.$$  \hspace{1cm} (65)

Within the framework of geometric algebra and using rotors instead of complex exponentials the wavefunction $\psi$ rotates around the direction of the external $B$ field. The resulting effect is much the same: the interaction of the field-components with the external field leads to a rotation of the spin vector around the magnetic axis with two opposite vectors of magnetic moment [43]. In a Stern-Gerlach experiment, in this case, the ensuing trajectory will either be deflected along the positive or the negative $y$ axis: exactly the result observed in the actual experiments [42].

6.3 Spin Isotropy

In standard theory, the spin of electrons is isotropic. This means, that the direction of the spin vector without an external magnetic field is undefined. It seems at first glance that the previous section, where the spin vector was oriented in a definite direction with respect to the vector of electron propagation, contradicts the model in standard theory. If, for example, the external magnetic field $\mathbf{B}$ is oriented along the $\mathbf{e}_1$ axis, then the static potential $\phi_B$ will be zero. Clearly, this contradicts the observations in Stern-Gerlach type experiments, where the split into two separate trajectories is independent of the orientation of the field.

The aim of this section is to show, how the concept of isotropic spin fits into the presented model of electrons. From preceding sections we know that electrons with
vanishing velocity do not possess field components to their energy density. If the plane of these field components is related to the direction of spin, then electrons of zero velocity do not possess spin.

As the electron only possesses spin, if it is in motion, the question arises, how the spin vector relates to the plane of the electromagnetic energy components. The electric $E$ and magnetic $H$ components are in the plane perpendicular to the velocity vector of the electron, the vector $E \times H$ can therefore either be parallel (positive helicity) or anti-parallel (negative helicity) to the velocity vector. Then the spin vector of a free electron is described by the following relations:

$$s_0^\pm = \pm \frac{1}{2} \psi e_3 \psi^\dagger = \pm \frac{1}{2} \rho_0 e_3.$$  \hspace{1cm} (66)

In this case the spin-vector of a single electron is isotropic with respect to the plane perpendicular to the direction of motion. As this direction is singled out due to the motion of the electron, the spin of a single electron cannot be completely isotropic, if spin is to be a consequence of electron motion. However, for a statistical manifold of $n^+$ spin-up ($s_0^+$) and $n^-$ spin-down ($s_0^-$) electrons, where $n^+ = n^-$ the manifold will be fully isotropic in 3-dimensional space. So far, the model is thus in accordance with experimental evidence.

Considering the experimental evidence further, it is inconceivable that the plane of the electromagnetic field components has a defined orientation, which is not perpendicular to the vector of velocity, without any external $B$ field, as this would lead not to two discrete experimental results but, depending on the orientation of the field, to more or less continuous results. However, it is not in contradiction with experiments, if the orientation is well defined and not perpendicular to the velocity direction within an external $B$ field.

This analysis shifts the focus on the process considerably, because in this case the key problem is not to find an orientation of the spin vector, which yields two discrete results in every possible measurements in an external gradient of $B$ (which, of course, will lead to the Pauli equation and Pauli matrices \cite{44, 45}), but to determine, how an external field $B$ changes the orientation of the field plane. If the external field rotates the field plane by an angle which is proportional to the angle between the external field vector $B$ and the vector of electron propagation $v_{el}$, then the result is exactly the result obtained in the previous section: the magnetic moment then is either positive or negative with respect to the plane perpendicular to the external field and the possible measurements are either a deviation in positive or in negative direction, as observed in a Stern-Gerlach experiment. We have assumed, in the previous section, that this angle is half the angle between the field vector and the velocity vector. This choice, however, is not compulsory. As the exact angle will have to be determined by a careful analysis of experimental results, it is well beyond the scope of this paper, which only seeks to establish, that experimental results in static magnetic fields are in accordance with the proposed model of extended electrons. In fact, as shown in the following, this angle is contained in a constant, which describes the rotation of the field components by a modified Landau-Lifshitz equation.
6.4 Spin Dynamics

In condensed matter theory the dynamics of a spin system is described by the semi-empirical Landau-Lifshitz equation, which reads [46]:

\[
\frac{\partial \vec{M}}{\partial t} = -\frac{\gamma}{1 + \alpha^2} \vec{M} \times \vec{H} - \frac{\gamma \alpha}{(1 + \alpha^2) M_S} \vec{M} \times (\vec{M} \times \vec{H}).
\]  

(67)

In this equation \(\vec{M}\) is the magnetization vector, \(\vec{H}\) the applied magnetic field, \(M_S\) the saturation magnetization, and \(\alpha\) and \(\gamma\) an empirical constant and the gyromagnetic ratio of the electron. As shown above, the field component \(\vec{S}\) of the electron in motion will precess around the magnetic vector if it is not parallel or antiparallel to the velocity. This is described by the first part of the equation. The second part is commonly associated with damping. Here, we propose a formulation, which is similar to the second component of the equation, but will lead to two discrete and anti-parallel induced spin directions. It includes the velocity vector of the electron to describe something akin to a torque acting on the field vector. The change of direction due to an external \(\vec{B}\) field is described by:

\[
\frac{d\vec{S}}{dt} = \text{const} \cdot \vec{S} \times (\vec{v} \times \frac{d\vec{B}}{dt}).
\]

(68)

If the field is switched on in a finite interval, and to first order in the approximation, the induced field vector within an external field is then described by:

\[
\vec{S}_{\text{induced}} = \text{const} \cdot \vec{S} \times (\vec{v} \times \vec{B}).
\]

(69)

The equation has two discrete solutions (see Fig. 1). Given now that the field vector precesses around the external field we obtain exactly two solutions with opposite sign, which, in a field gradient along the \(x\)-direction will lead to two deflections in a Stern-Gerlach experiment.

We conclude the presentation of a model of electron interactions with magnetic fields by pointing out that the key difference to standard models is that spin isotropy is taken to its logical extreme: the spin of an electron is only defined with respect
to the velocity vector of the electron, but not with respect to the external magnetic field. External fields lead, as in standard condensed matter physics, to a breaking of rotational symmetry. We may thus conclude that the model of electrons developed accounts for all known effects in static magnetic or electrostatic fields.

