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Selected Topics in Partial Differential Equations

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Abstract
Enstedt, M. 2011. Selected Topics in Partial Differential Equations. Acta Universitatis Upsaliensis. *Uppsala Dissertations in Mathematics* 70. x, 14 pp. Uppsala. ISBN 978-91-506-2193-8.

This Ph.D. thesis consists of five papers and an introduction to the main topics of the thesis. In Paper I we give an abstract criteria for existence of multiple solutions to nonlinear coupled equations involving magnetic Schrödinger operators. In paper II we establish existence of infinitely many solutions to the quasirelativistic Hartree-Fock equations for Coulomb systems along with properties of the solutions. In Paper III we establish existence of a ground state to the magnetic Hartree-Fock equations. In Paper IV we study the Choquard equation with general potentials (including quasirelativistic and magnetic versions of the equation) and establish existence of multiple solutions. In Paper V we prove that, under some assumptions on its nonmagnetic counterpart, a magnetic Schrödinger operator admits a representation with a positive Lagrange density and we derive consequences of this property.

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Till mamma och pappa

Preface

In the clearing stands a boxer and a fighter by his trade,
And he carries the reminders of every glove that laid him down,
Or cut him 'til he cried out in his anger and his shame,
"I am leaving, I am leaving." But the fighter still remains.

Simon & Garfunkel, The Boxer, 1969

This thesis will be presented to the Faculty of Science and Technology at Uppsala University, in candidacy, for the degree of Doctor of Philosophy. I have been employed at the Department of Mathematics for five years. My employment consisted of one year teaching, two years of advanced courses and two years of research.

The thesis consists of a brief introduction to the topic of the thesis, a summary in Swedish and a collection of selected publications between 2008 and 2010.

First of all I would like to express my deepest gratitude to my advisor Michael Melgaard. The warm hospitality from Yehuda Pinchover and the Department of Mathematics at Technion-Israel Institute of Technology during my visit was very much appreciated. I would like to thank Michael Benedicks, Royal Institute of Technology, for giving me the opportunity to participate in the program "Dynamics and PDE" at the Mittag-Leffler Institute. The School of Mathematical Sciences at Dublin Institute of Technology has shown me great hospitality during all my visits and for that I am very grateful.

I am thankful for having had the opportunity of participating in The National Graduate School in Scientific Computing (NGSSC).

Finally, and by no means the least, I would like to heartfully thank my family for all their support and patience over the years.

MATTIAS ENSTEDT
Uppsala, February 2011

List of Papers

This thesis is based on the following papers, which are referred to in the text by their Roman numerals.

I Enstedt, M., Melgaard, M. (2010) Abstract criteria for multiple solutions to nonlinear coupled equations involving magnetic Schrödinger operators (submitted manuscript).

II Enstedt, M., Melgaard, M. (2009) Existence of infinitely many distinct solutions to the quasi-relativistic Hartree-Fock equations. *International Journal of Mathematics and Mathematical Sciences*, 2009 (ID 651871).

III Enstedt, M., Melgaard, M. (2008) Existence of solution to Hartree-Fock equations with decreasing magnetic fields. *Nonlinear analysis*, 69(7):2125-2141.

IV Enstedt, M., Melgaard, M. (2010) Multiple solutions of Choquard type equations, (submitted manuscript).

V Enstedt M., Tintarev, K. (2009) Weighted spectral gap for magnetic Schrödinger operators with a potential term. *Potential Analysis*, 31(3):215-226.

It should be stressed that Paper I above can be used to extend the following paper, which is not included in the thesis.

Enstedt, M., Melgaard, M. (2008) Non-existence of a minimizer to the magnetic Hartree-Fock functional. *Positivity*, 12(4):653-666.

Contents

1. Introduction

The general topic of this Ph.D. thesis is partial differential equations (PDEs). This thesis deals with various problems originating in quantum mechanics and quantum chemistry. Also, problems within nonlinear analysis are studied. The introduction that follows is brief and by no means complete. For a more complete description the reader may consult the bibliography within each paper.

1.1 The time-independent Schrödinger equation

In this section we aim to give a very brief description of quantum mechanics. We refer to [Thi02] for a more complete treatment. Consider a system of N electrons interacting with K nuclei. Measurable quantities, such as energy, of this physical system, described by quantum mechanics (which is the underlying mathematical framework for many of branches of physics and chemistry), corresponds to self-adjoint operators acting on certain Hilbert spaces, which are subspaces of $L^2(\mathbb{R}^m)$, for some m depending on the number of electrons. In a typical situation, considering the nuclei as classical (the Born-Oppenheimer approximation) fixed at points $\mathbf{R} := (R_1, \cdots, R_K) \in \mathbb{R}^{3K}$, one has an energy operator, $H^{\mathbf{R}}$, of the form

$$\sum_n T_n + V(x_n) + \frac{1}{2} \sum_{m \neq n} W(x_n - x_m),$$

corresponding to an energy functional, $\mathscr{E}$, say, where T_n corresponds to the kinetic energy of particle n. Here $x_n \in \mathbb{R}^3$ corresponds to the position of particle n, V to some external potential and W is a potential describing the interaction between the particles. The time-independent Schrödinger equation reads

$$H^{\mathbf{R}} \psi = E \psi, \tag{1.1.1}$$

where the scalar E denotes the energy and ψ is a normalized function in the aforementioned Hilbert space. From this microscopic model one can derive many macroscopic properties.

