

MATHEMATICAL ANALYSIS OF EXTENDED SEMICONDUCTOR DEVICE MODELS

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1. INTRODUCTION

In this paper I present the basic ideas and results of my "applied mathematics" TMR project dealing with the modeling and the analysis of state-of-the-art semiconductor equations which incorporate e.g. phenomena like quantum tunneling of electrons that are not covered by classical models.

Standard semiconductor device models like the drift diffusion equations are based on a macroscopic description of the conduction electrons by quantities like charge and current densities that are directly related to measurements, e.g. of the current-voltage characteristic of a device. Due to their underlying physical assumptions, however, these classical models have fundamental limits of applicability which are exceeded by today's fabrication technology where phenomena like high density effects, temperature flows, quantum tunneling, etc. play an important role.

In order to overcome this problem classical (macroscopic) models can be supplied with "correction terms" essentially based on ad hoc assumptions on transport coefficients. These modifications allow to include some of the "new" phenomena. However the commonly used correction terms involve phenomenological constants to be adjusted for each specific situation and for some of the features of new devices this approach fails completely.

On the other hand, fully (many body) quantum mechanical models including all possible physical effects are much too complicated from the numerical point of view.

Hence there is a need to study rigorously the relation of different models in a hierarchy of complexity - both for justifying existing simplified models and for deriving new ones.

For that study we use "asymptotic analysis" : This means a mathematically strict analysis of the limit from one model to another as some physical parameters vanish or diverge.

The results presented in this paper are focussed on the **Schrödinger equation** as the "standard" quantum semiconductor model. We deal with the **derivation and analysis of relativistic/quantum mechanical correction terms**. In addition to their important applications these were challenging open mathematical problems as such.

Note that the goal of this kind of mathematical research is not to provide industry with simulation codes or

other "prêt-à-porter" results, but to lay the foundations to understand current technology and to initiate future developments. The combination of mathematical modeling, mathematical analysis and numerical simulation is at the core of modern Applied Mathematics and Industrial Mathematics and is thus are indispensable for every modern technology.

However, in Europe the role of basic research directed towards application is somewhat less accepted than e.g. in the USA, where companies like IBM, Lucent,... run large research laboratories for basic research and the military budget significantly contributes also to that end. Initiatives in the framework of the European Union, like the TMR programme, play a key role in order to foster this kind of "applicable mathematical basic research" in a joint European effort.

The research performed in the course of this TMR project is an example of this application driven basic research: the rigorous asymptotic analysis of generalized Schrödinger equations lays a sound foundation to the understanding of semiconductor models where effects are included that are important in state-of-the-art applications and future devices.

In particular, we consider three different situations : (1) the "**semiclassical limit**", i.e. the limit from quantum to classical mechanics for vanishing Planck's constant, (2) the "**nonrelativistic limit**", i.e. the limit from relativistic to nonrelativistic quantum mechanics for infinite speed of light and (3) the "**high density limit**", i.e. the limit from a nonlocal to a local exchange interaction for fermions at high density of particles. The general theory we developed in [GMMP] applies to many other examples of homogenization problems in physics, for instance the homogenization limits of wave equations or Maxwell equations in a periodic medium. There "Homogenization" means that we regard the physical quantities at a scale where the distance between two points of the periodic structure is undistinguishable and we look for new, in general "simpler" equations that contain this microscopic information in an "effective" way.

In the context of (1), i.e. the "semiclassical limits of quantum mechanics" according to the "correspondence principle" we work with a powerful tool in the asymptotic analysis of partial differential equations, the Wigner transform. This transform has been invented by the physicist E. Wigner in 1932 for this purpose, but only in the

last 10 years it's great potential as a mathematical method has been noticed and this TMR project has significantly contributed in setting up a rigorous mathematical framework. We develop a general theory [GMMP] and [M4] of it's use for homogenization limits of problems with a distinguished scale of oscillations. Also, we are able to deal with the nonlinear Schrödinger-Poisson system in a crystal and, for the first time, prove rigorously how to derive the semiclassical equations - a fundamental model in solid state physics [BMP2]. Starting from a Schrödinger equation for conduction electrons in a crystal we derive a Vlasov type equation for an isolated energy band.

