Studies in the Wigner-Poisson and Schrödinger-Poisson Systems

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Dissertation submitted to the Faculty of the Virginia Polytechnic Institute and State University in partial fulfillment of the requirements for the degree of

Doctor of Philosophy
in
Physics

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October 21, 1998
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Keywords : Wigner-Poisson, Schrödinger-Poisson, Quantum Transport Theory

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(ABSTRACT)

The need to model the quantum effects in semiconductor devices such as resonance tunneling diodes and quantum dots has lead to an intense study of the Wigner-Poisson (WP) and Schrödinger-Poisson (SP) systems. In this work we present the mathematical analysis of several related models for these systems. These include: a time-dependent model of dissipation in (SP), a quasi-linear (SP) system, a study of the stationary (WP)-(SP) problem with a discussion of the quantum analogue of classical BGK modes and a proof of existence of eigenfunctions for (SP) with periodic boundary conditions, and an examination of the stationary Wigner equations with "inflow" boundary conditions. Finally, a proposed numerical scheme for the stationary (SP) system with Boltzmann distribution functions is shown along with its corresponding Bloch equation.

ACKNOWLEDGEMENTS

I am indebted to many people who have shared with me their time, expertise and experience, to make my work possible. Some of them however, deserve special thanks.

First, I would like to thank my advisor, Prof. Paul Zweifel, for his encouragement, patience, and friendship. Moreover, I would like to thank both Prof. Horst Lange of the university of Köln and Prof. Reinhard Illner of the university of Victoria for their mathematical expertise and gracious hospitality through the years.

I would like to thank every member of the Center for Transport Theory and Mathematical Physics for their wonderful talks, lectures, and instruction over the years. This includes: Profs. Robert Bowden, George Hagedorn, Martin Klaus, Joseph Slawny, and Paul Zweifel. This thanks extends also to the many interesting guests which have visited through the years.

I am also grateful to Profs. John Ficenec and Lay Nam Chang for their time and insights. Acknowledgment is also due to the many friends and colleagues that I have come to know through the years here at Virginia Tech, they include: Armin Kargol, Syed Alwi Ahmad, Chopin Soo, Manash Mukherjee, and Clemmitt Sigler. I would also like to thank both Christa Thomas and Gloria Henneke for all their help and support.

Finally, this work could not have been completed without the love and support of my family. Last but not least, I would like to dedicate this work to the loving memory of my late grandmother, Dorothy Hudson.

Contents

Chapter 1

Introduction

1.1 Introduction and motivation

The Wigner–Poisson system describes the time evolution of a single particle density function in phase-space; its natural counterpart, Schrödinger–Poisson, describes a system of wave functions for this particle in a Hilbert space. (These systems will henceforth be referred to as (WP) and (SP) respectively.) This single particle description, however, is supposed to model in a self-consistent way an ensemble of indistinguishable self-interacting particles. The interaction is through a coulombic field, which itself depends on the density function in (WP) or the wave functions in (SP), and gives rise to a self-consistent potential which satisfies a Poisson equation. This in turn couples the potential to the evolution of the density (WP) or the states (SP). It is in this sense, that one refers to these systems as a mean-field or self-consistent theory. The physical motivation for the study of the (WP)–(SP) systems is clear. This theory has been put forth as a possible description of the quantum effects observed in semiconductor devices such as resonance tunneling diodes (RTDs) [1] or quantum dots [2]. The mathematical motivation is also quite clear; as an abstract theory it involves the rich use of nonlinear PDE theory, pseudo-differential operators (PDOs), harmonic anaylsis (through the use of the Wigner transform), and the mathematics of quantum mechanics. This motivation holds also for the many sub-topics and problems generated by the study of the (WP)-(SP) system and was the inspiration for this work.

1.2 Background

Since Neunzert's "reintroduction" of the (WP) system in the 1980's to the transport community, there has been an intense and prolific study of this problem along with its natural counterpart, the (SP) system. Of course, the mathematics culture had only "rediscovered" what the physics community had know for decades: that the rich techniques and complex structures arising from the Wigner phase-space representation of quantum mechanics was both a challenging and rewarding area of research. Following a preliminary investigation of the linear Wigner equation (often referred to as the quantum Liouville equation) by Markowich et al. [3, 4, 5] and others [6, 7]; the main task at hand, solving the still "open" (WP) problem was rigorously attacked. First to solve was Markowich et al. [8] in a seminal 1989 work, and later by Lange et al.[9] with an elegant clarifying proof. This in turn gave rise to a proliferation of spin-off topics of research.

First, remembering the physical motivations of this research, the study of finite regions or geometries now became germane and was investigated along with various boundary conditions. For example, the finite cube ($Q \subset \mathbb{R}^d$, $d = 1, 2, 3$) with periodic boundary conditions was considered in both [10] and [11]. Later Floquet or Bloch conditions (as referred to in physics) were also investigated, see [12]. Moreover, for this same geometry, combinations of the standard Dirichlet and Neumann boundary conditions were explored on Q in [13].

Second, seeing that most physical simulations of the (WP) system utilized (for the sake of convergence) a dissipative term in the evolution equation, various models for dissipation were proposed and undertaken. Since the fundamental nature of dissipation (at least at the quantum level) is largely unknown, these treatments were mostly vis-á-vis ad hoc means. There are, of course, many standard treatments; and one, the relaxation time approximation was studied by Arnold first for the linear Wigner equation [14] and then for the full (WP) system [15]. Using a more fundamental approach, Lange and Zweifel [16] investigated the full (WP) problem by considering an augmented hamiltonian operator for the corresponding (SP) system (i.e., a hamiltonian which consisted of both a self-adjoint term and a skew-adjoint term was considered). Lastly, a dynamic model of dissipation was presented in [17] and is shown in this work. Speculation still exists on the possible fundamental nature of an implementation of Fokker-Planck like terms to the (WP) system and what meaning (if any) their quantum counterparts might have.

Third, a natural question arose after the discovery of solutions of the (WP)-(SP) system, that of the existence of the ($\hbar \to 0$) classical limit and its relation to the classical Vlasov-Poisson system. The formal limit of (WP) had been known for years; but it was the work of P.L. Lions et al. [18] which clarified the true type of and conditions for convergence. Subsequently Markowich et al. [19] showed this convergence for the (3D) full-space (WP)-(SP) problem.

Fourth, the desire to model steady-state and thermal equilibrium conditions in semiconductor devices gave way to a study of time-independent and scattering models for (WP)-(SP). Due to the statistical nature of the system, different distribution functions were chosen. Markowich and Mauser in [20] investigated Boltzmann statistics for (SP) which gave rise to a self-consistent Bloch equation. Here they assumed that the self-consistent potential was independent of the inverse temperature $\beta = \frac{1}{kT}$ (a consequence of their existence proof). Two other studies of the time-independent (WP)-(SP) system were made; one using a variational technique [21] and another using a fixed-point argument [22]. Both modeled the stationary (SP) system under only general assumptions (which all known physical distributions satisfy) on the ensemble statistics and neither required any assumptions on the β dependence of the potential.

Fifth, numerical schemes were proposed and investigated. Perhaps viewed as "old hat" to the physics community it was not until the existence of solutions to (WP)-(SP) that rigorous treatment of convergence issues could be made. One proposed scheme by Arnold [23], on (WP) only, was that of the operator splitting method which utilized the Trotter product theorem. Another was the spectral method of Markowich and Ringhofer [24] for the time-dependent (WP)-(SP) system. Mauser et al. [25] proposed a method for the Bloch like system considered in [20] which by using an iterative scheme yielded a result for a β dependent potential. Yet another numerical study by Ringhofer et al. [26] introduced absorbing boundary conditions to the time-dependent (WP) problem mainly to combat specious reflections observed in simulations.

Sixth and last, there is the work in the physics literature. These studies, some predating the aforementioned works and many concurrent with them, have been primarily concerned with the simulation of semiconductor devices and for the most part, utilize solely the (WP) system, see refs. [27, 28, 29, 30] (to name a few).

1.3 Organization of this work

The organization of the rest of this work follows not only the time order in which these studies were made, but also parallels the natural progression of research of the previously mentioned works. Consequently, this work gives a global overview of subjects arising from the study of (WP)-(SP) systems.

We first give a brief overview in chapter two of the derivation of the (WP)-(SP) system. Here we shall state the necessary definitions and theorems. Moreover, one shall see how the "mean-field" system is derived utilizing the BBGKY (Bogoliubov-Born-Green-Kirkwood-Yvon) hierarchy.

In chapter three, a model for dynamic dissipation in the (SP) system will be presented. Here the evolution of a system (borrowed from a physical model of field modulation) with a given time-dependent dissipation function is considered. The corresponding (WP) system will also be derived and investigated. Using conservation and quasi-conservation laws, global existence and uniqueness is shown for the Cauchy problem associated with both the repulsive and attractive cases. (The attractive or "self-focusing" case requires an assumption of small initial data.)

In chapter four, we consider a quasilinear Schrödinger-Poisson system, that is, an (SP) system in which the self-consistent potential satisfies a Poisson equation involving a non-constant, field-dependent dielectric constant of the form $\epsilon(x, \nabla V) = \epsilon_0 + \epsilon_1 |\nabla V|^2$. A unique global strong solution is shown for initial data satisfying certain regularity conditions. This is done by using a sequence of Galerkin approximations along with their associated *a priori* bounds. From the details of this analysis a matrix approximation is seen and its computational value is discussed. Lastly, the one-dimensional version of this model is solved in explicit detail.