1.2 Magnetic Schrödinger operators

In Section 1.1 the operator $-\Delta$ is an example of how to described the kinetic energy of a particle in a physical system. To have an analogous description of kinetic energy when the system is exposed to an external magnetic field $\mathscr{B} : \mathbb{R}^3 \to \mathbb{R}^3$, we introduce the magnetic Laplace operator $\Delta_{\mathscr{A}}$. The operator is formally defined by $(\nabla + i\mathscr{A})^2$, and associated with the quadratic form (defined on $\mathbf{H}^1_{\mathscr{A}}(\mathbb{R}^3)$ which will be introduced below)

$$\phi \mapsto \int_{\mathbb{R}^3} |\nabla + i\mathscr{A}\phi|^2 \mathrm{d}x.$$

Here the magnetic potential $\mathscr{A}$ satisfies $\nabla \times \mathscr{A} = \mathscr{B}$, in general one does not make any regularity assumptions on the magnetic potential.
When working with the usual Laplace operator one knows that the Sobolev space $\mathbf{H}^1(\mathbb{R}^3)$, defined as the space of all functions which belong to $L^2(\mathbb{R}^3)$, have their first distribution derivatives in $L^2(\mathbb{R}^3)$ and is equipped with the inner product

$$\langle \phi, \psi \rangle_{\mathbf{H}^1(\mathbb{R}^3)} := \int_{\mathbb{R}^3} \phi \overline{\psi} + \nabla \phi \cdot \nabla \overline{\psi} \mathrm{d}x,$$

many times play an important part. Here $\overline{\psi}$ denotes the complex-conjugate of ψ. One therefore has to define an analogous space, which we will call a magnetic Sobolev space. We define

$$\mathbf{H}^1_{\mathscr{A}}(\mathbb{R}^3) := \left\{ \phi \in L^2(\mathbb{R}^3) : \nabla_{\mathscr{A}} \phi \in L^2(\mathbb{R}^3) \right\}$$

where $\nabla_{\mathscr{A}} := \nabla + i\mathscr{A}$, with norm

$$\|f\|_{\mathbf{H}^1_{\mathscr{A}}(\mathbb{R}^3)} := \left(\|f\|^2_{L^2(\mathbb{R}^3)} + \|\nabla_{\mathscr{A}} f\|^2_{L^2(\mathbb{R}^3)} \right)^{\frac{1}{2}}.$$

The diamagnetic inequality (see e.g. [LL01, EL89] and the references therein) states that, for a given $\mathscr{A} \in L^2_{\mathrm{loc}}(\mathbb{R}^3)$, that for all $\phi \in \mathbf{H}^1_{\mathscr{A}}(\mathbb{R}^3)$ we have that

$$|\nabla_{\mathscr{A}} \phi| \geq |\nabla |\phi||. \tag{1.2.1}$$

This inequality is very important and give us in combination with the Sobolev embedding theorem (see e.g. [Maz85, Ada75]) many useful properties. For more details one can, as an example, consult [BE10].

1.3 Quasirelativistic Schrödinger operators

In Section 1.2 we considered a way to describe the kinetic energy of a particle under the influence of an external magnetic field. If we want to take some additional effects into account one can consider the quasirelativistic energy that we will introduce in this section. We know that, appropriately defined, the Fourier-Plancherel transform, $\mathscr{F} : L^2(\mathbb{R}^3) \to L^2(\mathbb{R}^3)$, is a unitary isomorphism (cf. [Hör03, SW71]) and we may therefore define

$$\mathbf{H}^{\frac{1}{2}}(\mathbb{R}^3) := \left\{ f \in L^2(\mathbb{R}^3) : (1 + |\xi|^2)^{\frac{1}{4}} \mathscr{F} f(\xi) \in L^2(\mathbb{R}^3) \right\},$$

with the inner-product

$$\langle \phi, \psi \rangle_{\mathbf{H}^{\frac{1}{2}}(\mathbb{R}^3)} := \int_{\mathbb{R}^3} \mathscr{F}\phi(\xi)(1+|\xi|^2)^{\frac{1}{2}}\overline{\mathscr{F}\psi(\xi)}\mathrm{d}\xi,$$

we refer to [Fol99] for details.
We define the following sesquilinear form on $\mathbf{H}^{\frac{1}{2}}(\mathbb{R}^3) \times \mathbf{H}^{\frac{1}{2}}(\mathbb{R}^3)$:

$$\int_{\mathbb{R}^3} \mathscr{F}\phi(\xi)\overline{\mathscr{F}\psi(\xi)}\left(\left(\frac{1}{\alpha^2}+|\xi|^2\right)^{\frac{1}{2}} - \frac{1}{\alpha}\right)\mathrm{d}\xi$$

and using one of Kato's representation theorems, we can associate a quasirelativistic operator for the kinetic energy (see e.g. [EE87, RS78, BE10] for details). Here $\alpha > 0$ is Sommerfeld's structure constant, which is roughly equal to $\frac{1}{137}$.