In [BMP1] and [M5] we systematically study the non-relativistic limit (infinite velocity of light) from the Dirac equation to the Schrödinger equation. Here the electron is described by a 4-vector that represents the spin of fermions and a "negative energy component", i.e. "antimatter". In particular we rigorously derive first order (in the reciprocal speed of light) corrections of the Dirac equations, i.e. the Pauli equation containing a coupling of the electrons spin with the magnetic field. Our papers represent the first results for the case of time-dependent electro-magnetic potentials.

In [BM1] we deal with correction terms to the one-particle Schrödinger equation which are due to the Hartree-Fock ansatz in the reduction of the N-body problem. We use the method of deformations (local scaling transformations) for a rigorous derivation of the Slater exchange as a local approximation to the Hartree-Fock exchange in the thermodynamical limit (infinite number of particles). We use this method of deformations also for a rigorous derivation of kinetic energy functionals like the Thomas-Fermi equation and it's corrections as given by the von-Weizsäcker term [BGM1].

2. THE SCHRÖDINGER EQUATION AND ITS CONNECTIONS TO CLASSICAL PHYSICS

The standard form of the Schrödinger equation that governs the time evolution of a quantum particle described by it's "wave function" $\psi(x, t)$ reads

$$i\hbar \frac{\partial}{\partial t} \psi = -\frac{\hbar^2}{2} \Delta \psi + V(x, t) \psi = 0 \quad , \quad x \in \mathbb{R}_x^3, t \in \mathbb{R} \quad (2.1)$$

where x is the particle's "position" in the 3-dimensional space denoted by \mathbb{R}_x^3 and Δ denotes the Laplace operator, i.e. second order spatial derivatives. The independent variable t is the time and $\frac{\partial}{\partial t}$ denotes the time derivative. $V(x, t) \psi$ means the multiplication of the wavefunction with the potential $V(x, t)$ that models the interaction of the particle with the rest of the world (for instance a given electric field or other electrons,...) . For vanishing potential, i.e. $V(x, t) = 0$ the Schrödinger equation reduces to that of a free particle. \hbar is the (scaled) Planck constant, the fundamental constant of nature in quantum physics. Note that the wave function $\psi(x, t)$ at a position x at time t is a complex number, whereas physical "reality" - what we can measure - is described by real numbers. The crucial point is that the "physical" quantities like the "charge density" are given by expressions like $n = |\psi|^2$, i.e. the

square of the modulus, which is again a real number. In fact, this (charge) density

$$n(x, t) = |\psi(x, t)|^2 \quad (2.2)$$

is the probability of finding a particle at a time t at the position x .

In classical (statistical) mechanics the state of a particle is described by a "distribution function" $f(x, v, t) \geq 0$ which is the probability of finding a particle at a time t at the position x with the velocity v , i.e. at the point (x, v) in "phase space".

The time evolution of $f(x, v, t)$, $x \in \mathbb{R}_x^3$, $v \in \mathbb{R}_v^3$, $t > 0$ is given by the Liouville equation also called the Vlasov equation in this context

$$\frac{\partial}{\partial t} f + v \cdot \nabla_x f - \nabla_x V(x, t) \cdot \nabla_v f = 0 \quad (2.3)$$

Now the "density" $n(x, t)$ is given as a moment (marginal) of $f(x, v, t)$:

$$n(x, t) = \int_{\mathbb{R}_v^3} f(x, v, t) dv \quad (2.4)$$

In quantum mechanics, a joint "probability distribution in phase space" - i.e. a nonnegative function $f(x, v, t)$ that contains the physical information as moments like in (2.4) - is a priori not possible. This would violate the Heisenberg uncertainty principle which states that one cannot simultaneously measure exactly the position and the velocity of a quantum particle.

By the fundamental "correspondence principle" the equations of quantum mechanics should become the equations of classical mechanics for vanishing Planck constant, i.e. in the limit $\hbar \rightarrow \infty$.

However, comparing the Schrödinger equation (2.1) for the complex wave function $\psi(x, t)$ with the Vlasov equation (2.3) for the nonnegative distribution function $f(x, v, t)$, it is absolutely not obvious how the one equation can be derived from the other. Simply setting \hbar to zero in the Schrödinger equation makes no sense at all.