The theoretical underpinnings of stationary solutions to the (WP) problem are investigated in chapter five along with their (SP) consequences. A generalization to the classical form of stationary solutions to the Vlasov-Poisson system is presented and shown to be the quantum analogue of classical BGK (Berstein, Greene, Kruskal) modes [31]. In the context of the (WP)-(SP) problem, a complete set of commuting operators (CSCO) is shown to exist, assuming the existence of the self-consistent potential. Using this formalism a quantum Bloch-like equation is derived in place of the Wigner equation.

Next in chapter six, we consider the stationary states of an (SP) system on the finite cube Q with periodic boundary conditions. Certain properties on the given statistical distribution functions are assumed and an "energy" matrix is found (in the linear case this is just a diagonal matrix of the usual energy eigenvalues). Contrary to the usual variation principle used in many time-independent problems, an iteration technique is used utilizing the Schauder fixed point theorem (hence non-unique existence is shown). Bounds on eigenvalues are found and techniques for calculating eigenvalues numerically are discussed. Lastly, regularity of solutions is shown to be tied to certain convergence properties of the given statistical distributions evaluated at the solution eigenvalues.

In chapter seven, a model for the linear (given potential) Wigner equation with inflow boundary conditions is discussed. A brief explanation is given of the use and effectiveness of inflow conditions for the classical Liouville equation. Moreover, physical motivation for this model is also presented by way of a discussion of the generated current, and the possible relationship of the inflow boundary conditions with a corresponding quantum mechanical condition. Uniqueness of the generated current is also shown along with an analytical expansion of the Wigner function "solution". A recursion relation for this expansion is derived and certain convergence properties shown. Moreover, the regularity for the known solution and its relationship to the given inflow data is discussed.

Finally in chapter nine, we discuss conclusions from these studies and the possible future research of open problems generated from this work.

Following in appendix A, we present a possible numerical scheme for solving the time-independent (SP) system. A Bloch equation (generated from Boltzmann statistics) is derived and studied with this scheme in both the linear and self-consistent cases. A "master" equation for this system is shown; and the convergence of successive approximations is discussed.

Chapter 2

Derivation of the (WP)-(SP) system

2.1 The Wigner Formalism

In 1932, Wigner [32] introduced the following formula on phase space ($(x,p) \in \mathbb{R}^{3N} \times \mathbb{R}^{3N}$) to calculate expectation values of certain statistical quantities, and it has henceforth become known as the Wigner distribution $w(x,p)$

$$w(x,p) = \frac{1}{(2\pi\hbar)^{3N}} \int\limits_{\mathbb{R}^{3N}} dz e^{ipz/\hbar} \langle x - \frac{z}{2} |\rho| x + \frac{z}{2} \rangle \,. \tag{2.1.1}$$

Clearly, w is no more than the Fourier transform of the off-diagonal elements of the density matrix. A more modern approach would be the following [33]. Define the Wigner transform of an operator "A" on phase space to be "A_w"

$$A_w(x,p) = \sum_{k,l} A_{kl} \int\limits_{\mathbb{R}^{3N}} e^{ipz/\hbar} \psi_k(x - \frac{z}{2}) \overline{\psi}_l(x + \frac{z}{2}) dz \tag{2.1.2}$$

$$A_{kl} = (\psi_k, A\psi_l)_{L^2(\mathbb{R}^{3N})} \,, \tag{2.1.3}$$

where (ψ_k) is any orthonormal basis in L^2, the quantum state space. First defined in [34], it is clear that the Wigner function is $(2\pi\hbar)^{-3N}$ times the Wigner transform of the density operator ρ. Moreover, for any trace class operator it can be shown (see [35]) that

$$Tr(A) = \frac{1}{(2\pi\hbar)^{3N}} \int_{\mathbb{R}^{3N} \times \mathbb{R}^{3N}} A_w(x,p)\, dx\, dp \,, \tag{2.1.4}$$

as can the following relation for suitable A, B

$$Tr(BA) = Tr(AB) = \frac{1}{(2\pi\hbar)^{3N}} \int_{\mathbb{R}^{3N} \times \mathbb{R}^{3N}} A_w(x,p) B_w(x,p)\, dx\, dp \,. \tag{2.1.5}$$

(The first equality is well known and must hold given the second equality.) Clearly , these formulae are most useful in the calculation of statistical averages since

$$\langle A\rangle = Tr(\rho A) = \frac{1}{(2\pi\hbar)^{3N}}\int_{\mathbb{R}^{3N}\times\mathbb{R}^{3N}} \rho_w(x,p)A_w(x,p)\,dx\,dp\,; \tag{2.1.6}$$

moreover, since (at least formally) power series in $\hbar$ exist for ρ_w, A_w, one could conceivably compute quantum corrections for $\langle A\rangle_{\text{cl}}$.

The following formula is due to Groenewold [36] and it is integral in proving both the previous formulae and the derivation of the Wigner equation. It states that the Wigner transform of a product of operators AB is given by

$$\begin{aligned}(AB)_w &= A_w(x - \frac{\hbar}{2i}\nabla_p, p + \frac{\hbar}{2i}\nabla_x)B_w(x,p)\\ &= B_w(x + \frac{\hbar}{2i}\nabla_p, p - \frac{\hbar}{2i}\nabla_x)A_w(x,p)\,.\end{aligned} \tag{2.1.7}$$

For completion sake, we consider the Weyl transform which takes functions on phase-space $f(x,p)$ into a quantum mechanical operators $F(X,P)$ acting on the corresponding Hilbert space. It is defined to be

$$\Omega f = F(X,P) = \frac{1}{(2\pi\hbar)^{3N}}\int_{\mathbb{R}^{3N}\times\mathbb{R}^{3N}} e^{-i(\sigma\cdot X+\tau\cdot P)/\hbar}\phi(\sigma,\tau)\,d\sigma d\tau\,, \tag{2.1.8}$$

where

$$\phi(\sigma,\tau) = \int_{\mathbb{R}^{3N}\times\mathbb{R}^{3N}} e^{i(\sigma x+\tau p)}f(x,p)\,dx\,dp\,. \tag{2.1.9}$$

Using this definition in conjuction with the Wigner transform, one can show that they are mutual inverses:

$$(\Omega f)_w = f \quad\text{and}\quad \Omega A_w = A\,. \tag{2.1.10}$$

It is interesting to note that the Wigner transform of a density operator $\rho = |\psi\rangle\langle\psi|$ from a pure normalized state ψ in the Hilbert space $L^2(\mathbb{R}^{3N})$ *may* not necessarily be in L^1 of the corresponding phase-space, even though the Lebesgue integral exists and hence must equal one,

$$Tr(\rho) = \frac{1}{(2\pi\hbar)^{3N}}\int_{\mathbb{R}^{3N}\times\mathbb{R}^{3N}} \rho_w(x,p)\,dxdp = 1\,. \tag{2.1.11}$$

This fact follows from a harmonic analysis result of Simon [37] and can be easily seen by taking the Wigner transform of $\frac{1}{\sqrt{2}}e^{-x}H(x)$ where $H(x)$ is the Heaviside function. This naturally, begs the question of *which* space to pose an evolution of the Wigner function w. Of course one could consider the space of all phase-space functions which come from the Wigner transform of density matrices but this would be rather opaque. Luckily in a work by Narcowich et al. [38], one finds conditions (which are slightly more clear) on the phase-space functions themselves. They are:

(1) $\iint w(x,p)dx\,dp = 1$

(2) $\iint w(x,p)w[\psi](x,p)dx\,dp \geq 0$

(for every Wigner transform of a pure state ψ). A complete exegesis which hopefully clarifies the properties of both the Wigner and Weyl transforms can be found in Folland [39].

The Wigner equation (sometimes referred to as the quantum Liouville equation) describes the evolution of the Wigner function w, and is derived by first considering the evolution of the corresponding density operator ρ under the Schrödinger operator $\frac{1}{2}P^2 + V(x)$. In the Heisenberg representation we have

$$i\hbar\rho = H\rho - \rho H\,. \tag{2.1.12}$$

By taking the Wigner transform of both sides (2.1.12) and utilizing Groenewold's formula one finds that

$$i\hbar\partial_t\rho_w = -ip\cdot\nabla_x\rho_w + (V(x+\frac{\hbar}{2i}\nabla_p) - V((x-\frac{\hbar}{2i}\nabla_p))\rho_w\,. \tag{2.1.13}$$

Clearly, the term involving the potential must be understood as a pseudo-differential operator (PDO) on ρ_w. $\Theta(V)$ is then given by

$$\Theta(V)\rho_w = \int_{\mathbb{R}^{3N}} e^{i(p-p')z}(V(x+\frac{\hbar}{2i}z) - V(x-\frac{\hbar}{2i}z))\rho_w(x,z)\,dz\,dp' \tag{2.1.14}$$

with symbol

$$\delta V = V(x+\frac{\tau}{2}) - V(x-\frac{\tau}{2})\,. \tag{2.1.15}$$

Finally, the Wigner equation becomes

$$\partial_t w(x,p,t) + v\cdot\nabla_x w - \frac{i}{\hbar}\Theta(V)w = 0\,. \tag{2.1.16}$$

2.2 The (WP)-(SP) System

The (WP)-(SP) system is derived in much the same fashion as the linear Wigner equation. To see a full explanation of this derivation see Ref. [40] or for an overview Ref. [41]. This time we start with the N-body hamiltonian operator (representing indistinguishable particles in the Hilbert space $L^2(\mathbb{R}^{3N})$)

$$H = \sum_{i=1}^{N}\frac{1}{2}P_i^2 + V(x_i,\ldots,x_N)\,. \tag{2.2.1}$$

Here V is the interparticle internal potential which we shall assume only depends on binary interactions, i.e.