1.4 The basic model

We will now be more precise than in the previous sections. We still consider a system of N electrons interacting with K nuclei (static), with charge $Z_k > 0$ and position R_k. Define $Z := (Z_1, \dots, Z_K)$ and put $V(x) := -\sum_{k=1}^{N} \frac{Z_k}{|x-R_k|}$ along with $W(x) := \frac{1}{|x|}$. We can of course consider more general potentials V and W (which is done in certain papers in this thesis), but V and W as before are among the most common in physics and the discussions along with definitions in this section is mutatis mutandis (up to the fact that the problems has to be well-defined). Since systems of particles are usually found in their most stable state, the lowest E in (1.1.1), the ground state energy, is of fundamental interest. Equivalently, by a variational principle, we can define (still on a formal level) the following to be the ground state

$$E(N, \mathbf{Z}) := \inf_{\psi \in \mathscr{H} : \|\psi\|_{\mathbf{L^2}(\mathbb{R}^{3\mathrm{N}})} = 1} \mathscr{E}(\psi), \tag{1.4.1}$$

where $\mathscr{H}$ is defined as the N-fold antisymmetric tensor product of $\mathbf{H}(\mathbb{R}^3) \subset L^2(\mathbb{R}^3)$ and

$$\mathscr{E}(\psi) := \sum_{n=1}^{N} \mathfrak{s}[\psi(x1, \dots, x_{n-1}, \cdot, x_{n+1}, \dots, x_N)] + \int_{\mathbb{R}^3} V(x_n)|\psi|^2 \mathrm{d}x_n$$
$$+ \frac{1}{2}\sum_{m \neq n} \int_{\mathbb{R}^3 \times \mathbb{R}^3} W(x_n - x_m)|\psi|^2 \mathrm{d}x_n \mathrm{d}x_m. \tag{1.4.2}$$

Typically, the space $\mathbf{H}(\mathbb{R}^3)$ is defined depending on the the models we are working with and $\mathfrak{s} : \mathbf{H}(\mathbb{R}^3) \to \mathbb{R}$ is a quadratic form, corresponding to the kinetic energy. See Section 1.2 and Section 1.3 for examples of $\mathbf{H}(\mathbb{R}^3)$ and $\mathfrak{s}$.

1.5 Approximations

Let us now consider (1.1.1) in the hydrogen case (with appropriate units). It is special because it is exactly solvable. It can be shown that, the discrete spectrum, denoted spec_{d}, of $H_1 = -\Delta - |x|^{-1}$ acting on $L^2(\mathbb{R}^3)$ equals

$$\text{spec}_{\text{d}}(H_1) = \left\{ -\frac{1}{(2n)^2} : n = 1, 2, 3, \ldots \right\}.$$

When N increases the functional (1.4.2) will still be a quadratic form, which, in the situation, has to be considered a good property. The problem is connected to the space on which the minimization takes place. Therefore approximation is needed. We focus on the following approximation. In addition to the references in the papers we recommend [CLBM06, LBL05, Lie90, Lio88]. See also the quantum chemistry book [SO96].

1.5.1 The Hartree-Fock approximation

A so-called wave function method aim to find a approximation of the "true" ground state by reducing the complexity of the space upon which one aims to find critical points (the variational space). An example of this method is the Hartree-Fock approximation. The Hartree-Fock approximation consists of restricting the possible minimizers from all elements in $\mathscr{H}$ to all elements which can be written as

$$\Psi := \frac{1}{\sqrt{N!}} \det \phi_n(x_m),$$

where $\{\phi_n\}_{n=1}^N \in \mathbf{H}^N$ (with canonical inner-product) satisfies $\langle \phi_n, \phi_m \rangle_{L^2(\mathbb{R}^3)} = \delta_{nm}$. This motivates the following definition.

Definition 1. *The* **Hartree-Fock ground state energy** *is*

$$E := \inf \left\{ \mathscr{E}(\phi_1, \ldots, \phi_N) : (\phi_1, \ldots, \phi_N) \in \mathbf{H}^N, \langle \phi_m, \phi_n \rangle_{L^2(\mathbb{R}^3)} = \delta_{mn} \right\},$$

where

$$\begin{aligned} \mathscr{E} : \mathbf{H}^N \to \mathbb{R} : (\phi_1, \cdots, \phi_N) \mapsto & \sum_{n=1}^{N} \mathfrak{s}[\phi_n] + \int_{\mathbb{R}^3} V(x)\rho(x)\mathrm{d}x \\ & + \frac{1}{2} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} W_1(x - x')\rho(x)\rho(x') - |\tau(x, x')|^2 W_2(x - x')\mathrm{d}x\mathrm{d}x'. \end{aligned} \quad (1.5.1)$$

Here $\tau(x,x') = \sum_{n=1}^{N} \phi_n(x)\,\phi_n(x')$ *is the density matrix, and* $\rho(x) = \sum_{n=1}^{N} |\phi_n(x)|^2$ *the density associated to the state. The functions* W_1, W_2 *and* V *are real valued and defined on* $\mathbb{R}^3$. *If a minimizer exists then it is said that the molecule has a* **Hartree-Fock ground state**. *We will call other critical points of* $\mathscr{E}$ *for* **excited states**.

1.6 Some inequalities

Let us assume that we want to study the existence question of a Hartree-Fock ground state for $\mathscr{A} = \mathbf{0}$, $W_1 = W_2 = \frac{1}{|x|}$ and $V = -\frac{Z}{|x|}$ with $Z > 0$, say. Then the naive way, when one wants to study a minimizing sequence, is to prove that the sequence will be uniformly bounded in $\mathbf{H}^1(\mathbb{R}^3)$. Due to the non-negativity, from the Cauchy-Schwartz inequality, of the last term in (1.5.1) inequalities of the type

$$\int_{\mathbb{R}^3} \frac{|\phi|^2}{|x|}\mathrm{d}x \leq \varepsilon \int_{\mathbb{R}^3} |\nabla\phi|^2\mathrm{d}x + C(\varepsilon)\int_{\mathbb{R}^3} |\phi|^2\mathrm{d}x, \quad \phi \in \mathbf{C}_0^\infty(\mathbb{R}^3), \tag{1.6.1}$$