The mathematical tool that allows for a direct link between the Schrödinger equation (2.1) and the Vlasov equation (2.3) is given by "Wigner transforms" : E. Wigner introduced the so-called Wignerfunction [W] in the context of semiclassical quantum mechanics as follows :

Let $\psi \in L^2(\mathbb{R}^3)$ and \hbar be the (scaled) Planck constant. Then the Wigner transform $w^\hbar(x, v)$ of $\psi(x)$ is the "phase-space" function in $L^2(\mathbb{R}_x^3 \times \mathbb{R}_v^3)$ obtained from the "density matrix" $\psi(x) \bar{\psi}(y)$ by a change of coordinates to "center of mass and relative coordinates at a scale \hbar and a subsequent Fourier transform with respect to the relative coordinate :

$$w^\hbar(x, v) = (2\pi)^{-3} \int_{\mathbb{R}_\eta^3} \psi(x - \hbar \frac{\eta}{2}) \bar{\psi}(x + \hbar \frac{\eta}{2}) e^{i\eta \cdot v} d\eta \quad (2.5)$$

where $\bar{\psi}$ denotes the complex conjugate of ψ .

By the superscript \hbar of $w^\hbar(x, v)$ we stress the \hbar -dependence of the transform which was introduced in the change of variables in the argument of ψ .

Note that the dual variable v of the position x represents a velocity (strictly speaking an impulsion ξ), thus justifying the name "phase space" for $\mathbb{R}_x^3 \times \mathbb{R}_v^3$ although the function w^{\hbar} is real but not nonnegative, i.e. w^{\hbar} **has in general also negative values** - a fact that saves the Heisenberg principle.

The time evolution of the Wigner function $w^{\hbar}(x, v, t)$ as the transform (2.5) of the wave function $\psi^{\hbar}(x, t)$ is obtained by direct calculation from the Schrödinger equation. The result is the so called "Wigner equation", also called "Quantum-Vlasov" or "Quantum-Liouville" equation :

$$\frac{\partial}{\partial t} w^{\hbar} + v \cdot \nabla_x w^{\hbar} - \Theta^{\hbar}[V] w^{\hbar} = 0, \quad (2.6)$$

where $\Theta^{\hbar}[V]$ is a so called pseudo-differential operator containing the potential V in its symbol. This operator is local in position x and nonlocal in velocity v due to the Fourier transform in the definition of the Wigner function.

This equation is already "very similar" to the classical Vlasov equation (2.3). The important point is that for the Wigner function the position density $n(x, t)$ is again given by a moment (i.e. a marginal of the "distribution function", just like in the classical case (2.4)

$$n(x, t) = \int_{\mathbb{R}_v} w^{\hbar}(x, v, t) dv \quad (2.7)$$

with $n(x, t) \geq 0$, although $w^{\hbar}(x, v, t)$ will in general have also negative values.

The idea of Wigner functions has initiated a lot of work in the context of phase-space formulations of quantum mechanics. Only recently the community of mathematicians working on partial differential equations has realized the enormous potential of Wigner transforms as a very powerful tool in many new contexts also outside quantum mechanics. This TMR project has contributed both to the general theory [GMMP], [M4] and to the special case of the description of an electron in a crystal lattice as it is necessary for semiconductor structures [BMP2].

In general a "Wigner transform" consists of three steps

- **Quadratic form** taking the product of a function and a complex conjugate function
- **Doubling of coordinates** to center of mass and relative coordinates with a **scaling parameter** (\hbar)
- **Fouriertransform** w.r.t. the relative coordinate

An exhausting general survey of properties of different realizations of Wigner transforms is given in [GMMP] (and [M4] as a short reading).

The mathematically difficult task is to rigorously justify the transition from the Schrödinger equation (2.1) to the Vlasov equation (2.3) via the Wigner equation (2.6). In case that the **potential** $V(x, t)$ is **given**, we have a "**linear problem**" which is easier to tackle.