$$V(x_1, \dots, x_N) = \sum_{j,k=1}^{N} v(x_j, x_k)\,.$$

Next, as in the derivation of the Vlasov equation, we consider a BBGKY hierarchy of equations $d = 1, \dots, N$ for $\rho^{(1)}, \rho^{(2)}, \dots$ resulting from the following ansatz for the integral kernel of the density operator $\rho(r_1, \dots, r_N, s_1, \dots, s_N)$.

$$\rho^{(d)}(r_1, \dots, r_N, s_1, \dots, s_N) = \prod_{j=1}^{d} \rho^{(1)}(r_j, s_j, t)\,. \tag{2.2.2}$$

In the context of atomic physics this sometimes referred to as the "Hartree-Fock" or "molecular chaos" ansatz and denotes that the particles in a sub-ensemble of order "d" move in dependently of each other. At any rate, this leads to a hierarchy of equations of which the lowest order in "d" is

$$\begin{aligned} i\hbar\partial_t\rho^{(1)} &= -\frac{\hbar^2}{2}(\triangle_s - \triangle_r)\rho^{(1)} \\ &\quad -\frac{q}{4\pi}\int_{\mathbb{R}^3}(v(s,u) - v(r,u))\rho^{(2)}(r,u,s,u,t)\,du\,. \end{aligned} \tag{2.2.3}$$

Where the ansatz gives $\rho^{(2)} = \rho^{(1)}(r,s,t) \cdot \rho^{(1)}(u,u,t)$. This yields the following Heisenberg evolution equation for the d=1 kernel:

$$i\hbar\partial_t\rho^{(1)} = -\frac{\hbar^2}{2}(\triangle_s - \triangle_r)\rho^{(1)} - (v[\rho^{(1)}](s,u) - v[\rho^{(1)}](r,u))\rho^{(1)}\,, \tag{2.2.4}$$

where

$$v[\rho^{(1)}] = \frac{q}{4\pi}\int_{\mathbb{R}^3} v(x,u)\rho^{(1)}(u,u,t)\,du\,. \tag{2.2.5}$$

Now taking the Wigner transform of the lowest order terms and again utilizing (2.1.7) we find the following system

$$\partial_t\rho_w^{(1)} + \frac{p}{m}\cdot\nabla_x\rho_w^{(1)} - \frac{i}{\hbar}\Theta(v[\rho^{(1)}])\rho_w^{(1)} = 0\,. \tag{2.2.6}$$

Moreover, since $v(x,u) = \frac{1}{|x-u|}$, (Eq. 2.2.5) implies that the potential must satisfy

$$\triangle v(\rho^{(1)}) = q \cdot n(x,t)\,, \tag{2.2.7}$$

where $n(x,t)$, the number density is given by

$$n(x,t) = \rho^{(1)}(x,x,t) = \frac{1}{(2\pi\hbar)^3}\int_{\mathbb{R}^3}\rho_w^{(1)}(x,p,t)\,dp\,. \tag{2.2.8}$$

(2.2.7) is clearly the Poisson equation, and since we are now dealing with a one particle, mean-field description, we shall drop superscript on $\rho^{(1)}$. It is this system (2.2.6)-(2.2.8) that will henceforth be referred to as the Wigner-Poisson equation.

Finally, one may expand the kernel $\rho^{(1)}(r,s,t)$ in a series of states $\psi_n(x,t)$ weighted by λ_n (with the property $\sum \lambda_n = 1$) and arrive at the corresponding Schödinger-Poisson system:

$$
\begin{aligned}
\partial_t \Psi(x,t) &= -\frac{1}{2}\triangle\Psi + V(\Psi)\Psi &\quad (2.2.9)\\
\Psi &= (\psi_m)_{m\in\mathbb{N}} &\quad (2.2.10)\\
n(x,t) &= \sum \lambda_m |\psi_m(x,t)|^2 &\quad (2.2.11)\\
\triangle V &= -\epsilon n &\quad (2.2.12)
\end{aligned}
$$

Of course, for time-dependent problems one must define the initial condition from which these equations must evolve. For (2.2.6)-(2.2.8) we are given the “initial” density operator ρ_I from which we set $\rho_w(x,p,0) = [\rho_I]_w(x,p)$. Hence for (2.2.9)-(2.2.11) we are given a system of initial states of the form $\psi_m(x,0) = \phi_m(x)$ coming from the eigenfunctions of ρ_I.

Consequently, it is these two systems (with various additional terms and assumptions) that the rest of this work hopes to explore.

Chapter 3

Time-Dependent Dissipation in (WP)-(SP) Systems

3.1 Introduction

In a recent article [42] the following nonlinear Schrödinger equation was introduced:

$$i\beta\phi_t + \frac{i}{2}\beta_t\phi = -\frac{1}{2}\triangle\phi + \frac{1}{2}\beta^2\phi + \alpha|\phi|^2\phi \qquad (x \in \mathbb{R}^3, t \in \mathbb{R}). \tag{3.1.1}$$

Here β is a specific real function of t only and α a given function of x. In Ref. [42], equation (3.1.1) models beam propagation in a nonlinear medium where the extra terms involving β are designed to take into account fast longitudinal field oscillations; moreover, t represents a time-dilated spatial variable, and $\triangle$ is the 1-dimensional Laplacian. Now thinking of t as the time variable (with $x \in \mathbb{R}^3$), equation (3.1.1) can be interpreted as a cubic nonlinear Schrödinger equation modeling time-dependent dissipation (to be further explained in Sec. 3.3).

In this paper, we consider a generalized version of equation (3.1.1) which also includes a self-consistent potential V. In addition, we generalize the cubic nonlinearity to an arbitrary power and, for simplicity we take α to be a constant. Hence our equations become

$$\begin{aligned} i\beta\psi_t + \frac{i}{2}\beta_t\psi &= -\frac{1}{2}\triangle\psi + V(\psi)\psi + g\left(|\psi|^2\right)\psi && (3.1.2)\\ -\triangle V &= |\psi|^2 && (3.1.3)\\ \psi(x,0) &= \psi_0(x). && (3.1.4)\end{aligned}$$

Here $\alpha \in \mathbb{R}, p > 0, x \in \mathbb{R}^3, t \in \mathbb{R}^+$, and β is a real function on $\mathbb{R}^+$; $g(s) = \alpha s^p (s \geq 0)$. The term $\frac{1}{2}\beta^2\phi$ appearing in (3.1.1) has been omitted from (3.1.2) since it can be eliminated by use of the gauge transformation:

$$\psi = e^{\frac{i}{2}\int_0^t \beta(s)\ ds}\tilde{\psi}.$$

Equations (3.1.2)–(3.1.3) may also be written in the following form

$$\begin{aligned} i\phi_t &= -\frac{1}{2}\triangle\phi + \frac{1}{\beta}V\left(\frac{\phi}{\sqrt{\beta}}\right)\phi + \frac{1}{\beta}\cdot g\left(\frac{|\phi|^2}{\beta}\right)\phi && (3.1.5) \\ -\triangle V &= \frac{1}{\beta}|\phi|^2 && (3.1.6) \end{aligned}$$

by use of the transformation

$$\phi = \sqrt{\beta}\psi.$$

The self-consistent term $V(\psi)\psi$ is familiar from quantum transport theory [8] [9] [33] [40]. For the modified equation the introduction of β represents time-dependent dissipation; and in Sec. 3.3 we show that the probability density, $\int_{\mathbb{R}^3}|\psi|^2\,dx$, for this system is proportional to $\frac{1}{\beta}$. A model for a constant dissipation rate has been considered in Ref. [16]. This dissipation was implemented in a different manner from that presented here, namely by adding certain complex terms to the hamiltonian. Other models for dissipation in quantum mechanics have been treated in Refs. [43] and [49].

In Sec. 3.2 we derive the Wigner-Poisson equation associated with the Schrödinger-Poisson system (3.1.2)–(3.1.4) by utilizing the Wigner transform described in Ref. [33]. In Sec. 3.3 we obtain a conservation law for the probability density and an associated evolution law for a Liapounov functional [44] or "quasi-energy" of system (3.1.2)–(3.1.4). In Sec. 3.4 these laws are used to obtain global-in-time existence results for the Cauchy problem of the Schrödinger system (3.1.2)–(3.1.4); these results can be transferred to the associated Wigner equation along the same lines as in Ref. [9].

3.2 The Wigner Equation

The Wigner function, w, associated with the Schrödinger wave function ψ is given by (see Ref. [33]):

$$w(x,v,t) = \left(\frac{1}{2\pi}\right)^3 \int_{\mathbb{R}^3} e^{iv\eta}\bar{\psi}\left(x+\frac{\eta}{2},t\right)\psi\left(x-\frac{\eta}{2},t\right)\,d\eta. \tag{3.2.1}$$

Differentiating, and multiplying by $i\beta$ we get

$$i\beta\partial_t w(x,v,t) = \left(\frac{1}{2\pi}\right)^3 i\beta\int_{\mathbb{R}^3} e^{iv\eta}\left[\bar{\psi}_{+,t}\psi_- + \bar{\psi}_+\psi_{-,t}\right]\,d\eta \tag{3.2.2}$$

where

$$\psi_\pm = \psi\left(x\pm\frac{\eta}{2},t\right). \tag{3.2.3}$$

For the time-derivative terms in (3.2.2) we now use the Schrödinger equation (3.1.2); the terms $-\frac{1}{2}\triangle\psi + V(\psi)\psi$ lead to the usual Wigner operator $-iW_0 w$ [33] on the right-hand side of (3.2.2)

$$W_0 w = v \cdot \nabla_x w - i\Theta_0(V)w \tag{3.2.4}$$

where $\Theta_0(V)$ is the usual pseudo-differential operator with symbol [42] [8] [49]

$$\text{Sym } \Theta_0 = V\left(x + \frac{\eta}{2}, t\right) - V\left(x - \frac{\eta}{2}, t\right) \tag{3.2.5}$$

i.e.

$$\left(\Theta_0(V)w\right)(x,v,t) = \left(\frac{1}{2\pi}\right)^3 \int_{\mathbb{R}^3_\eta} e^{iv\eta}\left[V\left(x+\frac{\eta}{2},t\right) - V\left(x-\frac{\eta}{2},t\right)\right]\hat{w}(x,\eta,t)\, d\eta \tag{3.2.6}$$

and

$$\hat{w}(x,\eta,t) = \int_{\mathbb{R}^3_{v'}} e^{-iv'\eta} w(x,v',t)\, dv' \tag{3.2.7}$$

(We always assume $\hbar = 1$).