which can be found in e.g. [RS75, RM05], will be useful and important. Here $\varepsilon > 0$ and C is a function depending on ε. A way of looking at it is to consider the ground state question for the hydrogen atom, with charge Z of the nuclei which is placed at the origin, namely,

$$\inf_{\phi\in\mathbf{H}^1_{\mathscr{A}}(\mathbb{R}^3)} \left\{ \int_{\mathbb{R}^3} |\nabla_{\mathscr{A}}\phi|^2 + V|\phi|^2\mathrm{d}x : \|\phi\|_{L^2(\mathbb{R}^3)} = 1 \right\},$$

with V as above and $\mathscr{A} \in L^2_{\mathrm{loc}}(\mathbb{R}^3)$. The diamagnetic inequality and Hölder's inequality in combination with the classical Hardy inequality

$$\int_{\mathbb{R}^3} |\nabla\phi|^2 - \frac{|\phi|^2}{|x|^2}\mathrm{d}x \geq \frac{1}{4}\int_{\mathbb{R}^3} |\phi|^2\mathrm{d}x, \qquad \phi \in \mathbf{H}^1(\mathbb{R}^3), \tag{1.6.2}$$

allow us to conclude that

$$\int_{\mathbb{R}^3} |\nabla_{\mathscr{A}}\phi|^2 + V|\phi|^2\mathrm{d}x \geq \int_{\mathbb{R}^3} \left(\frac{1-4Z|x|}{4|x|^2}\right)|\phi|^2\mathrm{d}x \geq -Z^2. \tag{1.6.3}$$

Thus we have the existence of an infimum. Whether this infimum is attained or not is a different question.
In connection with this there are many natural questions. As an example, let us take $\mathbf{H}^{\frac{1}{2}}(\mathbb{R}^3)$ as the underlying space. This case will be very natural in connection to, for example, many type of quasirelativistic Schrödinger equations, quasirelativistic Hartree equations, quasirelativistic Hartree-Fock equations and quasirelativistic Choquard type equations. In this case one can rely

on methods from harmonic analysis to get

$$\int_{\mathbb{R}^3} |\xi||\hat{\phi}(\xi)|^2 \mathrm{d}\xi - \int_{\mathbb{R}^3} \frac{2|\phi|^2}{\pi|x|}\mathrm{d}x \geq 0, \qquad \phi \in \mathbf{H}^{\frac{1}{2}}(\mathbb{R}^3).$$

We refer to [Kat95] for details. This informs us that we have to impose a bound from below on the constant $\varepsilon > 0$ if we want to conclude something similar to (1.6.1). Hence we have weaker properties, in terms of these inequalities, when we consider problems involving quasirelativistic operators.

On the other hand, if we move our focus back to the magnetic case, when we use the diamagnetic inequality (1.2.1) in, for exampel (1.6.3), we, roughly speaking, use that we do not loose any strength in the inequality when we change our study from the magnetic case to the nonmagnetic case. We do not however, use the possibility that the magnetic field might, for specific magnetic fields, actually improve the Hardy constant ($\frac{1}{4}$ in (1.6.2)), at least on subsets of $\mathbb{R}^3$ or more generally, with a different Hardy constant, on subsets of $\mathbb{R}^N$. In connection to this it is natural to ask if, given a $\mathscr{A}$ and a V, there exist a positive function $\Lambda : \mathbb{R} \to \mathbb{R}$, say, with some regularity properties such that

$$\int_{\mathbb{R}^N} |\nabla_{\mathscr{A}}\phi|^2 + V|\phi|^2 \mathrm{d}x \geq \int_{\mathbb{R}^N} \Lambda(|\phi|)\mathrm{d}x.$$

This would inform us that we have, in some sense, a gap. If we are able to prove the existence of such a function we might ask if it is possible to actually find some lower bounds on Λ and using this, perhaps, improve some inequalities, for example, the Hardy inequality.

2. Summary of the papers

In this chapter we give a brief and by no means complete description of the content of the papers in this thesis. For a more complete list of references we refer to each paper.

2.1 Paper I

In Paper I [EM10a], joint with Michael Melgaard, we extend results by the authors in [EM08a] (note that the arguments can be used to extend results in [EM08b]). The main contribution of the paper is that it provides an abstract criteria for determining, for example, if a Hartree-Fock type system has infinitely many solutions. The criteria is general and will depend on, for example, the sign of the functions W_1 and W_2. One of the main results is the following theorem.

Theorem 2. *Let the general assumptions and Assumption 3.1 hold true. Then:*
1. Every minimizing sequence of the functional $\mathscr{E}(\cdot)-\gamma\|\cdot\|^2_{L^2(\mathbb{R}^3)^N}$, *is relatively compact in* $\mathscr{C}$. *In particular, there exists a minimizer* φ *of* $\mathscr{E}(\cdot)-\gamma\|\cdot\|^2_{L^2(\mathbb{R}^3)^N}$, *on* $\left\{(\phi_1,\ldots,\phi_N)\in\mathbf{H}^1_{\mathscr{A}}(\mathbb{R}^3)^N, \langle\phi_m,\phi_n\rangle_{L^2(\mathbb{R}^3)}=\delta_{mn}\right\}$ *and (up to unitary transformations) the components of* $\varphi=(\varphi_1,\ldots,\varphi_N)$ *satisfy the Hartree-Fock type equations*