However, for the modeling of semiconductors, we have to take into account the electrostatic repulsion of electrons among themselves. This means that the Schrödinger equation (2.1) governing the time evolution of the wave function ψ depends on the solution ψ of the equation : the problem becomes "nonlinear" ! This requires a self-consistent coupling of the Wigner equation to an equation for the potential $V(x, t)$. In the easiest approximation the potential is calculated from the charge density $n(x, t)$ by the Poisson equation :

$$\Delta V(x, t) = -(n(x, t) - C(x)) \quad (2.8)$$

where $C(x)$ stands for an eventual doping profile of a semiconductor device.

In section 4. we will consider an improved modeling of this selfconsistent coupling where the potential calculated from the Poisson equation is corrected by an additional "exchange potential".

For the "**nonlinear problem**", where the **potential** is not given but is calculated **self-consistently**, the classical limit $\hbar \rightarrow 0$ from the Schrödinger-Poisson system (2.1),(2.2), (2.8) to the Vlasov-Poisson system (2.3),(2.4), (2.8) has been an open problem for a long time, finally solved in [LP], [MM1].

For semiconductor modeling we have to regard the conduction electrons in a crystal. This yields a very interesting special case of a Schrödinger equation (2.1) with a potential that is periodic on a lattice. (In realistic models there is also an additional non-periodic potential.) In this case the classical limit of vanishing Planck constant has to be performed simultaneously with the homogenization of the periodic structure. This means that we look at the semiconductor on a scale where the distance between two atoms of the crystal lattice is too small to be resolved and we consider the periodic structure by "effective" macroscopic quantities.

Using adaptations and refinements of the idea of the Wigner transform (2.5) to the situation in a crystal we were able in [BMP2] to give the first rigorous derivation of the widely used "semiclassical equations" [AM] of solid state physics. The latter are a variant of the Vlasov equation (2.3) with the crucial difference that the distribution $f = f(x, k, t)$ has the velocity $v \in \mathbb{R}_v^3$ replaced by the "crystal momentum" $k \in B$, the bounded Brioullin zone, with $x \in \mathbb{R}$, $t > 0$:

$$\frac{\partial f}{\partial t} + \frac{1}{\hbar} \nabla_k E_m(k) \cdot \nabla_x f + \frac{1}{\hbar} \nabla_x V(x) \cdot \nabla_k f = 0, \quad (2.9)$$

subject to a periodic boundary condition in k .

Here $E_m(k)$ are the so called "energy bands" which are typical for a semiconducto [AM] and the k c dependent velocities $v_m(k)$ are given by $v_m(k) = \frac{1}{\hbar} \nabla_k E_m(k)$.

This equation has to be coupled to the Poisson equation (2.8) again, where the density $n(x, t) \geq 0$ is now given by

$$n(x, t) = \frac{1}{4\pi^3} \int_B f(x, k, t) dk \quad (2.10)$$

However, this inclusion of a non-periodic potential causes significant mathematical problems and the first result (in

3-dimensions) for a semiclassical limit to the semiclassical equations in a one band approximation with a field term was a major breakthrough given in the course of this TMR project [BMP2].

3. RELATIVISTIC CORRECTIONS OF THE SCHRÖDINGER EQUATION

In situations where electrons move very fast, the Schrödinger equation should be replaced by “relativistic models” which take into account the fact that there is no “instantaneous interaction” faster than the speed of light. This situation occurs not only for particles of cosmic radiation and in the mighty accelerators e.g. at CERN in Geneva, but also in every heavy atom the inner electrons cannot be described properly in a nonrelativistic theory which would not give the correct fine structure in the observed spectra.

One of the fundamental quantum mechanical and relativistic equations is the Dirac equation [D2] for the electron as a spinor. “Spinor” means that the scalar “wave function” ψ as it occurs in the Schrödinger equation is replaced by a vector Ψ which has 4 complex components.

These 4 components of Ψ correspond to an electron component and a “positron” component, both with two possible “spin directions”:

$$\Psi = \begin{pmatrix} \cdot \\ \cdot \\ \cdot \\ \cdot \end{pmatrix} = \begin{pmatrix} \text{electron, spin "up"} \\ \text{electron, spin "down"} \\ \text{positron, spin "up"} \\ \text{positron, spin "down"} \end{pmatrix} \quad (3.11)$$

It is one of the intrinsic peculiarities of relativistic quantum theory that in the Dirac equation a particle and its antiparticle occur intertwined.