We introduce $\Theta_1(g)$ to represent the pseudo-differential operator with symbol

$$\text{Sym } \Theta_1 = g(n_+) - g(n_-) \tag{3.2.8}$$

where $n_\pm = |\psi_\pm|^2$ and $g(s) = \alpha s^p$. Using these definitions and (3.2.2), we arrive at

$$\partial_t(\beta w) + v \cdot \nabla_x w - i\left(\Theta_0(V) + \Theta_1(g)\right) w = 0; \tag{3.2.9}$$

this can also be written in terms of $w^\beta := \beta w$

$$\partial_t w^\beta + \frac{1}{\beta} v \cdot \nabla_x w^\beta - i\left(\frac{1}{\beta^2}\Theta_0(V) + \frac{1}{\beta^{p+1}}\Theta_1(g)\right) w^\beta = 0. \tag{3.2.10}$$

For the numerical computation of solutions, it is more convenient to deal with the Fourier transformed Wigner equation [23]. Using (3.2.7) this equation is

$$\partial_t(\beta\hat{w}) + i\nabla_\eta \cdot \nabla_x \hat{w} - i\left[V_+ - V_- + g(n_+) - g(n_-)\right]\hat{w} = 0 \tag{3.2.11}$$

where $V_\pm = V\left(x \pm \frac{\eta}{2}, t\right)$.

The transformation $r = x + \frac{\eta}{2}, s = x - \frac{\eta}{2}$ has been used [3] to prove the equivalence of the Wigner-Poisson and Schrödinger-Poisson systems (for $\beta \equiv 1, \alpha = 0$). Defining

$$z(r,s,t) = \hat{w}\left(x(r,s), \eta(r,s), t\right) \tag{3.2.12}$$

we get analogously for z

$$i\partial_t(\beta z) = (H'_r - H'_s)z \tag{3.2.13}$$

where

$$H'_r = -\frac{1}{2}\triangle_r + V\left(\psi(r,t)\right) + g\left(n(r,t)\right). \tag{3.2.14}$$

3.3 Conservation and Quasi-Conservation Laws

In this section we consider (as a preparation for the existence results) some Liapounov type functionals of (strong) local solutions ψ of system (3.1.2)–(3.1.4) (see Sec. 3.4 for a definition of strong solutions). These functionals are important for the physical background of system (3.1.2)–(3.1.3). We define

$$P(t) = P(\psi; t) = \beta(t) \int_{\mathbb{R}^3} |\psi(x,t)|^2 \, dx \tag{3.3.1}$$

and

$$Q(t) = Q(\psi; t) = \int_{\mathbb{R}^3} \left\{ |\nabla \psi|^2 + |\nabla V|^2 + 2h(|\psi|^2) \right\} \, dx \tag{3.3.2}$$

where

$$h(s) = \int_0^s g(r) \, dr. \tag{3.3.3}$$

In the following theorem, we assume ψ to be any local strong solution (see Sec. 3.4) of (3.1.2)–(3.1.4) on a time interval $S_T = [0, T]$ $(T > 0)$ such that $P(t)$ and $Q(t)$ exist for all t in S_T. Consequently, all relevant expressions used in the following proof exist. We also assume that $\beta \in C^1[0, T]$.

Theorem 3.3.1. *The following conservation or quasi-conservation laws are valid:*

$$P(t) = \text{const.} \tag{3.3.4}$$

$$\partial_t \left(\beta Q(t) \right) = \beta_t \left\{ - \int_{\mathbb{R}^3} |\nabla V|^2 \, dx + 2 \int_{\mathbb{R}^3} \left[h(|\psi|^2) - g(|\psi|^2)|\psi|^2 \right] \, dx \right\} \tag{3.3.5}$$

for all $t \in S_T$, and any local strong solution ψ on S_T.

Proof. For any local strong solution we have the identity

$$\partial_t(\beta |\psi|^2) = \mathrm{Im}(\triangle \bar{\psi} \cdot \psi). \tag{3.3.6}$$

This follows from

$$\partial_t(\beta|\psi|^2) = \beta_t|\psi|^2 + 2\beta \mathrm{Re}(\psi_t \bar{\psi}) = \beta_t|\psi|^2 + 2\beta \mathrm{Im}(i\psi_t \bar{\psi}) = \beta_t|\psi|^2 - \beta_t|\psi|^2 - \mathrm{Im}(\triangle \psi \bar{\psi}) = \mathrm{Im}(\triangle \bar{\psi} \psi);$$

here we have used (3.1.2) as well as the fact that V and g are real functions.

From (3.3.6) we get

$$\begin{aligned}\partial_t P(t) &= \int_{\mathbb{R}^3} \partial_t(\beta|\psi|^2)\ dx \\ &= \mathrm{Im}\int_{\mathbb{R}^3} (\triangle\bar{\psi})\psi\ dx = -\mathrm{Im}\int_{\mathbb{R}^3} |\nabla\psi|^2\ dx = 0.\end{aligned}$$

Furthermore, we calculate that

$$\partial_t\left(\beta Q(t)\right) = \beta_t Q + \beta Q_t = \beta_t Q - 2\mathrm{Im}\int_{\mathbb{R}^3} i\beta\psi_t\triangle\bar{\psi}\ dx + 2\beta\int_{\mathbb{R}^3} g(|\psi|^2)|\psi|_t^2\ dx + 2\beta\int_{\mathbb{R}^3} V|\psi|_t^2\ dx,$$

and using equations (3.1.2), (3.1.3), (3.3.6), and some partial integration we arrive at

$$\begin{aligned}\partial_t\left(\beta Q(t)\right) &= \beta_t Q - \beta_t\int_{\mathbb{R}^3}|\nabla\psi|^2\ dx - 2\mathrm{Im}\int_{\mathbb{R}^3}\psi\triangle\bar{\psi}V\ dx - 2\mathrm{Im}\int_{\mathbb{R}^3}\psi\triangle\bar{\psi}g(|\psi|^2)\ dx + \\ &\quad 2\beta\int_{\mathbb{R}^3} g(|\psi|^2)|\psi|_t^2\ dx + 2\beta\int_{\mathbb{R}^3} V|\psi|_t^2\ dx \\ &= -\beta_t\int_{\mathbb{R}^3}|\nabla V|^2\ dx + 2\beta_t\int_{\mathbb{R}^3}\left[h(|\psi|^2) - g(|\psi|^2)|\psi|^2\right]\ dx. \qquad \square\end{aligned}$$

Remark. Theorem 3.3.1 implies that

$$\int_{\mathbb{R}^3}|\psi(x,t)|^2\ dx = \frac{C}{\beta(t)} \tag{3.3.7}$$

on any time interval S_T where ψ exists as a local strong solution. If we assume β to be a positive increasing function, (3.3.7) implies that the probability density of the system decreases with time, illustrating the dissipation in the model. Moreover, (3.3.5) implies an *a priori* bound for the terms comprising $Q(t)$ when the right-hand side of (3.3.5) is non-positive. The last assertion is true if, *e.g.*, $\alpha \geq 0$, $p \geq 1$, and $\beta_t \geq 0$. This follows from

$$2\beta_t\int_{\mathbb{R}^3}\left[h(|\psi|^2) - g(|\psi|^2)|\psi|^2\right]\ dx = 2\alpha\beta_t\frac{1-p}{1+p}\int_{\mathbb{R}^3}|\psi|^{2(p+1)}\ dx.$$

We note that $\psi \in L^{2(p+1)}(\mathbb{R}^3)$ for strong solutions ψ (See Sec. 3.4).

3.4 Global Existence

Now we present some global existence results for the system (3.1.2)–(3.1.4). These results follow partially from the theory for the nonlinear Schrödinger equation (without the potential V and for the case $\beta \equiv 1$) and partially from results of the Wigner-Poisson system (for the case $\beta \equiv 1$ and $\alpha = 0$) (see Refs. [9] and [45]). To proceed we first need some notation and definitions.

Let $T(t)$ $(t \in \mathbb{R})$ be the group generated by $\frac{i}{2}\triangle$ on $L^2(\mathbb{R}^3)$, and

$$U(t,s) = T\left(\int_s^t \frac{dr}{\beta(r)}\right) \tag{3.4.1}$$

be the evolution operator for the linear equation

$$i\phi_t = -\frac{1}{2\beta}\triangle\phi \tag{3.4.2}$$

which belongs to (3.1.2). Here $\beta : \mathbb{R}^+ \to \mathbb{R}$ is any continuously differentiable positive real function. By a *strong solution* (H^2-solution) of (3.1.2)–(3.1.3) on a finite interval $S_T = [0,T]$ we mean a function $\psi \in C\left(S_T, H^2(\mathbb{R}^3)\right) \bigcap C^1\left(S_T, L^2(\mathbb{R}^3)\right)$ such that (3.1.2)–(3.1.3) is fulfilled in the L^2-sense (for a given $\psi_0 \in H^2(\mathbb{R}^3)$) and $V = G * |\psi|^2 \in H^2(\mathbb{R}^3)$ with $G(x) = \frac{1}{4\pi} \cdot \frac{1}{|x|}$. A strong solution is *global* if it exists on any time interval S_T $(T > 0)$.