$$\begin{cases} F\varphi_n+(\lambda_n-\gamma)\varphi_n=0, \\ \langle\varphi_m,\varphi_n\rangle_{L^2(\mathbb{R}^3)}=\delta_{mn}, \end{cases} \tag{2.1.1}$$

where F *is the Fock type operator (associated with* $\mathscr{E}(\cdot)-\gamma\|\cdot\|^2_{L^2(\mathbb{R}^3)^N}$*) and the numbers* $-(\lambda_n-\gamma)$ *are the* N *lowest eigenvalues of* F.
2. There exists a sequence $\{\varphi^{(k)}\}_{k=1}^{\infty}$, *with entries* $\varphi^{(k)}=(\varphi_1^{(k)},\ldots,\varphi_N^{(k)})$, *of solutions (on different levels of energy) of the Hartree-Fock type equations (2.1.1) which satisfy the constraints* $\langle\varphi_m^{(k)},\varphi_n^{(k)}\rangle_{L^2(\mathbb{R}^3)}=\delta_{mn}$ *for all* $1\le m,n\le N$ *and, furthermore, the Lagrange multipliers* $\lambda_n^{(k)}-\gamma$ *are positive.*

Moreover, depending on the assumptions one can derive various properties of the solutions, we refer to the paper for complete details.

2.2 Paper II

In Paper II based on [EM09], joint with Michael Melgaard, we give the first proof of existence of multiple solutions to the quasirelativistic Hartree-Fock equations.

Theorem 3. *Let us assume that the total nuclear charge* $Z_{\mathrm{tot}} = \sum_{k=1}^{K} Z_k$ *satisfies* $Z_{\mathrm{tot}} < Z_{\mathrm{c}} := 2/(\alpha\pi)$ *(where* α *is the Sommerfeld's structure constant) and let* $N \in \mathbb{N}$ *satisfy* $N-1 < Z_{\mathrm{tot}}$*. We define* $V := -\sum_{k=1}^{N} \frac{Z_k}{|x-R_k|}$*, with* $R_k \in \mathbb{R}^3$ *and* $W := \frac{1}{|x|}$*. Then:*
1. Every minimizing sequence of the quasirelativistic Hartree-Fock functional $\mathscr{E}(\cdot)$ *is relatively compact in the Stiefel type manifold*

$$\mathscr{C} := \left\{ (\phi_1, \ldots, \phi_N) \in \mathbf{H}^{\frac{1}{2}}(\mathbb{R}^3)^N : \langle \phi_n, \phi_m \rangle_{L^2(\mathbb{R}^3)} = \delta_{nm} \right\}.$$

In particular, there exists a minimizer φ *of* $\mathscr{E}(\cdot)$ *on the admissible set* $\mathscr{C}$ *and (up to unitary transformations) the components of* $\varphi = (\varphi_1, \ldots, \varphi_N)$ *will satisfy the quasirelativistic Hartree-Fock equations*

$$\begin{cases} F\varphi_n + \lambda_n \varphi_n = 0, \\ \langle \varphi_m, \varphi_n \rangle_{L^2(\mathbb{R}^3)} = \delta_{mn}, \end{cases}$$

where F *is the quasirelativistic Fock operator (see the paper for the exact construction) and the numbers* $-\lambda_n$ *are the* N *lowest negative eigenvalues of the operator* F*.*
2. There exists a sequence $\{\varphi^{(k)}\}_{k\geq 1}$*, with entries* $\varphi^{(k)} = (\varphi_1^{(k)}, \ldots, \varphi_N^{(k)})$*, of distinct solutions of the quasirelativistic Hartree-Fock equations (in the sense above) which satisfy the constraints* $\langle \varphi_m^{(k)}, \varphi_n^{(k)} \rangle_{L^2(\mathbb{R}^3)} = \delta_{mn}$*, for all* $1 \leq m,n \leq N$ *and, furthermore, the Lagrange multipliers* $\lambda_n^{(k)}$ *are nonnegative and positive, when* $Z_{\mathrm{tot}} = N$ *and* $Z_{\mathrm{tot}} > N$*, respectively. Moreover, the following properties are valid as* $k \to \infty$*:*

$$\begin{array}{rcl} \lambda_n^{(k)} & \longrightarrow & 0, \quad \mathscr{E}(\varphi^{(k)}) \longrightarrow 0, \\ \varphi^{(k)} & \longrightarrow & 0 \text{ weakly in } \mathbf{H}^{1/2}(\mathbb{R}^3)^N. \end{array}$$

It is should be stressed that there exist regularity and decay results for these equations, we refer to the paper for more details.

2.3 Paper III

In Paper III based on [EM08a], joint with Michael Melgaard, we study the existence of a ground state for the magnetic Hartree-Fock equations for a class of magnetic fields.

Theorem 4. *Assume that* $Z_{\text{tot}} = \sum_{k=1}^{K} Z_k > N-1$*, where* $Z_k > 0$*. Let* $V = -\sum_{k=1}^{N} \frac{Z_k}{|x-R_k|}$*, with* $R_k \in \mathbb{R}^3$ *and assume that* $W = \frac{1}{|x|}$*. If Assumption 1.1 holds true then there exists a Hartree-Fock ground state, which is also a solution to the Hartree-Fock equation.*

2.4 Paper IV

In Paper IV [EM10b], joint with Michael Melgaard, we study quasirelativistic and magnetic versions of the so-called Choquard equation. The positivity that was mentioned in Section 1.6 does not hold. This will have a significant impact on the analysis of the problem. We present a criteria, to conclude existence of infinitely many solutions to the corresponding version of the Choquard equations, with general potentials. As a special case of the results in this paper we have the following.