6.5 Rotations and Wavefunction Symmetry

The distinguishing property of fermions is that their wavefunction changes its sign upon a rotation by $2\pi$. To see that this is also the case for our wavefunctions, we study a rotation of the spin vector $s$ of the free electron. In geometric algebra a rotation of a vector is accomplished by a two-sided multiplication with a rotator $R$ ([27], p. 274):

$$s' = RsR^\dagger. \tag{70}$$

The one-sided rotator $R$ for a rotation of $\theta$ can be described as the exponent:

$$R = R(\theta) = \exp -B\theta/2, \quad B^2 = -1. \tag{71}$$

Since the spin vector is given by:

$$s = \rho_0 e^\pm = \psi e^\pm \psi^\dagger, \tag{72}$$

the wavefunction must transform in the following way:

$$s' = R(\theta)\psi \left[ e^\pm \right] \psi^\dagger R^\dagger(\theta) \Rightarrow \psi' = R(\theta)\psi. \tag{73}$$

That the wavefunction transforms via a one-sided and not a two-sided rotation is crucial for its symmetry properties. Assume now that the angle of rotation $\theta = 2\pi$. Then the spin vector will make a full rotation and revert to its original state. But this is not true for the wavefunction, since:

$$\psi' = \exp -B\pi \psi = [\cos(\pi) - B\sin(\pi)] \psi = -\psi. \tag{74}$$

One could thus conclude that also the general symmetry of the wavefunction, which in many-electron systems is the basis of its construction from Slater determinants, comes from geometrical properties of the wavefunction as a sum of scalar and bivector terms. We shall use this property in our construction of the many-electron wavefunction.

6.6 Vector Potential and Wavelength

An interesting variation of the same topic is the behavior of electrons in an Aharonov-Bohm experiment. There, the magnetic field $B$ is actually zero, while the vector potential $A$ is non-zero. As measured orginally by Chambers [47] in 1960, and more recently by Osakabe et al. in 1986 [48], the vector potential affects the phase of the
electron. The effect can be formalised as a change of the wavevector in an external field $A$ with:

$$k(A) = k_0 + \alpha A. \tag{75}$$

Here, $\alpha$ is assumed to be a constant. That the potential must affect the wavevector or the local distribution of the electron density and the related potentials can be inferred from the description of a free electron after it has passed a region with non-vanishing potential $A$. In this case the wavefunction $\psi_S(z, t)$ corresponds to the original wavefunction $\psi_{S0}(z, t)$ augmented by an additional, and $A$ dependent phase. For simplicity we assume that $A$ is parallel to $e_3$, then we get:

$$\psi_S(A, z, t) = \psi_{S0}(z, t) \cdot \exp \left( i \alpha \int_{z_0}^{z} A(z) \, dz \right). \tag{76}$$

Here, we have assumed that $A$ is only non-zero from $z_0$. Using the formulation of $\psi_{S0}$ for a free electron derived above, we may write for the wavefunction $\psi_S(z_0$ is set to zero for convenience):

$$\psi_S(A, z, t) = \exp \left[ \left( \frac{2\pi}{\lambda_0} + \alpha A \right) \left( z - 2\pi \nu_0 t \right) \right]. \tag{77}$$

Clearly the wavelength has been changed. If $A$ is positive then the energy density in the region of the vector potential has been increased. If this affects the electron, then it must lead to an increase of the wavevector. The constant $\alpha$ must therefore be positive. In atomic units and comparing with the experimental phase shifts one finds 1. However, since the electron charge is negative we get for the wavefunction $\psi$ in an external vector potential the result:

$$\psi_S(A, z, t) = \exp \left[ \left( \frac{2\pi}{\lambda_0} - A \right) \left( z - 2\pi \nu_0 t \right) \right]. \tag{78}$$

The density and field components of the electron in this case are described by:

$$\rho^{1/2} = \rho_0^{1/2} \cos \left[ \left( \frac{2\pi}{\lambda_0} - A \right) \left( z - 2\pi \nu_0 t \right) \right],$$

$$S^{1/2} = \rho_0^{1/2} \sin \left[ \left( \frac{2\pi}{\lambda_0} - A \right) \left( z - 2\pi \nu_0 t \right) \right]. \tag{79}$$

In an Aharonov-Bohm experiment with two different pathways characterized by opposite values of $A$ within the interval $z_0, z_1$, the two partial waves at a point $z$ will be:

$$\psi^+_S(A, z, t) = \rho^{1/2} \exp \left( \frac{2\pi}{\lambda_0} z - (z_1 - z_0) A - 2\pi \nu t \right),$$

$$\psi^-_S(A, z, t) = \rho^{1/2} \exp \left( \frac{2\pi}{\lambda_0} z + (z_1 - z_0) A - 2\pi \nu t \right). \tag{80}$$
A superposition of the two partial waves at \( z \) will consequently lead to an oscillating amplitude, described by:

\[
\psi_S = \frac{1}{2} (\psi^+ + \psi^-) = \rho^{1/2} \exp \left( \frac{2\pi}{\lambda_0} z - 2\pi n t \right) \cos(z_1 - z_0) A
\]

\[
= \left( \rho^{1/2} + i S^{1/2} \right) \cos(z_1 - z_0) A. \tag{81}
\]

This oscillation can then be measured, as in the case of electron density waves at surfaces, as an \( A \) and \( z_1 - z_0 \) dependent density variation at a detector screen.

A generalisation of this result into a Schrödinger equation which includes an external vector potential is not as straightforward as in the case of electrostatic fields. The reason is that \( A \) is not generally a vector, but a bivector, properly written as \( i A \) (this follows from the fact that in a relativistic framework it has to be a complex field [27]). We start by writing the wavefunction in a more transparent form as:

\[
\psi_S = \rho_0^{1/2} \left[ \cos ((k - iA) \cdot x - \omega t) + i \sin ((k - iA) \cdot x - \omega t) \right]. \tag{82}
\]

Here, \( x \) is a three-dimensional position vector, and \( i \) is the pseudoscalar \( e_1 e_2 e_3 \). If we assume that the vector potential in the region of interest is constant, then a first derivative of this wavefunction leads to the following result:

\[
\nabla \psi_S = \rho_0^{1/2} \left[ -(k - iA) \sin ((k - iA) \cdot x - \omega t) + (ik + A) \cos ((k - iA) \cdot x - \omega t) \right]
\]

\[
= \rho_0^{1/2} \left[ -k \sin \phi + A \cos \phi + i(k \cos \phi + A \sin \phi) \right]. \tag{83}
\]

For brevity we have written \( \phi \) for the argument of the periodic functions in the last line. It can clearly be seen that the inclusion of a general vector potential into the Schrödinger equation requires that it has a different nature than the terms related to the wavevector \( k \). The gradient of \( \psi_S \) in this case is a multivector composed of even (the bivector terms) and odd (the vector terms) elements. For the second derivative one obtains with the same procedure:

\[
\nabla^2 \psi_S = \rho_0^{1/2} \left( -k^2 - A \cdot k - k \cdot A + A^2 \right) \psi_S. \tag{84}
\]