We would like to prove that (3.1.2)–(3.1.4) has a unique global strong solution for a given $\psi_0 \in H^2(\mathbb{R}^3)$. To reach this result we need following assumptions:

$$\alpha > 0, \quad 0 \le p < 2 \tag{P}$$

$$\alpha < 0, \quad 0 \le p < \tfrac{2}{3} \tag{N$_1$}$$

$$\alpha < 0, \quad \tfrac{2}{3} \le p < 2,\ \beta_t \ge 0 \text{ on } \mathbb{R}^+. \tag{N$_2$}$$

Remark. In (N_2) the assumption $\beta_t \ge 0$ is made to simplify the proof of this case in the following theorem. Furthermore, we note that one could formulate other more complicated conditions on β such that the global existence result again would be true.

Theorem 3.4.1. *Let $\psi_o \in H^2(\mathbb{R}^3), \beta \in C^1(\mathbb{R}^+, \mathbb{R})$ be real and positive and either $\alpha = 0$ or one of the conditions (P) or (N_1) hold. Then there exists a unique global strong solution ψ of (3.1.2)–(3.1.4). If (N_2) is true, then there exists a $\delta_0 > 0$ such that the same result follows if either*

$$|\alpha| \;\; or \;\; \|\psi_0\|_{L^2} \;\; or \;\; \|\nabla\psi_0\|_{L^2} + \|\nabla V_0\|_{L^2} \le \delta_0. \tag{3.4.3}$$

Proof (of Theorem 3.4.1). We first sketch a proof of the existence of a *local* strong solution on a small time interval $S_{T_0} = [0, T_0]$. This proof uses a technique developed in Ref. [45] and [9] (see also Refs. [46, 47]). To show the existence of a local strong H^2-solution one must first prove the existence of a unique local (weak) H^1-solution on the small time interval S_{T_0}; this is a function $\psi \in C\left(S_{T_0}, H^1(\mathbb{R}^3)\right) \bigcap C^1\left(S_{T_0}, H^{-1}(\mathbb{R}^3)\right)$ satisfying (3.1.2)–(3.1.4) in the (weak) H^1-sense. This follows from a slight variation and combination of the proofs of Theorem 3.10 of Ref. [9] and Theorem 4.3.1 of Ref. [45]; first one writes (3.1.2) in the form

$$i\phi_t = -\frac{1}{2\beta}\triangle\phi + \mathcal{J}(\phi) \tag{3.4.4}$$

where the nonlinearity $\mathcal{J}$ is given by

$$\mathcal{J}(\phi) = \frac{1}{\beta}V(\frac{\phi}{\sqrt{\beta}})\phi + \frac{1}{\beta}g(\frac{|\phi|^2}{\beta})\phi \tag{3.4.5}$$

with $V(\psi) = G * |\psi|^2$. The H^1-Lipschitz properties of $\mathcal{J}$ is proved as in Ref. [45] or Ref. [9] by estimating the time dependent factors by a constant C_{T_0} on the time interval S_{T_0}. For the proof of the Lipschitz property of the term $\alpha|\psi|^{2p}\psi$ one needs the assumption $0 \leq p < 2$ (see Ref. [45]). To get the local H^1-solution one applies Banach's fixed-point theorem and the Lipschitz properties of $\mathcal{J}$ to the "mild" version of (3.4.4), namely

$$\phi(t) = U(t,0)\phi_0 - i\int_0^t U(t,s)\mathcal{J}\left(\phi(s)\right)\, ds. \tag{3.4.6}$$

Next, to get the local strong H^2-solution (for $\psi_0 \in H^2(\mathbb{R}^3)$) one needs to show that for $u \in H^2(\mathbb{R}^3)$ with $\|u\|_{H^2} \leq M$,

$$\|\mathcal{J}(u)\|_{L^q} \leq C(M)(1 + \|u\|_{H^2}) \tag{3.4.7}$$

for some $q > 2$ (see Theorem 5.5.1 of Ref. [45]). This is true for $\mathcal{J}$ by remarks 5.2.9 of Ref. [45] and the fact that $G \in L^r(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ for any $r < 3$; also one needs the boundedness of $\frac{1}{\beta}$ and β_t on any finite time interval. A crucial estimate essential to proving the H^2-bound in Theorem 5.5.1 is the following well-known decay property of the group $T(t)$ on $L^2(\mathbb{R}^n)$:

$$\|T(t)\|_{B(L^q(\mathbb{R}^n),L^p(\mathbb{R}^n))} \leq (4\pi|t|)^{n(\frac{1}{p}-\frac{1}{2})}$$

($2 \leq p \leq \infty$, $t \in \mathbb{R}\setminus\{0\}$, $\frac{1}{p}+\frac{1}{q} = 1$, see Ref. [45], Prop. 3.2.1). This is applied to values of the form $t - s$ $(0 \leq s \leq t)$ of the time variable. In our case this is true analogously on any finite time interval $S_T = [0,T]$, since on S_T one has $0 < \beta(t) \leq \beta_T$ for some $\beta_T > 0$, and thus for $0 \leq s < t$,

$$\|U(t,s)\|_{B(L^q(\mathbb{R}^3),L^p(\mathbb{R}^3))} \leq \left(4\pi\int_s^t \frac{d\tau}{\beta(\tau)}\right)^{3\left(\frac{1}{p}-\frac{1}{2}\right)} \leq \left(\frac{\beta_T}{4\pi(t-s)}\right)^{3(\frac{1}{2}-\frac{1}{p})}$$

which is enough to give the desired result in our case.

Now to arrive at the global strong H^2-solution, we need an *a priori* $H^2 - norm$ estimate for the local strong H^2-solution on any finite time interval $S_T = [0,T]$. By the proof of Theorem 3.3.1 it is clear that any local strong H^2-solution satisfies the conservation and quasi-conservation laws (3.3.4) and (3.3.5). Note that $\psi \in L^{2(p+1)}(\mathbb{R}^3)$ if $\psi \in H^2(\mathbb{R}^3)$; this follows from the Sobolev embedding $H^2(\mathbb{R}^3) \subset L^{2(p+1)}(\mathbb{R}^3)$ $(\forall p \geq 0)$. From (3.3.4) we know that the L^2-norm of any local strong solution is bounded, i.e.

$$\|\psi(t)\|_{L^2} \leq C(T)\ (\forall t \in S_T), \tag{3.4.8}$$

where $C(T)$ depends continuously on T.

First we consider an H^1-bound on the solution ψ. For this bound we consider the different signs of α, noting that for $\alpha = 0$ we just have a special case of Theorem 3.10 of Ref. [9]. For assumption (P) ($\alpha > 0$, $0 \le p < 2$) we have by integrating (3.3.5)

$$\begin{aligned} Q(t) &\le \frac{\beta(0)}{\beta(t)}Q(0) + \frac{1}{\beta(t)}\int_0^t \beta_t(s)\left\{-\int |\nabla V|^2 \, dx + 2\alpha\frac{1-p}{1+p}\int |\psi|^{2(p+1)} \, dx\right\} \, ds \\ &\le C_T\beta(0)Q(0) + C_T\int_0^t Q(s) \, ds. \end{aligned} \tag{3.4.9}$$

Hence by Gronwall's Lemma this implies the H^1-bound on S_T:

$$\|\psi(t)\|_{H^1} \le C(T). \tag{3.4.10}$$

Next considering (N_1), we again integrate (3.3.5); now using the Gagliardo-Nirenberg inequality (see Ref. [48]):

$$\int |\psi|^{2(p+1)} \, dx \le C\left\{\int |\psi|^2 \, dx\right\}^{1-\frac{p}{2}}\left\{\int |\nabla\psi|^2 \, dx\right\}^{\frac{3p}{2}} \tag{3.4.11}$$

along with the quantity derived from (3.3.4) :

$$\int |\psi|^2 \, dx = \frac{\beta(0)}{\beta(t)}\int |\psi_0|^2 \, dx \tag{3.4.12}$$

leads to (with $\beta_0 := \beta(0)$):

$$\beta(t)Q(t) \le \beta_0 Q(0) + \int_0^t |\beta_t(s)|\left\{\int |\nabla V|^2 \, dx + 2|\alpha|\frac{1-p}{1+p}C\left[\frac{\beta_0}{\beta(s)}\int |\psi_0|^2 \, dx\right]^{1-\frac{p}{2}}\left[\int |\nabla\psi|^2 \, dx\right]^{\frac{3p}{2}}\right\} \, ds. \tag{3.4.13}$$

Since $\frac{3p}{2} < 1$, we can use Young's inequality ($ab \le \epsilon a^r + C_\epsilon b^{r'}$; $r, r' \ge 1, \frac{1}{r} + \frac{1}{r'} = 1$) with $r = \frac{2}{3p}$ to get from (3.4.11)–(3.4.13) the following:

$$\int \left\{|\nabla\psi|^2 + |\nabla V|^2\right\} \, dx \le C_{T,p,\alpha}\left(1 + \epsilon\|\psi_0\|_{L^2}^{\sigma}\int |\nabla\psi|^2 \, dx\right) + \tilde{C}_{T,p,\alpha}\|\psi_0\|_{L^2}^{\sigma}\int_0^t\int \left\{|\nabla\psi|^2 + |\nabla V|^2\right\} \, dx \, ds \tag{3.4.14}$$

Here $\sigma = \frac{2(2-p)}{2-3p}$. Once again Gronwall's lemma gives that (3.4.14) implies (3.4.10) if ϵ is chosen small enough.