Theorem 5. *Let the general assumption hold true. Furthermore, in the quasirelativistic case assume that Assumption 3.1 holds true and in the magnetic case assume that Assumption 3.4 holds true. Then the equation*

$$\begin{cases} L_{\#}\phi + V\phi - |\phi|^2 * W\phi = -\lambda\phi, \\ \|\phi\|_{L^2(\mathbb{R}^3)} = 1, \end{cases} \tag{2.4.1}$$

has infinitely many solutions for $L_{\text{cm}} = -\Delta_{\mathscr{A}} = (\nabla + i\mathscr{A})^2$*, with* $\mathscr{A} \in L^2_{\text{loc}}(\mathbb{R}^3)$*, or* $L_{\text{cq}} = \sqrt{-\alpha^{-2}\Delta + \alpha^{-4}} - \alpha^{-2}$ *(with* α *being Sommerfeld's structure constant).*

In the paper various symmetry and decay properties of the solutions are proven, see the paper for details.

2.5 Paper V

In Paper V [ET09], joint with Kyril Tintarev, we study the quadratic form

$$\mathfrak{q}_{\mathscr{A},V} : C_c^\infty(\Omega) \to \mathbb{R} : u \mapsto \int_\Omega |\nabla_{\mathscr{A}} u(x)|^2 + V(x)|u(x)|^2 \mathrm{d}x.$$

Later on we need $\mathscr{B} := \operatorname{curl} \mathscr{A}$. We prove the following statement on the spectral gap.

Theorem 6. *Suppose that* $\Omega \subset \mathbb{R}^N$ *is a domain and that* $V \in L^\infty_{\text{loc}}(\Omega)$ *is such that* $\mathfrak{q}_{0,V} \geq 0$*. Let* $\mathscr{A} \in \mathscr{K}(\Omega)$*, where*

$$\mathscr{K}(\Omega) = \begin{cases} \cup_{a>2} L^a_{\text{loc}}(\Omega, \mathbb{R}^N) & N = 2, \\ L^N_{\text{loc}}(\Omega, \mathbb{R}^N) & N \geq 3. \end{cases}$$

If curl $\mathscr{A} \neq 0$*, in the sense of distributions, on* Ω*, the quadratic form* $\mathfrak{q}_{\mathscr{A},V}$ *has a weighted spectral gap in* Ω*. That is, there exist a positive continuous function* W*, such that*

$$\mathfrak{q}_{\mathscr{A},V}(u) \geq \int_\Omega W(x)|u(x)|^2 \mathrm{d}x, \qquad u \in C_c^\infty(\Omega),$$

hold true.

Using an estimate on the gap that is derived in the paper we may derive the following.

Theorem 7. *Let* $\Omega \subset \mathbb{R}^N \setminus B_r(0)$*,* $r > 0$*,* $N > 2$*, and let* $V = -\left(\frac{N-2}{2}\right)^2 |x|^{-2}$*. We have that*

$$\mathfrak{q}_{\mathscr{A},V}[u] \geq \frac{\varepsilon}{\varepsilon+1} \int (b - \varepsilon(N-2)^2/4r^{-2})|u|^2 \mathrm{d}x.$$

For $N > 2$*, setting* $\varepsilon = 2br^2/(N-2)^2$*, we arrive at*

$$\mathfrak{q}_{\mathscr{A},V}[u] \geq \frac{b}{2} \frac{2br^2/(N-2)^2}{1+2br^2/(N-2)^2} \int |u|^2 \mathrm{d}x.$$

This also implies that the best Hardy constant in the problem is greater or equal to

$$\left(\frac{N-2}{2}\right)^2 + \frac{b^2}{2b + r^{-2}(N-2)^2}.$$

In addition we prove the following result within the theory of nonlinear magnetic Schrödinger equations.

Theorem 8. *Assume that* $\mathscr{B}$ *is an exact and continuous 2-form on* $\mathbb{R}^N$*. Let* $\mathscr{B}$ *and* $V \in \mathscr{V}$ *be* $\mathbb{Z}^N$*-periodic and assume that* V *belongs to*

$$\left\{ V \in L^\infty_{\mathrm{loc}}(\mathbb{R}^N) : \mathfrak{q}_{0,V} \geq 0 \right\}.$$

Then there exists a minimizer for

$$\inf \left\{ \mathfrak{q}_{\mathscr{A},V}[u] : \int_{\mathbb{R}^N} |u(x)|^p \mathrm{dx} = 1 \right\},$$

which is, up to a multiple, a solution to

$$-\Delta_{\mathscr{A}} u + Vu = |u|^{p-2}u,$$

with $p \in (2, 2^*)$ *and* $N > 2$*.*

3. Summary in Swedish (Svensk sammanfattning)

Denna avhandling behandlar områdena partiella differentialekvationer och analys.