To account for the changes in the local derivatives compared to the frequency in a Schrödinger-type equation one consequently has to set:

\[
i \frac{\partial \psi_S}{\partial t} = \frac{1}{2} \left( i \nabla - A \right)^2 \psi_S. \tag{85}
\]

Including also a scalar potential \( V \), we obtain:

\[
i \frac{\partial \psi_S}{\partial t} = \frac{1}{2} \left( e_i \frac{i \partial}{\partial x_i} - A \right)^2 \psi_S + V \psi_S. \tag{86}
\]

The equation is equal to the general non-relativistic Schrödinger equation for electrons in the presence of electrostatic and vector potentials. The suggested extended model of electrons is thus fully compatible with the non-relativistic theoretical framework of quantum mechanics.
7 Electrons in Dynamic External Fields

Based on these findings one may equally analyze the effect of an external electromagnetic field on the velocity of electrons. The electromagnetic field shall be described by a bivector $iS^{1/2}_{em} e_3$, which propagates in $e_3$ direction with velocity $c$, the velocity of light in a vacuum. The bivector $iS^{1/2}_{em} e_3$ encaptures electromagnetic $E$ and $H$ fields perpendicular to $e_3$. Since there is no real component of the electromagnetic field vector, the field can also not act directly on the real part of the electron’s wavefunction, or its density distribution. However, we found in the analysis of the electron’s acceleration in an external field that the time derivative of the field components and the density components are equal and of opposite sign. One may infer from that finding that an external and oscillating field $S$ will lead to an oscillating field $\rho$ via something akin to the Newtonian principle: for every action (here, a variation of field intensity due to an impinging electromagnetic field), there is a reaction (here, a variation of mass density of the electron). To see whether such an assumption is justified we consider an electromagnetic field propagation in $z$-direction with the field vector $S_{em}$ given by:

$$S_{em}(z, t) = S_0(t) \sin^2 \left( \frac{2\pi}{\lambda} z - 2\pi vt \right).$$

(87)

Given that the field propagates with relativistic velocity we assume, for this treatment, that the electron velocity is very small and that in effect the propagating EM field interacts at a given point with the electron, which perceives the presence of the field more or less as a time-dependent variation. At a point $z_0, \phi_0 = (2\pi/\lambda)z_0$ this means:

$$\dot{S}_{em}(z_0, t) = \dot{S}_0(t) \sin^2 (\phi_0 - 2\pi vt) - 4\pi \nu S_0(t) \sin (\phi_0 - 2\pi vt) \cos (\phi_0 - 2\pi vt).$$

(88)

If the effect of the electron’s density is equal to the change of the external field

$$d\dot{\rho}_{el}(z_0, t) = -\dot{S}_{em}(z_0, t),$$

(89)

then the density change at $z_0$, which we assume to be initially constant and $\rho_0$, will be:

$$d\rho_{el}(z_0, t) = \rho_0 - S_0(z_0, t) \sin^2 (\phi_0 - 2\pi vt).$$

(90)

According to the relation between density and field components this also leads to a change of the internal potentials $S_{el}$ of the electron, described by:

$$dS_{el}(z_0, t) = S_0(z_0, t) \sin^2 (\phi_0 - 2\pi vt).$$

(91)

The limit of energy adsorption from the electromagnetic field is reached, when the electron density has reached the limit:

$$\rho_{el}(z_0, t_f) = \rho_0 - S_0(z_0, t_f) = 0.$$
While this seems a coincidence at first view—the amplitude $S_0$ could in principle be arbitrary and the electron adsorb less energy than required to reach this threshold—on reflection it is quite understandable. After all, the external field $S_{ph}$ will have been created by the reverse effect, i.e. an electron being decelerated and emitting a photon in the process. Such an emission process is equivalent to an adsorption process with a negative time coordinate. From a physical point of view it is therefore symmetric.

However, it has to be acknowledged that this particular point deserves a more careful analysis, which has to be given in future. The second point, which has not been treated is the transfer of frequency, due to the external $S$ field, to a change in wavelength, or a local change of electron density and field amplitudes after adsorption of energy. So far, this point has been omitted since we have analysed energy transfer processes at one particular coordinate $z_0$ only. To determine the phase difference between different points at the moment, when the electron acceleration is terminated ($t = t_f$), we calculate the density at the point $z + dz$. From the equations derived so far it is clear that:

$$\phi_0 - 2\pi v t_f = \frac{\pi}{2}, \quad S_0(z_0, t_f) = \rho_0. \quad \text{(93)}$$

Calculating now the density at $z_0 + dz$ and $t = t_f$ we get:

$$\rho_{el}(z_0 + dz, t_f) = S_0(z_0, t_f) - S_0(z_0 + dz, t_f) \sin^2 \left( \frac{\pi}{2} + \frac{2\pi}{\lambda} dz \right)$$

$$= S_0(z_0, t_f) - S_0(z_0 + dz, t_f) \cos^2 \left( \frac{2\pi}{\lambda} dz \right). \quad \text{(94)}$$

Setting now:

$$S_0(z_0 + dz, t_f) \approx S_0(z_0, t_f) = \rho_0 \quad \text{(95)}$$

we obtain for the amplitude of the density at the point $z_0 + dz$ the result:

$$\rho_{el}(z_0 + dz, t_f) = \rho_0 \sin^2 \left( \frac{2\pi}{\lambda} dz \right). \quad \text{(96)}$$

The local distribution of the density is then equal to the local distribution of a wave with velocity $v = h/m\lambda$. A similar result is obtained for the field component of electron propagation. Since both components show the same properties as an electron wave in motion with velocity $v$ it is safe to conclude that the adsorption of the $S$ field leads to an acceleration of the electron until it reaches a velocity which is corresponding to the frequency of the incident dynamic field.

As both components comply with the standard form for the wavefunction, we may write the electron wavefunction after acceleration as:

$$\psi_S(v) = \rho^{1/2}(v) + iS^{1/2}(v) = \rho_0 \exp i \left( \frac{2\pi}{\lambda} z - 2\pi v t \right). \quad \text{(97)}$$

One may now analyze the problem of an electron in motion undergoing accelerations due to impinging photons. Given that the wavefunction is linear, a subsequent acceleration will change it in exactly the same manner as the first one. This means, that
one can actually analyze electron-photon interactions from the viewpoint of the conservation of energy and momenta. This is, how one commonly accounts for Compton scattering [49].