Finally for (N_2), we consider the two cases: $\frac{2}{3} \le p \le 1$ and $1 < p < 2$ (for both $\alpha < 0$). But before we can proceed, we need the following local version of Gronwall's lemma:

Lemma 3.4.2. *Let $\phi \in C[0,T)$ $(0 < T \le \infty)$, $\phi(t) \ge 0$, and let there be positive constants A, B, γ such that*

$$\phi(t) \le A + B\phi(t)^\gamma \qquad (\forall t \in [0,T)).$$

If one of the following conditions

(i) $0 \leq \gamma < 1$

(ii) $\gamma = 1,\ B < 1$

(iii) $\gamma > 1$, *and there is an* $\epsilon_0 \in (0,1)$ *such that*

$$B\phi(0)^{\gamma-1} < \epsilon_0 < 1, BA^{\gamma-1} < \epsilon_0(1-\epsilon_0)^{\gamma-1}$$

is valid, then there exists a constant $M > 0$ *such that*

$$\phi(t) \leq M \qquad (\forall t \in [0,T))\,.$$

Proof. We prove Lemma 3.4.2 in the case when (iii) is true only, since the case (ii) is trivial and in case (i) the assertion follows by a straightforward application of Young's inequality. Let (iii) hold. Since ϕ is continuous and $B\phi(0)^{\gamma-1} < \epsilon_0$ there is a $t_1 > 0$ such that $B\phi(t)^{\gamma-1} < \epsilon_0$ for $0 \leq t \leq t_1$. For $t \in [0, t_1]$ we then have:

$$\phi(t) \leq A + B\phi(t)^{\gamma-1}\phi(t) < A + \epsilon_0\phi(t)$$

which implies $\phi(t) < M := \frac{A}{1-\epsilon_0}$. Thus one has that

$$Z := \{t \mid 0 \leq t < T, \phi(t) < M\} \neq \emptyset.$$

Let $t^* = \sup Z$. We show that $t^* = T$ (from which the assertion follows). Assume $t^* < T$; then there exists a sequence $t_n \in Z$ such that $t_n \to t^*$. This means that $\phi(t^*) \leq M$. If $\phi(t^*) < M$ there would be a $\delta > 0$ with $\phi(t^* + \delta) < M$ contrary to the definition of t^*. Thus $\phi(t^*) = M$, and $t^* < T$ implies

$$M = \phi(t^*) \leq A + B\phi(t^*)^{\gamma-1}\phi(t^*) = A + B\left(\frac{A}{1-\epsilon_0}\right)^{\gamma-1} M < A + \epsilon_0 M = (1-\epsilon_0)M + \epsilon_0 M = M,$$

a contradiction. $\square$

For the first case ($\alpha < 0$, $\beta_t \geq 0$, $\frac{2}{3} \leq p \leq 1$) we deduce from (3.3.5),(3.4.9),and (3.4.11) that

$$\beta Q(t) \leq \beta_0 Q(0). \tag{3.4.15}$$

Since $\beta(0) \leq \beta(t)(\forall t \in [0,T])$,(3.4.15) implies for $\phi(t) := \int\{|\nabla\psi|^2 + |\nabla V|^2\}\, dx$ that

$$\phi(t) \leq \phi(0) + \frac{2|\alpha|}{p+1}\int |\psi|^{2(p+1)}\, dx \leq \phi(0) + \frac{2|\alpha|}{p+1}\|\psi_0\|_{L^2}^{\sigma_0}\left\{\int |\nabla\psi|^2\, dx\right\}^{\frac{3p}{2}} \tag{3.4.16}$$

where $\sigma_0 = 2 - p$. From (3.4.16) it follows that

$$\phi(t) \leq \phi(0) + \frac{2|\alpha|}{p+1}\|\psi_0\|_{L^2}^{\sigma_0}\phi(t)^{\frac{3p}{2}}.$$

Hence, case (iii) of Lemma 3.4.2 implies (3.4.12) if $|\alpha|$ or $\|\psi_0\|_{L^2}$ or $\|\nabla\psi_0\|_{L^2}+\|\nabla V_0\|_{L^2}$ is sufficiently small (the values being proportional to the constants A,B and $\psi(0)$ in Lemma 3.4.2(iii)).

In the second case ($\alpha < 0$, $\beta_t \geq 0$ and $1 < p < 2$), we proceed similarly as in (3.4.14) and (3.4.16) again using (3.4.11). Let $\tilde{\phi}(t) = \sup_{0\leq s\leq t} \phi(t)$. From (3.3.5) we get (since $\beta_t \geq 0$):

$$\phi(t) \leq \phi(0) + \frac{2|\alpha|}{p+1}\|\psi_0\|_{L^2}^{\sigma_0}\phi(t)^{\frac{3p}{2}} + 2|\alpha|\frac{p-1}{p+1}\|\psi_0\|_{L^2}^{\sigma_0}\frac{1}{\beta(t)}\int_0^t \beta_t(s)\phi(s)^{\frac{3p}{2}}\, ds. \qquad (3.4.17)$$

Now let $0 \leq t \leq \tau \leq T$, τ arbitrary; then from (3.4.17) we arrive at

$$\phi(t) \leq \phi(0) + \frac{2|\alpha|}{p+1}\|\psi_0\|_{L^2}^{\sigma_0}\left\{1 + (p-1)\frac{1}{\beta(t)}\int_0^t \beta_t(s)\, ds\right\}\tilde{\phi}(\tau)^{\frac{3p}{2}}$$

for all $t \in [0, \tau]$. This implies

$$\tilde{\phi}(\tau) \leq \phi(0) + 2|\alpha|\frac{p}{p+1}\|\psi_0\|_{L^2}^{\sigma_0}\tilde{\phi}(t)^{\frac{3p}{2}}$$

which again by Lemma 3.4.2(iii) gives the desired estimate (3.4.10) if $|\alpha|$ or $\|\psi_0\|_{L^2}$ is small enough.

The existence of an *a priori* H^2-bound

$$\|\psi(t)\|_{H^2} \leq C(T)$$

on any time interval [0,T] where the local strong solution ψ exists, follows from Ref. [9] (for the $V\cdot\psi$ term) and Ref. [45] (for the $\alpha|\psi|^{2p}\psi$ term) by just applying the Laplacian $\triangle$ to the right hand side of the mild version (3.4.6) of (3.1.2)–(3.1.4) and then estimating as in Ref. [9] or Ref. [45]'s proof of Theorem 5.2.1, Remark 4.3.2 (here again $G \in L^q(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ for any $q \in [1, 3)$). □

Remark. The proof of Theorem 3.4.1 shows that in some cases one has the estimate

$$\int \{|\nabla\psi|^2 + |\nabla V|^2\}\, dx \leq \frac{C}{\beta(t)} \qquad (\forall t \in \mathbb{R}^+),$$

e.g. in the case $\alpha > 0$, $\beta_t \geq 0$, $1 \leq p < 2$, which includes the repulsive (or defocusing) cubic nonlinear Schrödinger equation ($p = 1$).

Chapter 4

The Quasi-Linear (SP) System

4.1 Introduction

The Schrödinger-Poisson (SP) system of equations has been used extensively during the past several years to describe electron plasmas in semiconductors when quantum effects are important, as in the case of microstructures [40]. Surveys of mathematical methods used to treat (SP), or the equivalent Wigner-Poisson (WP) system, can be found in Refs. [54] and [55]. (See also Ref. [35] and the literature cited in Refs. [54],[55] and [35].)

The detailed analysis of the (SP) system set on the unit cube subject to periodic boundary conditions appears in [10]. (The one-dimensional (WP) problem had previously been considered in [11].)

In this chapter, we study a modified version of (SP) on the unit cube, taking into account a field-dependent dielectric constant of the form

$$\epsilon(x, \nabla V) = \epsilon_0 + \epsilon_1 |\nabla V|^2, \tag{4.1.1}$$

where the electric potential V satisfies the Poisson equation

$$-\nabla \cdot (\epsilon(x, \nabla V) \nabla V) = n - n^*. \tag{4.1.2}$$

Here n is the charge density which derives from the Schrödinger wave function by

$$n = \sum \lambda_m |\psi_m|^2 \tag{4.1.3}$$

where λ_m is the probability of the initial state $\varphi_m(x)$ and $\psi_m(x,t)$ is the solution of the time-dependent Schrödinger equation with initial value φ_m :

$$i\partial_t \psi_m = -\frac{1}{2}\Delta \psi_m + (V + \tilde{V})\psi_m, \tag{4.1.4}$$

$\psi_m(x,0) = \varphi_m(x)$.

The function n^* is a given, time-independent, dopant density which may be represented as

$$n^* = n_D^+ - n_A^- \tag{4.1.5}$$

where n_D^+ is the density of donors and n_A^- the density of acceptors [57]; $\tilde{V}$ is a given time-independent bias voltage.

We always impose charge neutrality:

$$\int_Q (n - n^*)\, dx = 0. \tag{4.1.6}$$

Equations (4.1.2) and (4.1.4) are to be solved subject to periodic boundary conditions on the unit cube $[0,1]^d$, $d = 1,2,3$.

The form, Eq.(4.1.1), of the dielectric constant is more-or-less standard in nonlinear optics [50, 52]. Physical models including terms like n^* and $\tilde{V}$ have been presented in [57] (and references therein).

In the present work we prove that (SP) as described above has a unique, global strong solution for any initial data satisfying certain regularity conditions. In Sec. 4.2 we provide a number of preliminary details concerning the nature of solutions as well as preliminary lemmata.

In Sec. 4.3 we define a Galerkin sequence for (SP), and prove existence results for each order. Sec. 4.4 deals with conservation laws and *a priori* bounds of the Galerkin sequence. These are then used for proving global existence. Finally, in Sec. 4.5, we derive a matrix approximation of the Poisson equation for computational purposes.