Som ett specialfall av resultaten i delar av denna avhandling visar vi följande resultat inom kvasirelativistisk Hartree-Fockteori samt starkare resultat för den magnetiska versionen av teorin. Låt N vara ett positivt heltal och $Z = (Z_1, \ldots, Z_K)$, $Z_k > 0$. Introducera den kvasirelativistiska Hartree-Fock funktionalen $\mathscr{E} : \mathbf{H}^{1/2}(\mathbb{R}^3)^N \to \mathbb{R}$:

$$(\phi_1, ..., \phi_N) \mapsto \alpha^{-1} \sum_{n=1}^{N} \left(\int_{\mathbb{R}^3} |\mathscr{F}\phi_n|^2 \,\mathrm{d}\mu(\xi) - \int_{\mathbb{R}^3} \alpha^{-1} |\phi_n|^2 \,\mathrm{d}x \right)$$

$$+ \int_{\mathbb{R}^3} V_{\mathrm{en}}(x)\rho_{\mathscr{D}}(x)\,\mathrm{d}x + \frac{1}{2}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} V_{\mathrm{ee}}(x-x')\big(\rho(x)\rho(x') - |\mathscr{D}(x,x')|^2\big)\,\mathrm{d}x\mathrm{d}x',$$

där

$$\mathscr{D}(x,x') = \sum_{n=1}^{N} \phi_n(x)\overline{\phi_n(x')},$$

och

$$\rho_{\mathscr{D}}(x) = \sum_{n=1}^{N} |\phi_n(x)|^2.$$

Här har vi att $R_n \in \mathbb{R}^3$, $n = 1, \ldots, N$ och

$$\mathrm{d}\mu(\mathrm{k}) := \sqrt{|\mathrm{k}|^2 + \alpha^{-2}}\mathrm{dx}, \tag{3.0.1}$$

med $\alpha > 0$. De vanligaste exemplen av potentialer (från fysiken men, resultaten håller för större klasser) V_{ee} samt V_{en} är givna av

$$V_{\mathrm{ee}}(x) := \frac{1}{|x|} \text{ och } V_{\mathrm{en}}(y) = \sum_{k=1}^{K} V_k(y), V_k(y) := -\frac{Z_k\alpha}{|y-R_k|}.$$

Under några tekniska antaganden svarar kritiska punkter, till den kvasirelativistiska Hartree-Fock funktionalen, på

$$\mathscr{C} := \left\{ \{\phi\}_{n=1}^{N} \in \mathbf{H}^{1/2}(\mathbb{R}^3)^N : \langle \phi_m, \phi_n \rangle_{L^2} = \delta_{mn} \right\},$$

mot lösningar till

$$\begin{cases} F\varphi_n + \lambda_n \varphi_n = 0, \\ \langle \varphi_m, \varphi_n \rangle_{L^2(\mathbb{R}^3)} = \delta_{mn}, \end{cases}$$

där $\varphi = (\varphi_1, \dots, \varphi_N)$, $(\lambda_1, \dots, \lambda_N) \in \mathbb{R}^N$ och F är Fockoperatorn associerad med

$$\begin{aligned} \mathfrak{f}[\phi, \psi] &:= \alpha^{-1}\tilde{\mathfrak{t}}_0[\phi, \psi] + \int_{\mathbb{R}^3} V_{\mathrm{en}}(x)\phi(x)\overline{\psi}(x)\,\mathrm{d}x \\ &+ \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \frac{\rho_{\mathscr{D}}(x)\phi(y)\overline{\psi}(y)}{|x-y|}\,\mathrm{d}x\mathrm{d}y - \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \mathscr{D}(x,y)\frac{\phi(y)\overline{\psi}(x)}{|x-y|}\,\mathrm{d}y\mathrm{d}x. \end{aligned}$$

Där vi har definierat

$$\tilde{\mathfrak{t}}_0[\phi, \psi] := \int_{\mathbb{R}^3} \phi\overline{\psi}\sqrt{|\xi|^2 + \alpha^{-2}}\mathrm{d}\xi - \alpha^{-1}\int_{\mathbb{R}^3} \phi\overline{\psi}\mathrm{d}x.$$

Man kan vidare visa olika egenskaper för egenvärdena och egenfunktionerna.

I andra delar av avhandlingen finns bland annat följande resultat. Introducera

$$\mathfrak{q}_{\mathscr{A},V} : C_c^\infty(\Omega) \to \mathbb{R} : u \mapsto \int_\Omega |\nabla_{\mathscr{A}} u(x)|^2 + V(x)|u(x)|^2\mathrm{d}x.$$

Här är Ω en öppen sammanhängande delmängd av $\mathbb{R}^N$ och $\mathscr{A}$ är en 1-form (associerade med en exakt 2-form $\mathscr{B}$). För $\mathfrak{q}_{0,V}$ existerar, under tekniska antaganden, en välkänd representation i termer av en positiv densitet. Vi generaliserar, under vissa tekniska restriktioner, denna identitet till

$$\mathfrak{q}_{\mathscr{A},V}[u] = \int_\Omega \left|\nabla_{\mathscr{A}}\left(\frac{u}{v}\right)\right|^2 v^2\mathrm{d}x, \qquad u \in C_c^\infty(\Omega).$$

Som en konsekvens av detta visar vi att när $\mathfrak{q}_{0,V} \geq 0$ och $\mathscr{A}$ uppfyller några svaga lokala integrabilitetsvillkor samt rot $\mathscr{A} \neq 0$ (i svag mening) gäller det att

$$\mathfrak{q}_{\mathscr{A},V}(u) \geq \int_\Omega W(x)|u(x)|^2\mathrm{d}x, \qquad u \in C_c^\infty(\Omega),$$

för en positiv och kontinuerlig funktion W. Vidare visar vi som ett exempel på våra resultat att, för speciella $\mathscr{B}$, olikheten

$$\int_\Omega |\nabla_{\mathscr{A}} u(x)|^2\mathrm{d}x - \left(\frac{N-2}{2}\right)^2 \int_\Omega \frac{|u(x)|^2}{|x|^2}\mathrm{d}x \geq C\int_\Omega |u(x)|^2\mathrm{d}x, u \in C_c^\infty(\Omega),$$

av Hardy typ håller (för vissa $C > 0$) på vissa komplementmängder till öppna bollar innehållande origo.