8 The Hydrogen Atom

It is straightforward to apply the Schrödinger equation of the electron, developed in previous sections, to the problem of a central potential and to restrict the problem to finding solutions of the equation:

\[
\left(-\frac{1}{2}\nabla^2 - \frac{1}{r}\right) \psi_S = i \frac{\partial \psi_S}{\partial t} = \epsilon \psi_S. \tag{98}
\]

However, even though we have shown how the frequency of the electron changes in an external electrostatic field, we have done so only for one particular value of the electrostatic potential. We have not analysed, whether the electron can have a single energy value, described by \(\epsilon\), in an environment, where the electrostatic potential varies within the mass distribution of a single electron. In particular, since we expect in such an environment that the frequency changes continuously. Within the present framework the Schrödinger equation, which describes the energy levels within a hydrogen atom, is due to a slightly different physical situation than treated previously. This situation is captured in postulate 4: In equilibrium, the energy density throughout the space occupied by a single electron is invariant. It can be argued that such a postulate is necessary to account for the—experimentally observed—stability of hydrogen. Let us assume that the postulate is not valid. We may then write the equation in the following way:

\[
\left(-\frac{1}{2}\nabla^2 - \frac{1}{r}\right) \psi_S = \epsilon(r) \psi_S. \tag{99}
\]

If a particular infinitesimal density component \(d\rho\) is found at a radius \(r\), its energy value is described by \(\epsilon(r)\). Now if \(\epsilon(r)\) varies with the radius, for example becoming more negative with decreasing \(r\), then the system can lower its energy if \(d\rho\) migrates to a position closer to the nucleus. In this case the general principle of energy minimization requires that the electron density collapses to an infinitesimal shell around the nucleus. Since this is not, what we observe, postulate 4 must be correct. And in this case the energy value \(\epsilon\) must be constant throughout the system.

The standard solution for the non-relativistic hydrogen problem is the following (we give its standard textbook format):

\[
\psi_{nlm}(r, \theta, \phi) = C_{nlm} \exp\left(-\frac{2r}{n a_0}\right) L_{n-l-1}^{2l+1}\left(\frac{2r}{n a_0}\right) \times P_m^l(\cos \theta) \exp(im\phi). \tag{100}
\]

Here, \(C_{nlm}\) is a normalization constant. Since the hydrogen atom is neutral, the total electron charge within its shell must be equal to unity. \(a_0\) is the Bohr radius, or
Density components, as analyzed in great detail in the preceding sections, are reflected by the real components of electron wavefunctions, while the imaginary components relate to the electron’s fields. This allows to decompose the wavefunction of the hydrogen electron into:

\[
\rho^{1/2} = U_{nlm}(r, \vartheta) \cos m\varphi, \\
S^{1/2} = U_{nlm}(r, \vartheta) \sin m\varphi.
\]

(102)

Here, the important result is that in general the electron within a hydrogen atom also possesses density components and field components, related to its state of motion. Doran and Lasenby have given a fully relativistic treatment of the hydrogen problem within geometric algebra, based on previous work of Eddington [50, 51], and found that the general solutions have to be described by multivectors. This indicates the same feature: a presence of density components and field components (see p. 294 of [27]).

The field plane is perpendicular to the direction of \( \mathbf{e}_\varphi \). It should be kept in mind that this wavefunction describes an electron without spin; the components \( m \neq 0 \) relate to additional motion of the electron around its \( z \)-axis. Including spin into this description requires to modify all states, also the groundstate \( m = 0 \). As the groundstate solution of hydrogen is radially symmetric, and as the spin-component of the wavefunction is decoupled from the local component and has exactly two solutions, we may account for spin by the component:

\[
\chi^\pm = \frac{1}{\sqrt{2}} (1 \pm \mathbf{e}_\vartheta \wedge \mathbf{e}_\varphi),
\]

\[
\psi_{nlm}^\pm(r, \vartheta, \varphi, \sigma) = \frac{1}{\sqrt{2}} U_{nlm}(r, \vartheta) e^{im\varphi} (1 \pm \mathbf{e}_\vartheta \wedge \mathbf{e}_\varphi).
\]

(103)

For the groundstate wavefunction \( m = 0 \) the result will thus be:

\[
\psi_{n0}^\pm(r, \vartheta, \varphi, \sigma) = \frac{1}{\sqrt{2}} U_{n0}(r, \vartheta)(1 \pm \mathbf{e}_\vartheta \wedge \mathbf{e}_\varphi).
\]

Writing the local part of the wavefunction as a multivector leads to the following formulation:

\[
\psi_{nlm} = U_{nlm}(r, \vartheta)(\cos m\varphi + \mathbf{e}_r \wedge \mathbf{e}_\vartheta \sin m\varphi).
\]

(104)

The complete solution including spin then can be written as the following multivector:

\[
\psi_{nlm}^\pm = \frac{U_{nlm}(r, \vartheta)}{\sqrt{2}} \times \{ \cos m\varphi + i \left[ (\mathbf{e}_\varphi \mp \mathbf{e}_\vartheta) \sin m\varphi \mp \mathbf{e}_r \cos m\varphi \right] \}.
\]

(105)
9 The Hydrogen Molecule and Density Functional Theory

A hydrogen molecule or a helium atom poses the additional problem to reconcile postulate 4 with the existence of one coherent electron density throughout the system. In principle, the problem can be solved using standard DFT based on the Kohn-Sham equations [9]. However, the Kohn-Sham formulation of DFT seems, from the outset, somewhat cumbersome, since it requires the self-consistent calculation of every single-electron state in a system. The computational effort required as the system size increases then rapidly becomes prohibitive. This has led to extensive research into the possibility of a so-called orbital-free formulation of DFT [52]. The key problem in this line of research is the kinetic energy functional, which to date cannot be described in a completely transferable manner. Given the preceding presentation, it seems quite unlikely that a relation, based on electron density alone, could actually account for all aspects of a many-electron system. If magnetic properties play a role at all, then according to this model they must enter the theoretical description. This applies not only to magnetic material, but also to non-magnetic solids, as the minimum energy state of the system is a consequence of the existence of an equal number of spin-up and spin-down electrons. However, the many-electron problem was encoded by Levy, Perdew and Sahni (LPS) in 1984 in an equation based only on the density [10] (see (4)).