The Dirac equation for Ψ is the “relativistic version of the Schrödinger equation” and it can be coupled to the Maxwell equations for the electromagnetic field in a similar way as we have coupled the Poisson equation (2.8) to the Schrödinger equation (2.1). Indeed, the Schrödinger-Poisson system is (formally) obtained as the “nonrelativistic limit” $c \rightarrow \infty$ of the nonlinear Dirac-Maxwell system, i.e. when the speed of light c tends to infinity.

In this project, however, we deal with the mathematically easier “linear case”, i.e. the case where the electromagnetic potential is given, e.g. the situation of a single electron in an external electromagnetic field. This is consistent with our assumption of bounded potentials which would not hold for the case of the selfconsistent Coulomb interaction among an ensemble of electrons, where the potential is given by the Poisson equation.

However, we are able, for the first time, to deal with the general case of time dependent potentials. All preceding literature treats the nonrelativistic limit in the mere “static case”, i.e. for time independent fields.

The Pauli equation (3.14) is an approximation of the Dirac equation (3.12) in two respects: on the one hand it is basically a first order approximation (in $1/c$), on the other hand it is an equation for the 2 spinor of the electron component of the 4 spinor of the Dirac equation (cp (3.11)), in fact, the positron components can be neglected in most problems of solid state physics.

The Dirac equation for a relativistic particle with spin in a given electromagnetic field is given by

$$i\hbar\partial_t\Psi = -i\hbar\gamma^0\gamma^k\partial_k\Psi + m_0c^2\gamma^0\Psi - qA_k\gamma^0\gamma^k\Psi - qV\Psi \quad (3.12)$$

The unknown Ψ is the 4-vector of the “Spinorfield” which is complex valued like the “wave function” ψ occurring in the Schrödinger equation (2.1), i.e. $\Psi(x, t) \in \mathcal{C}^4$, $t \in \mathbb{R}$ is the time, $x = (x_1, x_2, x_3) \in \mathbb{R}_x^3$ is the particles position. ∂_k stands for $\frac{\partial}{\partial x_k}$, where k denotes the 3 spatial dimension indices 1, 2, 3. The summation convention for indices is used, e.g. $\gamma^k A_k$ stands for $\sum_{k=1}^3 \gamma^k A_k$.

The 4×4 Dirac matrices $\gamma^\mu \in \mathcal{C}^{4 \times 4}$, $\mu = 0, \dots, 3$, are closely related to the 2×2 Pauli matrices $\sigma^k \in \mathcal{C}^{2 \times 2}$, $k = 1, 2, 3$.

$V(t, x)$ is the (time-dependent) electric potential and $A_k(x, t) \in \mathbb{R}$, $k = 1, 2, 3$, are the components of the magnetic potential where $\vec{A}(x, t) = (A_1, A_2, A_3)^\top$ is the magnetic potential vector. The electric field \vec{E} and the magnetic field \vec{B} are related to the potentials by the definition

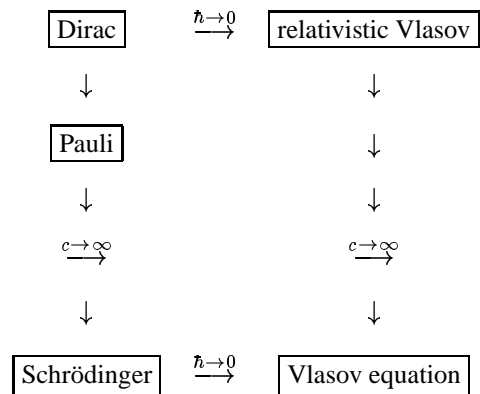
$$\vec{E}(x, t) = -\vec{\nabla}V - \partial_t\vec{A} \quad , \quad \vec{B}(x, t) = \text{curl}\vec{A} \quad (3.13)$$

The physical constants in (3.12) are $M = m_0c/\hbar$, $g = e/\hbar$, where m_0 is the electron’s rest mass, c is the velocity of light, \hbar is the Planck constant and e is the unit charge.