Bibliography

[Ada75] Robert A. Adams, *Sobolev spaces*, Academic Press [A subsidiary of Harcourt Brace Jovanovich, Publishers], New York-London, 1975, Pure and Applied Mathematics, Vol. 65.

[BE10] A.A. Balinsky and W.D. Evans, *Spectral analysis of relativistic operators*, Imperial College Press, London, 2010.

[CLBM06] Eric Cancès, Claude Le Bris, and Yvon Maday, *Méthodes mathématiques en chimie quantique. Une introduction*, Mathématiques & Applications (Berlin) [Mathematics & Applications], vol. 53, Springer, Berlin, 2006.

[EE87] D. E. Edmunds and W. D. Evans, *Spectral theory and differential operators*, Oxford Mathematical Monographs, The Clarendon Press Oxford University Press, New York, 1987, , Oxford Science Publications.

[EL89] Maria J. Esteban and Pierre-Louis Lions, *Stationary solutions of nonlinear Schrödinger equations with an external magnetic field*, Partial differential equations and the calculus of variations, Vol. I, Progr. Nonlinear Differential Equations Appl., vol. 1, Birkhäuser Boston, Boston, MA, 1989, pp. 401–449.

[EM08a] M. Enstedt and M. Melgaard, *Existence of solution to Hartree-Fock equations with decreasing magnetic fields*, Nonlinear analysis **69** (2008), no. 7, 2125–2141.

[EM08b] ———, *Non-existence of a minimizer to the magnetic Hartree-Fock functional*, Positivity **12** (2008), no. 4, 653–666.

[EM09] ———, *Existence of infinitely many distinct solutions to the quasi relativistic Hartree-Fock equations*, International Journal of Mathematics and Mathematical Sciences **2009** (2009), doi:10.1155/2009/651871.

[EM10a] ———, *Abstract criteria for multiple solutions to nonlinear coupled equations involving magnetic Schrödinger operators*, Manuscript (2010).

[EM10b] ———, *Multiple solutions of Choquard type equations*, Manuscript (2010).

[ET09] M. Enstedt and K. Tintarev, *Weighted spectral gap for magnetic Schrödinger operators with a potential term*, Potential Anal. **31** (2009), no. 3, 215–226.

[Fol99] Gerald B. Folland, *Real analysis*, second ed., Pure and Applied Mathematics (New York), John Wiley & Sons Inc., New York, 1999, Modern techniques and their applications, A Wiley-Interscience Publication.

[Hör03] Lars Hörmander, *The analysis of linear partial differential operators. I*, Classics in Mathematics, Springer-Verlag, Berlin, 2003, Distribution theory and Fourier analysis, Reprint of the second (1990) edition.

[Kat95] Tosio Kato, *Perturbation theory for linear operators*, Classics in Mathematics, Springer-Verlag, Berlin, 1995, Reprint of the 1980 edition.

[LBL05] Claude Le Bris and Pierre-Louis Lions, *From atoms to crystals: a mathematical journey*, Bull. Amer. Math. Soc. (N.S.) **42** (2005), no. 3, 291–363 (electronic).

[Lie90] Elliott H. Lieb, *The stability of matter: from atoms to stars*, Bull. Amer. Math. Soc. (N.S.) **22** (1990), no. 1, 1–49.

[Lio88] P.-L. Lions, *Hartree-Fock and related equations*, Nonlinear partial differential equations and their applications. Collège de France Seminar, Vol. IX (Paris, 1985–1986), Pitman Res. Notes Math. Ser., vol. 181, Longman Sci. Tech., Harlow, 1988, pp. 304–333.

[LL01] Elliott H. Lieb and Michael Loss, *Analysis*, second ed., Graduate Studies in Mathematics, vol. 14, American Mathematical Society, Providence, RI, 2001.

[Maz85] Vladimir G. Maz'ja, *Sobolev spaces*, Springer Series in Soviet Mathematics, Springer-Verlag, Berlin, 1985, Translated from the Russian by T. O. Shaposhnikova.

[RM05] G. Rozenblum and M. Melgaard, *Schrödinger operators with singular potentials*, Stationary partial differential equations. Vol. II, Handb. Differ. Equ., Elsevier/North-Holland, Amsterdam, 2005, pp. 407–517.

[RS75] Michael Reed and Barry Simon, *Methods of modern mathematical physics. II. Fourier analysis, self-adjointness*, Academic Press [Harcourt Brace Jovanovich Publishers], New York, 1975.

[RS78] ______, *Methods of modern mathematical physics. IV. Analysis of operators*, Academic Press [Harcourt Brace Jovanovich Publishers], New York, 1978.

[SO96] Attila Szabo and Neil Ostlund, *Modern quantum chemistry*, Dover publications, inc, New York, 1996.

[SW71] Elias M. Stein and Guido Weiss, *Introduction to Fourier analysis on Euclidean spaces*, Princeton University Press, Princeton, N.J., 1971, Princeton Mathematical Series, No. 32.

[Thi02] Walter Thirring, *Quantum mathematical physics*, second ed., Springer-Verlag, Berlin, 2002, Atoms, molecules and large systems, Translated from the 1979 and 1980 German originals by Evans M. Harrell II.