9.1 Modified Density Equation Including Spin

Within the present context, there are two problems with the equation: (i) It describes a bosonic system, since all properties, related to the spin of electrons, are absent from the formulation. (ii) It does not account for the difference in nature of field components (a bivector) and mass components (a scalar). It is hard to see, therefore, how this relation could be complete. However, it should be possible, given the analysis contained in this paper, to accurately describe a non-relativistic many-electron system in its groundstate by the following coupled equations:

\[
\Psi = \rho^{1/2} + i e_s S^{1/2},
\]

\[
\left[ -\frac{1}{2} \nabla^2 + v_{\text{ext}} + v_{\text{eff},0} + i e_v v_i \right] \Psi = \mu \Psi,
\]

\[
\rho_0 = \Psi^\dagger \Psi,
\]

\(v_{\text{eff},0}\) combines the Hartree potential and the cohesive potential defined in Sect. 5, but does not contain exchange-correlation potentials. Exchange and correlation potentials encode the difference between non-interacting and interacting electrons. In this equation electron interactions beyond \(v_{\text{eff},0}\) are part of the bivector potential \(i e_v v_i\), since they are due to field-mediated interactions within the electron distribution. The direction of the unit vector \(e_v\) and the intensity of the potential \(v_i\) will depend on the system under consideration and have to be determined self-consistently. The bivector part of the many-electron wavefunction, the product of unit vector \(e_s\) and electromagnetic intensity \(S^{1/2}\) are equally system and location dependent and have to be determined by self-consistent iterations. The equation couples field terms to density.
terms also via a bivector potential. The resulting mass and field components of the wavefunction $\Psi$ then give the conventional mass density $\rho_0$. Even though both $e_S$ and $e_v$ will vary from one point to the next, the set of coupled equations is still much simpler than the full many-body treatment of a many electron system in standard theory.

The justification to write the wavefunction of a many-electron system in this way rests on three results of previous sections: (i) The wavefunction of any single—and extended—electron complies with a Schrödinger equation. A system composed of an aggregate of more than one electron then should also comply with a Schrödinger-like equation. (ii) The construction of a wavefunction from scalar and bivector components ensures that the $4\pi$-symmetry of the wavefunction will be retained, which is the key property of the wavefunctions of fermions. (iii) The interaction between field components and mass components implies bivector potentials in a crystal field of interactions. Without such a potential many-body effects could not be included in the description.

One can decompose the equation into scalar and bivector components to make transparent, in comparison with the LPS equation, what the additional components actually are. For the scalar part we get:

$$\left[ -\frac{1}{2} \nabla^2 + v_{\text{ext}} + v_{\text{eff},0} - \mu \right] \rho^{1/2} = e_v \cdot e_S v_i S^{1/2}. \quad (107)$$

The change is thus not simply a potential term of the same general form as the effective or external potential. Such a behavior could be encoded e.g. in a density dependent exchange correlation potential. However, here we have an additional term which will act as a source for the electron density distribution. This source term depends on the direction of the bivector potential as well as the field components of electron motion. It is thus clearly beyond current models in DFT. The bivector equation is equally instructive. It can be written:

$$\left[ -\frac{1}{2} \nabla^2 + v_{\text{ext}} + v_{\text{eff},0} - \mu \right] i e_S S^{1/2} = e_v \wedge e_S v_i S^{1/2} - i e_v v_i \rho^{1/2}. \quad (108)$$

This is, in essence, a vector-equation with purely imaginary variables. It thus introduces directional effects into the density equation, and couples density components and field components. Also this equation is clearly beyond current formulations in DFT. In imaginary components and replacing the wedge product by the cross product ($a \wedge b = i a \times b$), we get:

$$\left[ -\frac{1}{2} \nabla^2 + v_{\text{ext}} + v_{\text{eff},0} - \mu \right] e_S S^{1/2} = e_v \times e_S v_i S^{1/2} - e_v v_i \rho^{1/2}. \quad (109)$$

It can also be seen that either the field component $S$ or the bivector potential $v_i$ by itself will not alter the general equation. Only the field components of electron energy and the bivector potential of the solid together could give an accurate account of the charge distribution for electrons with spin. It is also clear, by comparing with the hydrogen problem, that the potential $v_i$ is absent in the groundstate of the hydrogen electron: it is thus genuinely of many-body origin.
In a slightly more compact form, which differentiates between vector and scalar components of the equation, we may write the following coupled set of equations, where the local dependency of components has been made explicit for clarity:

\[
\Lambda(r) = e_S S^{1/2}, \\
\Pi(r) = e_v v_i, \\
v_0(r) = v_{\text{ext}} + v_{\text{eff},0}, \\
\left[-\frac{1}{2} \nabla^2 + v_0(r) - \mu\right] \rho^{1/2}(r) = \Pi(r) \cdot \Lambda(r), \\
\left[-\frac{1}{2} \nabla^2 + v_0(r) - \mu\right] \Lambda(r) + \rho^{1/2}(r) \Pi(r) = \Pi(r) \times \Lambda(r).
\]  

(110)

(111)

In general, the formulation is still much simpler than present formulations of many-body theory. The simplification comes from the fact that the model wavefunction contains only four (the amplitudes \( \rho^{1/2} \) and \( S^{1/2} \) and the vector of unit length \( e_S \)) independent variables, which can be mapped onto a grid in real space. It is thus much easier to evaluate in a general minimization problem even though it captures all physical properties of the system. Using, for example, a real-space method and a grid spacing of about 0.2 to 0.3 Å, it should become computational routine to simulate systems of more than one million atoms: an increase of the current limit of DFT of a factor of about one thousand. In this case, mesoscopic systems will come into the range of \textit{ab-initio} methods and biological systems should be tractable by theoretical means.

The indispensable first step for such a theoretical framework will be to determine the bivector potential and the effective potential in a simple system, say a system of constant electron density. Only after such a potential has actually been determined can the framework be applied to more complex systems with variable electron density. While it cannot be guaranteed that this approach will lead to a reliable method for computing the physical properties of many electron systems, it seems justified to develop its consequences and to compare the results to standard methods. The gain in theoretical efficiency, if successful, would be quite substantial.

9.2 Many-Body Wavefunction

The groundstate wavefunction of an \( N \)-electron system can be written as:

\[
\Psi_{MB} = \Psi(x_1, x_2, x_3, \dots, x_N).
\]  

(112)

Here, the variables \( x_i \) combine local \( (r_i) \) and spin \( (\sigma_i) \) variables. The wavefunction \( \Psi_{MB} \) thus contains at least \( 3N \) variables, the position vectors of all \( N \) electrons, \( r_1 \) to \( r_N \). The main condition imposed upon the wavefunction due to the Pauli principle is that it must be antisymmetric: an exchange of two variable (or two electrons) \( x_i \) and \( x_j \) \((i \text{ and } j)\) changes the sign of the wavefunction from plus to minus and vice versa. A general form of the wavefunction complying with this condition is its construction
via Slater determinants [53]:

\[ \Psi_{MB} = \sum_{\kappa} C_\kappa \text{Det} | \psi_1(x_1), \psi_2(x_2), \psi_3(x_3), \ldots, \psi_N(x_N) |. \]  (113)