4.2 Preliminary Details

We shall prove results on the existence, uniqueness and approximation of solutions of (SP) in one, two and three dimensions. This means we seek a wave function $\Psi = (\psi_m)_{m\in\mathbb{N}}$ and a self-consistent potential $V = V(\Psi)$ satisfying the system

$$i\partial_t\psi_m = -\frac{1}{2}\Delta\psi_m + (V(\Psi) + \tilde{V})\psi_m, \quad m \in \mathbb{N} \tag{4.2.1}$$

$$-\nabla\cdot(\epsilon_0 + \epsilon_1|\nabla V|^2)\nabla V = n - n^* \tag{4.2.2}$$

$$n(x,t) = \sum \lambda_m|\psi_m|^2 \tag{4.2.3}$$

$$\psi_m(x,0) = \phi_m(x) \tag{4.2.4}$$

subject to periodic boundary conditions on the unit cube $Q = [0,1]^d$, $d = 1,2,3$. We note ϵ_0, ϵ_1 are given positive constants and (λ_m) is a specified sequence of non-negative numbers satisfying $\sum \lambda_m = 1$.

Sometimes, for simplicity of presentation only, we shall take $\lambda_1 = \lambda = 1$, $\lambda_m = 0$, $m > 1$. Also, we take $\tilde{V} = 0$ and $n^* = 1$ since the more general case is treated similarly under some obvious technical assumptions. The charge neutrality condition, (4.1.6) now reads

$$\int_Q n(x,t)\,dx = 1. \tag{4.2.5}$$

(noting Eq. (4.2.3), this is the same as the statement that Ψ is normalized to one.)

We also assume. without loss of generality, that

$$\int_Q V(x,t)\,dx = 0 \tag{4.2.6}$$

since the solution of Poisson's equation is determined only up to an arbitrary additive constant.

We introduce the following spaces:

$$X^k = \{\Psi = (\psi_m)_{m\in\mathbb{N}}; \psi_m \in H^k_{\text{loc}}(\mathbb{R}^n), \psi_m(x) = \psi_m(x+l),\ l \in \mathbb{Z}^d\} \tag{4.2.7}$$

where the periodicity condition is satisfied in the L^2-sense. X^k is a Hilbert space with norm

$$||\Psi||^2_{X^k} = \sum_{m\in\mathbb{N},|\alpha|\le k} \lambda_m ||D^\alpha \psi_m||^2_{L^2} < \infty. \tag{4.2.8}$$

(If $\lambda_m = 0$ for some m, the corresponding ψ_m is taken equal to zero.) We shall write X for X^0 and $||\Psi||$ for $||\Psi||_{X^0}$.

By a solution of (SP) on a time interval [0,T] we mean a pair

$(\Psi(x,t), V(x,t))$ solving (4.2.1)-(4.2.4) a.e. on $Q \times [0,T]$ such that

$$\Psi \in C^1([0,T], X) \cap C([0,T], X^2);$$

$$V \in C([0,T], H^2(Q)); \quad \int_Q V\,dx = 0. \tag{4.2.9}$$

A global, strong solution is a strong solution on [0,T] for any $T > 0$.

For the subsequent section we need some lemmata which we now state. Recall that the spatial dimension is denoted by d, $d = 1, 2$ or 3.

Lemma 4.2.1 *There is a constant $C > 0$ such that for any $u \in W^{1,r}(Q)$ we have*

$$||u||_{L^p(Q)} \leq C||u||_{W^{1,r}(Q)} \tag{4.2.10}$$

for $d > r$ and $1 \leq p \leq \frac{dr}{d-r}$; furthermore,

$$||u||_{L^\infty(Q)} \leq C||u||_{W^{1,r}(Q)} \tag{4.2.11a}$$

if $r > d$. Also, for any u such that $\int_Q u\,dx = 0$ we have

$$||u||_{L^p(Q)} \leq C||\nabla u||^{\alpha}_{L^r(Q)}||u||^{(1-\alpha)}_{L^q} \tag{4.2.11b}$$

with $\alpha \in [0,1]$ and $\frac{1}{p} = \alpha(\frac{1}{r} - \frac{1}{d}) + \frac{1-\alpha}{q}$ $(1 \leq p \leq \infty, \quad 1 \leq q \leq \infty)$, and $1 - \frac{d}{r} \notin \mathbb{N} \cup \{0\}$; if $1 - \frac{d}{r} \in \mathbb{N} \cup \{0\}$ α has to satisfy $0 \leq \alpha < 1$.

Finally, we have Poincaré's inequality

$$||u||_{L^p} \leq C||\nabla u||_{L^p}$$

for $u \in W^{1,p}$ such that $\int_Q u\,dx = 0$.

Proof. See Refs. [51, p.164] and [91, p.218].

Lemma 4.2.2 *Let $n \in C_{\text{per}}(Q)$. Then there exists a unique weak solution $V \in W^{1,4}_{\text{per}}(Q)$ of Eq. (4.2.2), satisfying $\int_Q V\,dx = 0$, that is*

$$\int_Q (\epsilon_0 + \epsilon_1|\nabla V|^2)\nabla V \cdot \nabla\Phi\,dx - \int (n-1)\Phi\,dx = 0 \tag{4.2.12}$$

for every $\Phi \in C^\infty_{\text{per}}(Q)$.

Proof. Eq. (4.2.12) is the Euler equation of the Lagrange functional

$$L(V) = \frac{\epsilon_0}{2}\int_Q |\nabla V|^2\,dx + \frac{\epsilon_1}{4}\int_Q |\nabla V|^4\,dx - \int (n-1)V\,dx \tag{4.2.13}$$

for $V \in W^{1,4}_{\text{per}}(Q)$ and $n \in \left(W^{1,4}_{\text{per}}(Q)\right)^* = W^{-1,4/3}(Q)$. The condition on n is satisfied because, by hypothesis, $n \in C_{\text{per}}(Q)$.

The existence of a weak solution now follows from a theorem of [56, p.4] as a minimizer of $L(V)$ on the set

$$M = \{V \in W^{1,4}_{\text{per}}(Q);\ \int_Q V\,dx = 0\}. \tag{4.2.14}$$

For this, $L(V)$ and M must satisfy

(i) M is a weakly closed subset of a reflexive Banach space B;

(ii) $L(V)$ is weakly lower semi continuous on M, that is, for any sequence $(V_m) \subset M$ and any $V \in M$ such that $V_m \to V$ weakly in B, we have $L(V) \leq \liminf_{m\to\infty} L(V_m)$.

(iii) L is coercive, i.e., $L(V) \to \infty$ as $||V||_B \to \infty$, $V \in M$.

These conditions can be proved easily for our situation by using Hölder's, Young's and Poincaré's inequalities on M. The weak lower semi continuity then follows from the fact that the first two terms of $L(V)$ give rise to an equivalent norm in the Banach space, while the last term is actually weakly continuous.

Finally, uniqueness follows from Lemma 4.2.3 below.

Lemma 4.2.3 *For any two functions $u, v \in W^{1,4}_{per}(Q)$ we have*

$$\int_Q \{[\epsilon_0 + \epsilon_1|\nabla u|^2]\nabla u - [\epsilon_0 + \epsilon_1|\nabla v|^2]\nabla v\} \cdot \nabla(u-v)\, dx \geq$$
$$\epsilon_0||\nabla(u-v)||^2_{L^2} + \frac{\epsilon_1}{4}||\nabla(u-v)||^4_{L^4}. \qquad (4.2.15)$$

Proof. Let $p = \nabla u$, $q = \nabla v$, and

$$I := |p|^4 + |q|^4 - \langle p, q\rangle(|p|^2 + |q|^2) = \langle |p|^2 p - |q|^2 q, p - q\rangle.$$

By using Young's inequality we get

$$\begin{aligned} |p-q|^4 &= |p|^4 + |q|^4 + 4\langle p,q\rangle^2 + 2|p|^2|q|^2 - 4\langle p,q\rangle(|p|^2+|q|^2) \\ &\leq 4\left[|p|^4 + |q|^4 - \langle p,q\rangle(|p|^2+|q|^2)\right] = 4I. \end{aligned}$$

The left-hand side of (4.2.15) is equal to $\epsilon_0||\nabla(u-v)||^2_{L^2} + \epsilon_1 \int_Q I\, dx$, and thus $\geq \epsilon_0||\nabla(u-v)||^2_{L^2} + \frac{\epsilon_1}{4}||\nabla(u-v)||^4_{L^4}$. □

Lemma 4.2.4 *Let $n \in C^\infty_{per}(Q)$. Then the solution given by Lemma 4.2.2 is in $W^{3,2}_{per}(Q) \cap W^{1,\infty}_{per}(Q)$. Also,*

$$\int_Q (1 + |\nabla V|)^2 \sum_{i,j} (\partial_{x_i x_j} V)^2\, dx$$

exists.

Remark. It would be sufficient to assume $n \in C^{1,\alpha}_{\text{per}}(Q)$ for this result, but the statement given here is sufficient for our purposes.

Proof *(of Lemma 4.2.4)* We apply Theorems of Refs. [51] and [53]. First we use Théorèmes 5.1 and 5.2 of Chapter IV, Ref. [53]. The ellipticity conditions which are needed there are satisfied because Eq. (4.2.2) is of the form

$$\sum_{i=1}^{n} \partial_{x_i} a_i(x, \nabla V) + a(x) = 0 \tag{4.2.16a}$$

of these theorems, namely

$$a_i(x,p) = (\epsilon_0 + \epsilon_1 |p|^2) p_i, \qquad a(x) = 1 - n. \tag{4.2.16b}$$

The conditions (3.1), (3.2) and (5.7) of Ref. [51] are straightforward to verify. Théorèmes 5.1 and 5.2 also require that the weak solution of Lemma 4.2.2 lies in $L^\infty(Q)$. This is satisfied because of the inequality (4.2.11a) of Lemma 4.2.1.