There are two physically important limits of the Dirac equation (3.12) which were both dealt with in the course of this TMR project:

- The “classical limit” $\hbar \rightarrow 0$ (with c fixed), which is rigorously performed in [GMMP] using Wigner-transform techniques.
- The “nonrelativistic limit” $c \rightarrow \infty$ (with \hbar fixed) is the limit where the velocity of light tends to infinity and “instantaneous interactions” are considered. It is the subject of [BMP1], [M5]

The following graph shows the relation between the linear Dirac equation (3.12) and its approximations in the two abovementioned limits.



In this project we have been concerned with all these limits besides the limit from a relativistic Vlasov equation (where the velocity is bounded by the speed of light c) to the nonrelativistic Vlasov equation (2.3).

The “total” nonrelativistic limit $c \rightarrow \infty$ of the Dirac equation (3.12) yields scalar “Schrödinger equations” of

the type (2.1) where the spin does no longer occur and , in our scaling, the magnetic field has vanished (in contrast to other possible scalings of the equation where the relativistic dynamics of the electron are somewhat decoupled of the relativistic nature of the magnetic field.)

By "semi-nonrelativistic approximations" we denote approximations of the Dirac equation (3.12) which retain terms "of the size $1/c$ and smaller" and we use the name "Pauli equation" for equations "at first order in $1/c$ " (where the smaller terms of the size $(1/c)^2$ have been neglected) containing the spin-magnetic field coupling term with the famous factor $1/2$:

$$i\hbar\partial_t\phi = (i\hbar\vec{\nabla} + 1/c\vec{A})^2\phi - V\phi - 1/c\hbar\frac{1}{2}\sigma^k B_k\phi \quad (3.14)$$

Here in the Pauli equation (3.14) $\phi(x, t)$ is the 2-spinor of the "electron component" of $\Psi(x, t)$, i.e.

$$\phi = \begin{pmatrix} \cdot \\ \cdot \end{pmatrix} = \begin{pmatrix} \text{electron, spin "up"} \\ \text{electron, spin "down"} \end{pmatrix} \quad (3.15)$$

The crucial role of "asymptotic analysis" is to derive and justify such approximate models like the Pauli equation which are "correct at first order" in a small parameter and simpler to deal with than the underlying "correct" model.

The existing mathematically rigorous results for non-relativistic limits treat the mere static case, i.e. time-independent electromagnetic potentials and the methods developed in [BMP1] have opened new doors to an analysis of the time-dependent case, including the Dirac-Maxwell system.

4. MODELLING MANY ELECTRON SYSTEMS BY ONE-PARTICLE SCHRÖDINGER EQUATIONS

Up to now we have taken for granted that we work with "one particle" equations, i.e. the wave function $\psi(x, t)$ was depending on a single position x .

However, in the modeling of a semiconductor we have to consider many conduction electrons interacting with each other via the electric repulsion by Coulomb's law. Hence our starting point has actually to be many body quantum mechanics where the fundamental equation is the N particle Schrödinger equation for the N particle wave function $\Psi(x_1, \dots, x_N)$. We regard the time-independent case only, where we have to deal with the stationary N particle Schrödinger equation

$$H^N \Psi = E\Psi \quad (4.16)$$

with the N -body Hamilton operator

$$H^N := -\sum_{i=1}^N \Delta_i + \sum_{i=1}^N \sum_{j < i; j=1}^N V(x_i - x_j), \quad (4.17)$$

where we could eventually also add "local external potentials" $\sum_{i=1}^N U_{ext}(x_i)$.

By the "Pauli principle" it is forbidden that two electrons are in the same state. This implies that the N -fermion wavefunction $\Psi(x_1, \dots, x_N)$ has to be "antisymmetric", i.e. it changes sign when we interchange two arguments

x_j and x_k and it is zero whenever two positions x_j and x_k are equal. Mathematically this requirement is fulfilled if we assume Ψ to be a "Slater determinant" $\Psi(x_1, \dots, x_N) = \det(\psi_j(x_i))$.

Let $\psi_j(x)$, $j = 1, \dots, N$ be such "one particle" wave functions describing the ground state of N electrons.