For a hydrogen molecule the many-body wavefunction of the system, including the spin functions \( \alpha \) and \( \beta \), is given by [54]:

\[ \Psi(\mathbf{r}_1, \mathbf{r}_2, \sigma_1, \sigma_2) = C \begin{vmatrix} \psi_{100}(\mathbf{r}_1)\alpha(\sigma_1) & \psi_{100}(\mathbf{r}_2)\alpha(\sigma_2) \\ \psi_{100}(\mathbf{r}_1)\beta(\sigma_1) & \psi_{100}(\mathbf{r}_2)\beta(\sigma_2) \end{vmatrix}. \]  (114)

The total (groundstate) wavefunction is therefore:

\[ \Psi(\mathbf{r}_1, \mathbf{r}_2, \sigma_1, \sigma_2) = C \psi_{100}(\mathbf{r}_1-\mathbf{R}_1)\psi_{100}(\mathbf{r}_2-\mathbf{R}_2) \times \left[ \alpha(\sigma_1)\beta(\sigma_2) - \beta(\sigma_1)\alpha(\sigma_2) \right]. \]  (115)

Since a hydrogen molecule in its groundstate does not interact with a magnetic field, one may omit the spin-components of the wavefunction and write:

\[ \Psi_{H_2}(\mathbf{r}) = \psi_{100}(\mathbf{r}-\mathbf{R}_1)\psi_{100}(\mathbf{r}-\mathbf{R}_2) = \rho_0^{1/2}(\mathbf{r}), \]  (116)

where we have assumed that the nucleus of the first atom is at \( \mathbf{R}_1 \) and the nucleus of the second atom at \( \mathbf{R}_2 \). However, including spin becomes necessary if one considers the gradual transition from the hydrogen molecule to two hydrogen atoms [55]. In this wavefunction we may account for spin in a similar way as for the hydrogen atom, with the only difference that now we have two centers which serve as the origin of radial unit vectors. These unit vectors are symbolized by \( \mathbf{e}_r^1 \) and \( \mathbf{e}_r^2 \), respectively

\[ \Psi_{H_2}(\mathbf{r}, \sigma) = \frac{1}{2} \psi_{100}(\mathbf{r}-\mathbf{R}_1)\psi_{100}(\mathbf{r}-\mathbf{R}_2) \times \left[ \left( 1 + i\mathbf{e}_r^1 \right) \left( 1 - i\mathbf{e}_r^2 \right) - \left( 1 - i\mathbf{e}_r^1 \right) \left( 1 + i\mathbf{e}_r^2 \right) \right]. \]  (117)

In its triplet state the spin component of the two electron wavefunction is symmetric, while the local component becomes antisymmetric. In this case one has to construct the charge and spin densities from the 1\( s \) and 2\( s \) orbitals, respectively.

10 Discussion

We have on purpose avoided any reference to classical mechanics in this work on electrons. The reason is that we think that mechanics has obscured the meaning of certain formulations in quantum mechanics. In that respect, we also think that the name quantum mechanics carries a wrong message, and that it is better to talk about either wavedynamics or microdynamics, although this might be a secondary issue. The primary issue, we hope to have clarified in this paper, is that electrons are not mechanical objects. This, of course, is well known. However, so far no detailed account existed, how density and spin properties of single electrons might be distributed in space and time without any measurement. We think that the concept of an extended
electron, introduced here, might be easier to reconcile with experimental results at the atomic scale, with density functional theory, and with visualizations of physical processes. It is often the picture in the mind, which leads to new insights, and not the mathematical formalism. Whether this electron model describes the real electron or not, is a moot point. As demonstrated, it leads to the same numerical results as the standard model, it accounts for most experimental results obtained so far, it gives a consistent interpretation of the electron wavefunction, and it allows to picture atomic-scale processes in space and time. Even if it were not real, this electron seems quite a useful model.

It is instructive to look at the presented material from the viewpoint of basic principles. Quite apart from the historical development of modern electron theory, this should allow us to appreciate the importance or unimportance of specific findings. The first fundamental finding, and which made a wave theory of electrons initially necessary, is actually electron diffraction. That this was initially a hypothesis in a PhD thesis of Louis de Broglie, makes it all the more remarkable. In a modern context, one could say it is the observation of standing waves on a metal surface, which leaves no other conclusion but to assign wave properties to electrons. In this respect it is hard to overestimate the importance of the experiments coming out of Don Eigler’s lab in the early 1990s.

As a second fundamental finding one has to nominate photoelectric currents as interpreted by Einstein with the help of Planck’s hypothesis. Here, it is found that the frequency of the electron waves can be altered by electrostatic fields, as existing within a metal crystal. This finding paves the way for the formulation of the initial Schrödinger equation, which can be used to determine the emission frequencies of hydrogen atoms, admittedly one of the great problems of 19th century physics. However, this finding alone does not allow for a treatment of interactions with electromagnetic fields.

Here, we need the third fundamental finding, which we consider to be the Aharonov-Bohm effect. Only in this context can it be understood that the vector potential changes the wavelength and thus has to be treated differently than, e.g. the changes in an electrostatic potential, where the frequency is affected. It is also quite interesting that this effect was a theoretical prediction based on the Schrödinger equation and formulated long after the equation had been used to solve the hydrogen problem. The Aharonov-Bohm effect is as important as the photoelectric effect. Without it, the only way to include vector potentials in the Schrödinger equation would be via a classical Hamiltonian \( H = [p - (e/c)A]^2 \) [39], and the correspondence principle. This, in turn, would require to treat the electron as a classical point-particle and lead to inconsistencies in the suggested theoretical model.

The most intriguing part of the framework seems to concern the possibility of constructing wavefunctions from density and field components and, by the reverse process, of decomposing wavefunctions into density and field components. This should add substantial physical insight to any theoretical result obtained e.g. within a many-body framework. In the final analysis we think that the role and the actual—i.e. physical—content of the wavefunctions have not been sufficiently clear. An example of this lack of clarity in our view is the famous Schrödinger-cat thought experiment [56]. There, a superposition of two states, a living cat and a dead cat, collapses into
one final state upon measurement, i.e. the interaction of an electron with an external field. The important feature of the experiment lies in its statistical interpretation of the wavefunction. As we do not know, which state the electron is in, the cat could be said to be dead and alive at the same time—which seems quite impossible for a living organism. However, as shown in the treatment on spin and its interaction with a magnetic field, the electron wavefunction within the present framework will always indicate a well defined physical state, as described by time and space dependent density and field components. The statistics in this case do not enter via some unknown “quantum” property of electrons, but are due either to a variation of the electron’s properties in space and time (which, for example, prevents us seeing the density variations of a surface-state electron if it is not scattered on a defect, and makes us detect standing waves at a step edge or a single atom [41]), or to a lack of knowledge about the individual electron (which makes us detect two deflection spots in a Stern-Gerlach experiment [42]). In this case, if the life of a cat is related to one particular electron state, then this cat is definitely dead or alive, but never both. If we have to describe it as a superposition of alive and dead, then we have to concede that we do not know exactly which electron we are talking about, or at which precise moment our measurement is taken. This is, in essence, the same lack of information encountered in statistical thermodynamics. Incidentally, this view is very close to the one advocated by Schrödinger [56].

However, we have to concede that the model does not provide a comprehensive theory for the observed self-interference of single electrons [15]. Interference here is due to the spacetime variations of the electron’s wavefunction and its geometric characteristics upon scattering. How a single electron could change its wave pattern by interacting with an environment which is well separated from any one of its possible trajectories, cannot be answered within this model. The only way, it seems, that such behavior could be reconciled with the present model, is by invoking a detection loophole. If, for example, the impacts detected depend on a threshold energy of the impinging density wave and the state of the atoms making up the detector, then it seems possible that detection is actually a very rare and, due to the excitations of the detector atoms, essentially stochastic event and that most density waves remain undetected, but do contribute to the interference pattern. That such a scenario is not as inconceivable as it might seem, can be inferred from scanning tunneling microscopy experiments, where only a tiny fraction, or $10^{-5}$ of the actual current in the tunnel junction is detected in the experiments [57].

In a wider context, there is a long tradition in experimental physics, starting with Alain Aspect’s experiments in the 1980s [58], on the non-locality of quantum mechanics, formalized in the Bell inequalities [59, 60]. These experiments remain beyond the scope of this presentation, although it cannot at present be excluded that non-local correlations could play a role in the properties of the bivector potential in many-electron systems. Given the role of non-local correlations, for example in the construction of kinetic energy density functionals [61], such a possibility should certainly not be excluded. From a different point of view, it can be said that the Bell inequalities [59] are violated, whenever a system violates at least one of following two conditions: (i) Its interactions are strictly local, and (ii) its spin is counterfactual definite (see [62] and references therein). Counterfactual definite means that an electron possesses a particular (= definite) spin, regardless of whether it is measured or
not. Quantum mechanics, for example, violates both of these conditions: the first, in the collapse of the wavefunction (which is non-local), the second, in the dependence of spin on a measurement (as spin is generally isotropic without a measurement). This question requires a very detailed and careful analysis, which shall be pursued in a follow-up paper.

From the viewpoint of condensed matter theory and computational methods the extension of the equation derived by Levy, Perdew, and Sahni [10], via a distribution of density and field properties, given in (111), is certainly the most important aspect of the model. It seems at first view surprising that one may describe systems composed of a large number of electrons by a wavefunction with only four variables, i.e., the amplitudes of density and field components, and the direction of the field. In particular, since the standard model in many-body physics requires at least $3N$ variables. While the final proof that the model is suitable also for many-body systems will have to come from the application of the model, its predictions, and its agreement with experimental measurements, it can be analyzed, where the actual gain in efficiency could potentially come from. From the viewpoint of DFT, the key problem in orbital free models always was the kinetic energy functional [52]. In the Kohn-Sham formulation of DFT, this problem is transferred to the exchange-correlation functionals, which describe the difference in kinetic energy between interacting and non-interacting electrons [9]. In the present model, the kinetic energy density is given by the Laplace operator acting on the density and field components of electrons, e.g. in a solid. It is thus different from the von Weizsäcker or the Thomas-Fermi kinetic energy densities [6]. However, as shown in the derivation of the free electron and the hydrogen atom, it reverts to these limiting cases with a vanishing bivector potential in case of single electrons.

In many-body theory, the many-body aspect is usually encoded in the construction from single-electron states; here, the many-body aspect is accounted for by the bivector potential and by the phase coherence of densities and field components. The present model of a many-body system in a sense does not know of single, i.e., isolated electrons, since every single electron is connected to adjacent electrons via coherent density functions and fields. In the present model, the many-body aspect of a system is thus encoded in its coherence, and in its common energy or chemical potential $\mu$. Since it does not know of single electron states, it also does not require to build up the many-body wavefunction from Slater determinants defined via a $3N$-variable space. It is thus much closer to DFT than existing many-body formulations, even though electron correlations within solids should be accurately described. Considering, that phase coherence of $\Psi$ also plays a role across the boundary of a periodic system, most principles known to condensed matter theorists which come from periodic boundary conditions should be applicable. However, since the potential efficiency is much higher, in particular in the description of large systems, it should also be possible, without lack of precision, to simulate very large systems, i.e. mesoscopic systems and mesoscopic timescales.

DFT continues to be a project in development. In essence, its successful application to most problems in solid state physics and physical chemistry has made it an indispensable tool of theorists today. However, the current efforts to determine the kinetic energy of a many electron system [61, 63] and to go beyond Kohn-Sham theory
also reveal that the present theoretical framework is not an endpoint in the development. One of the motivations to develop this theoretical model of electrons was the attempt to understand, from the very principles of modern physics, why an electron appears such a strange entity. The hope was that a better understanding of fundamental processes and effects may lead to a better formulation of the many-electron problem. The bivector potential $\Pi$, introduced in this paper, is a genuinely novel concept. It arises naturally, as seen, if one tries to generalize the LPS equation for a spin system. What the exact form of this potential is and how it can be formalized in terms of spin-densities, remains to be seen.

We have briefly mentioned in this paper that a relativistic theoretical framework, based on the Dirac equation and geometric algebra, has been developed by Hestenes and others [26, 27]. However, we have not extended the present framework to the relativistic domain. A reason for this omission is that a non-relativistic framework seems to be sufficient for the time being, in particular in view of applications in condensed matter. In this respect it is also worth reflecting the fact that the Schrödinger equation, contrary to the wave equation, is actually Galilei-invariant (under a kinematic transformation of the wave function, see [39], p. 516). Which means that it remains unchanged for systems at low velocity, which applies to practically all systems studied under laboratory conditions. Under these conditions the first postulate of the theory of relativity remains thus valid, while the second postulate is also valid, since the speed of light is much larger than the velocity of electrons. Imposing an additional Lorentz-invariance on the systems under consideration in DFT seems thus unnecessary at this point. The only real motivation for developing such a Lorentz-invariant model of electrons for applications in condensed matter physics would be, if the description in this manner could be made substantially simpler. At present, this seems not the case. However, we shall return to this problem in future publications.