The Hartree-Fock (HF) model is the system of "one-particle equations" obtained by plugging the ansatz of a Slater determinant for Ψ into the equation (4.16) and making a variation principle for minimizing the total energy. This yields the following system of N equations for the (ψ_j) , $j = 1, \dots, N$'s :

$$-\frac{\Delta}{2}\psi_j + V_{local}(x)\psi_j + V_j(x, (\psi_k))\psi_j = \lambda_j\psi_j, \quad (4.18)$$

where we have chosen a scaling such that $\hbar^2/m = 1$. The potential V_{local} includes eventual external potentials (nuclei, electric field,...) whereas the selfconsistent potential V_j depends non-linearly on the whole set (ψ_k) and couples the N equations. It consists of the "direct Coulomb" term and the nonlocal exchange potential $V_{j,ex}$ which is different for each j .

Especially when N becomes very large, this HF model becomes too tedious for practical calculations. In solid state physics and in particular in semiconductor modeling we have to deal with extremely high numbers N of electrons and it is necessary to replace the HF system by simpler equations which allow for practical calculations, in particular for the exchange term $V_{j,ex}$ which is given by

$$(V_{ex}\psi_j)(x) := -\sum_{k=1}^N \int \frac{\psi_j(x')\overline{\psi_k(x')}{|x-x'|} \psi_k(x) dx' \quad (4.19)$$

This term not only couples the N equations, but is different for each of the equations, what we will call "nonlocal in the state" ψ_j . In addition, this term is "nonlocal in position" x .

In Density Functional Theory (DFT), $V_{j,ex}$ is approximated by a potential of the form $V(x, n)$ which does not depend on the ψ_j individually but only on their density function $n(x) = \sum_j |\psi_j(x)|^2$.

An astonishingly simple approximation of the exchange potential is due to Slater [S1] who replaces the complicated expression (4.19) by a simple third root of the density :

$$(V_{ex}\psi_j)(\mathbf{x}) \simeq -Cn^{1/3}(\mathbf{x}) \psi_j(\mathbf{x}) \quad (4.20)$$

(where $C > 0$ is a constant).

This term has the additional advantage that it models the exchange interaction without wave functions and can hence be used also in "classical" models. In particular in models invoking Fermi-Dirac statistics an exchange term should be included for reasons of consistency with the underlying Pauli principle.

The correct selfconsistent coupling of a one-particle Schrödinger equation (2.1) is hence given by a potential $V(x)$ that consists of the "direct Coulomb part" calculated

from the charge density $n(x)$ (2.2) via the Poisson equation (2.8) minus an exchange correction (4.20) which is a local function of $n(x)$.

$$V(x) = \int_{\mathbb{R}^3} \frac{1}{|x-x'|} n(x') dx' - Cn^{1/3}(x) \quad (4.21)$$

This different modeling can result in significant differences in the numerical simulations of semiconductor devices; e.g. in simulations of a resonant tunneling diode the inclusion of the exchange correction can influence the appearance of a hysteresis-like bistability of the steady state which in turn influences the current-voltage characteristic of the device. This is a typical example of the role of improved models obtained by corrections to “standard models”.

It is the goal of [BM1] to rigorously justify the replacement of (4.19) by (4.20) in the limit of high densities, i.e. $N \rightarrow \infty$ for fixed volume. (cp. [LS1]).

In the course of this TMR project we have introduced the method of deformations (local scaling transformations) [DaM] to this problem by using the basic idea of physicists, in particular Slater [S1] in a mathematically rigorous way : starting from the free electron approximation (plane waves) we use deformations to deal with rigorous derivations [BM1] for these models in the “high density limit”.

In a follow up works , [BGM1], [BGM2] we have started an extension on of the use of deformations for rigorously deriving other models of density functional theory (DFT), in particular the well known approximations for the kinetic energy as given by Thomas-Fermi (TF) theory [LS1] and it’s improvements such as the TF-von Weizsäcker (TFvW) [BGM1] and TFvW-Dirac (TFvWD) model (cf [D1]).

Again, these simplified models, where the energy is a function of the density n only instead of the many body wave function Ψ , are valid in the asymptotic regime $N \rightarrow \infty$ which corresponds to the “high density limit” since we keep the volume where the particles are contained fixed.

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