Acknowledgements This paper captures the essence of about fifteen years of research into electron properties from three perspectives: standard quantum mechanics, density functional theory, and experiments at the atomic scale. It contains thus all the increments in understanding brought about by discussions with colleagues over the years. Of all the colleagues I should thus acknowledge I can name only one: Jaime Keller, who introduced me to geometric algebra. The draft of this paper was carefully read by Iain R. McNab and Krisztian Palotas, who I have to thank for their contribution and their valuable suggestions. I also have to thank Air France: it was on a night flight from Paris to Beijing, when the first ideas to this concept crystallized in my mind. And finally, I have to thank the Royal Society for continued financial support.

References

1. Hohenberg, P., Kohn, W.: Phys. Rev. B 136, 864 (1964)
2. Thomas, L.H.: Proc. Cambr. Philos. Soc 23, 542 (1927)
3. Fermi, E.: Rend. Accad. Naz. Lincei 6, 602 (1927)
4. Fermi, E.: Z. Phys. 48, 73 (1928)
5. Zhou, B., Wang, Y.A.: J. Chem. Phys. 124, 081107 (2006)
6. Wang, Y.A., Govind, N., Carter, E.A.: Phys. Rev. B 60, 16350 (1999)
7. von Weizsäcker, C.F.: Z. Phys. 96, 431 (1935)
8. Perdew, J.P., Constantin, L.A.: Phys. Rev. B 75, 155109 (2007)
9. Kohn, W., Sham, J.S.: Phys. Rev. A 140, 1136 (1965)
10. Levy, M., Perdew, J.P., Sahni, V.: Phys. Rev. A 30, 2745 (1984)
11. March, N.H.: Phys. Lett. A 113, 446 (1986)
12. March, N.H.: J. Comput. Chem. 8, 375 (1987)
13. Holas, A., March, N.H.: Phys. Rev. A 44, 5521 (1991)
14. Misner, C.W., Thorne, K.S., Zurek, W.H.: Phys. Today 62, 40 (2009)
15. Donati, O., Missiroli, G.F., Pozzi, G.: Am. J. Phys. 41, 639 (1973)
16. Gabrielse, G., Hanneke, D., Kinoshita, T., Nio, M., Odom, B.: Phys. Rev. Lett. 97, 030802 (2006)
17. de Broglie, L.: La Reinterpretation de la Mecanique Ondulatoire. Gauthier-Villars, Paris (1971)
18. Valentini, A.: Phys. World 22, 32 (2009)
19. Bohm, D.: Phys. Rev. 85, 166 (1952)
20. Bohm, D.: Phys. Rev. 85, 180 (1952)
21. Hestenes, D.: J. Math. Phys. 14, 893 (1973)
22. Hestenes, D.: Found. Phys. 15, 63 (1985)
23. Hestenes, D.: Found. Phys. 20, 1213 (1990)
24. Eigler, D.: in “Quantum Leaps” on BBC2, May 23, 2002. Quote courtesy of Mike Ross, IBM Almaden
25. Nikolic, H.: Found. Phys. 37, 1563 (2007)
26. Hestenes, D., Sobczyk, G.: Clifford Algebra in Geometric Calculus. Reidel, Dordrecht (1984)
27. Doran, C., Lasenby, A.: Geometric Algebra for Physicists. Cambridge University Press, Cambridge (2002)
28. Hofer, W.A.: Physica A 256, 178 (1998)
29. Keller, J.: Theory of the Electron. Kluwer, Dordrecht (2001)
30. Gull, S., Lasenby, A., Doran, C.: Found. Phys. 23, 1175 (1993)
31. Gull, S., Lasenby, A., Doran, C.: Found. Phys. 23, 1293 (1993)
32. Born, M.: Z. Phys. 37, 863 (1926)
33. Born, M.: Z. Phys. 38, 803 (1926)
34. Born, M.: Gött. Nachr. Math. Phys. Kl. 1, 146 (1926)
35. Davisson, C., Germer, L.H.: Nature 119, 558 (1927)
36. Abraham, M., Becker, R.: Electricity and Magnetism. Blackie, London (1937)
37. Lorentz, H.A.: Theory of Electrons, 2nd edn. (1915). Reprint Dover, New York (1997)
38. Perdew, J., Zunger, A.: Phys. Rev. B 23, 5048 (1981)
39. Jackson, J.D.: Classical Electrodynamics. Wiley, New York (1999)
40. Delamotte, B.: Am. J. Phys. 72, 170 (2004)
41. Crownie, M.F., Lutz, C.P., Eigler, D.M.: Nature 363, 524 (1993)
42. Gerlach, W., Stern, O.: Z. Phys. 9, 353 (1922)
43. Challinor, A.D., Lasenby, A.N., Gull, S.F., Doran, C.J.L.: Phys. Lett. A 218, 128 (1996)
44. Uhlenbeck, G.E., Goudsmit, S.: Naturwissenschaften 47, 953 (1925)
45. Pauli, W.: Z. Phys. 41, 81 (1927)
46. Landau, L.D., Lifshitz, E.M.: Phys. Z. Sowjetunion 8, 153 (1935)
47. Chambers, R.C.: Phys. Rev. Lett. 5, 3 (1960)
48. Osakabe, N., et al.: Phys. Rev. A 34, 815 (1986)
49. Compton, A.H.: Phys. Rev. 21, 483 (1923)
50. Eddington, A.S.: Relativity Theory of Protons and Electrons. Cambridge University Press, Cambridge (1936)
51. Kilmister, C.W.: Eddington’s Search for a Fundamental Theory: A Key to the Universe. Cambridge University Press, Cambridge (1994)
52. Wang, Y.S., Carter, E.A.: In: Progress in Theoretical Chemistry and Physics, pp. 157–184. Kluwer, Dordrecht (2000)
53. Slater, J.C.: Phys. Rev. 34, 1293 (1929)
54. Kantorovic, L.: Quantum Theory of the Solid State: An Introduction. Kluwer, Dordrecht (2004)
55. Gunnarson, O., Lundqvist, B.: Phys. Rev. B 13, 4274 (1974)
56. Schrödinger, E.: Naturwissenschaften 23, 807 (1935), 823; 844
57. Hofer, W.A., Fisher, A.J.: Phys. Rev. Lett. 91, 036803 (2003)
58. Aspect, A., et al.: Phys. Rev. Lett. 47, 460 (1981)
59. Bell, J.S.: Physics I, 195 (1964)
60. Bell, J.S.: Speakable and Unspeakable in Quantum Mechanics. Cambridge University Press, Cambridge (1987)
61. Perdew, J.P., Ruzsinszky, A., Constantin, L.A., Sun, J., Csonka, G.I.: J. Chem. Theory Comput. 5, 902 (2009)
62. Blaylock, G.: Am. J. Phys. 78, 11 (2009)
63. Cangi, A., Lee, D., Elliott, P., Burke, K.: (2010). 1002.1351 [cond-mat]