We remark that these two theorems give regularity only on the interior of the region in which the weak solution exists. Thus, to apply these results, we extend the weak solution V of Lemma 4.2.2 from $W^{1,4}_{\text{per}}(Q)$ to a weak solution in $W^{1,4}(\tilde{Q})$, where $\tilde{Q}$ is the union of 3^d copies of Q with Q itself in the center. We will write Q_j, $j = 1, \dots, 3^d$ for these copies of Q, with $Q_1 = Q$. A weak solution in $W^{1,4}(\tilde{Q})$ is defined as in (4.2.12), but with test functions $\varphi \in C_0^\infty(\tilde{Q})$.

The weak solution V given by Lemma 4.2.2 is a continuous function (by Sobolev embedding; see Lemma 4.2.1, (4.2.11)). We can therefore extend V by periodicity to $\tilde{Q}$, and denoting the extension again by V, we see that $V \in W^{1,4}(\tilde{Q})$ (and also $V \in W^{1,2}(\tilde{Q})$) since $W^{1,4}_{\text{per}}(Q)$ consists of all functions which lie in $W^{1,4}_{\text{loc}}(Q)$ and are 1-periodic. Also, the extension is a weak solution in $W^{1,4}_{\text{per}}(Q_j)$ in the sense of (4.2.12) on each Q_j ($j = 1, \dots, 3^d$). Setting

$$L_j(V, \varphi) = \int_{Q_j} (\epsilon_0 + \epsilon_1 |\nabla V|^2) \nabla V \cdot \nabla \varphi \, dx$$

and $L(V, \varphi) = \sum_{j=1}^{3^d} L_j(V, \varphi)$ we have to show that

$$L(V, \varphi) = \int_{\tilde{Q}} (n-1) \varphi \, dx \tag{4.2.12a}$$

for all $\varphi \in C_0^\infty(\tilde{Q})$.

Let $\varphi \in C_0^\infty(\tilde{Q})$ be given, and let $\epsilon > 0$ (sufficiently small) and $\delta > 0$ be arbitrary but fixed. As $C^\infty_{\text{per}}(Q)$ is dense in $W^{1,4}(Q)$ in the $W^{1,4}(Q)-$norm, we may find a $C^\infty_{\text{per}}(\mathbb{R}^d)$- function $\tilde{V}$ such that for any $k = 1, \dots, d$ we have

$$4 \cdot 3^{d-1} ||\varphi||_{L^\infty(\tilde{Q})} \sum_k ||V_k - \tilde{V}_k||_{L^\infty(Q)} < \delta \tag{4.2.12b}$$

where $V_k = (\epsilon_0 + \epsilon_1 |\nabla V|^2) \partial_{x_k} V, \quad \tilde{V}_k = (\epsilon_0 + \epsilon_1 |\nabla \tilde{V}|^2) \partial_{x_k} \tilde{V}$; here, we have again used Lemma 4.2.1.

Now, for every sufficiently small $\epsilon > 0$, we construct continuous functions $\zeta_\epsilon \in W^{1,2}(\tilde{Q})$ such that:

$0 \leq \zeta_\epsilon(x) \leq 1 \quad (\forall x \in \tilde{Q})$
$\lim_{\epsilon \to 0} \zeta_\epsilon(x) = 1$ in the open core of each Q_j
$\operatorname{supp} \partial_{x_k} \zeta_\epsilon = [-1, 2]^{d-1} \times ([-2\epsilon, -\epsilon] \cup [\epsilon, 2\epsilon] \cup [1-2\epsilon, 1-\epsilon] \cup [1+\epsilon, 1+2\epsilon])$
(we shall denote these sets by $T_k(\epsilon)$; note that the union of
intervals refers to the variable x_k)
$|\partial_{x_k} \zeta(x)| \leq \dfrac{1}{\epsilon}$ for all $x \in T_k(\epsilon)$ $(k = 1, \dots, d)$.

In the three-dimensional case, an example of such a function is

$$\zeta_\epsilon(x) = \xi(x_1)\xi(x_2)\xi(x_3)$$

with

$$\xi(t) = \begin{cases} 1 \text{ for } |t| \geq 2\epsilon \text{ or } |t-1| \geq 2\epsilon \\ 0 \text{ for } |t| \leq \epsilon \text{ or } |t-1| \leq \epsilon \ (t \in [-1,2]) \\ \frac{1}{\epsilon}|t| - 1 \text{ for } \epsilon \leq t \leq 2\epsilon \text{ or } -2\epsilon \leq t \leq -\epsilon \\ \frac{1}{\epsilon}|t-1| - 1 \text{ for } \epsilon \leq t-1 \leq 2\epsilon \text{ or } -2\epsilon \leq t-1 \leq -\epsilon. \end{cases}$$

We now use that the left-hand side of (4.2.12) is zero when we insert any test function from $C_{\text{per}}(Q)$, and *a fortiori* also zero for any test function in $C_{\text{per}}(Q_j)$ when integrating over Q_j $(j = 1, \dots, 3^d)$. For simplicity of notation, we only discuss 3 dimensions. In this case, we get

$$\begin{aligned} L(V, \varphi) - \int_{\tilde{Q}} (n-1)\, dx &= \sum_{j=1}^{3^d} \left\{ L_j(V, \varphi) - \int_{Q_j} (n-1)\varphi \ dx \right\} \\ &= I_1^\epsilon + I_2^\epsilon + I_3^\epsilon + I_4^\epsilon + I_5^\epsilon \end{aligned}$$

where

$$\begin{aligned} I_1^\epsilon &= \sum_j \left\{ \sum_k \int_{Q_j} V_k \partial_{x_k}(\varphi\zeta_\epsilon)\, dx - \int_{Q_j} (n-1)(\varphi\zeta_\epsilon)\, dx \right\} \\ I_2^\epsilon &= \sum_k \int_{\tilde{Q}} V_k (\partial_{x_k}\varphi)(1-\zeta_\epsilon)\, dx \\ I_3^\epsilon &= -\sum_k \int_{T_k^\epsilon} \tilde{V}_k \cdot \varphi \partial_{x_k} \zeta_\epsilon\, dx \\ I_4^\epsilon &= -\sum_k \int_{T_k^\epsilon} (V_k - \tilde{V}_k)\varphi \cdot \partial_{x_k}\zeta_\epsilon\, dx \\ I_5^\epsilon &= -\int_{\tilde{Q}} (n-1)\varphi\,(1-\zeta_\epsilon)\, dx. \end{aligned}$$

The term I_1^ϵ vanishes by the weak solution property on any Q_j; we have I_2^ϵ, $I_5^\epsilon = o(1)$ as $\epsilon \to 0$, because $\zeta_\epsilon \to 1$ a.e. on $\tilde{Q}$. From (4.2.12b), I_4^ϵ is bounded by δ, as

$$|I_4^\epsilon| \leq \frac{1}{\epsilon} ||\varphi||_{L^\infty(\tilde{Q})} \sum_k ||V_k - \tilde{V}_k||_{L^\infty(Q)} 3^{d-1} 4\epsilon < \delta.$$

The term I_3^ϵ is $o(1)$ for $\epsilon \to 0$, too, since this is true for each term in the sum defining I_3^ϵ. Consider, e.g., the term for $k = 1$ and recall that $d = 3$. Abbreviating $\chi := \varphi\tilde{V}_1$, and using the example function from above for ζ_ϵ, we have

$$\begin{aligned}
\int_{T_1^\epsilon} \chi(x) \partial_{x_1} \zeta_\epsilon(x)\, dx &= \frac{1}{\epsilon} \int_0^\epsilon \left\{ \int_{-1}^2 \int_{-1}^2 \chi(x_1 + \epsilon, x_2, x_3)\, dx_2 dx_3 \right\} dx_1 \\
&- \frac{1}{\epsilon} \int_0^\epsilon \left\{ \int_{-1}^2 \int_{-1}^2 \chi(x_1 - 2\epsilon, x_2, x_3)\, dx_2 dx_3 \right\} dx_1 \\
&+ \frac{1}{\epsilon} \int_0^\epsilon \left\{ \int_{-1}^2 \int_{-1}^2 \chi(x_1 + 1 + \epsilon, x_2, x_3)\, dx_2 dx_3 \right\} dx_1 \\
&- \frac{1}{\epsilon} \int_0^\epsilon \left\{ \int_{-1}^2 \int_{-1}^2 \chi(x_1 + 1 - 2\epsilon, x_2, x_3)\, dx_2 dx_3 \right\} dx_1.
\end{aligned}$$

As $\epsilon \to 0$, and by the continuity of χ, the right hand side converges to $\eta(0) - \eta(0) + \eta(1) - \eta(1) = 0$, where

$$\eta(t) := \int_{-1}^2 \int_{-1}^2 \chi(t, x_2, x_3)\, dx_2 dx_3.$$

We arrive at

$$|L(V, \varphi) - \int_{\tilde{Q}} (n-1)\, \varphi\, dx| \leq \delta$$

for any $\delta > 0$. This implies (4.2.12a).

We are now in position to use (4.2.12a) and the Theorems from Ref. [53]. These results imply that the solution is in $W^{2,2}_{\text{per}}(Q) \cap W^{1,\infty}_{\text{per}}(Q)$ and satisfies

$$\int_Q (1 + |\nabla V|)^2 \sum_{i,j} (\partial_{x_i x_j} V)^2\, dx < \infty, \qquad \int_Q |\nabla V|^4\, dx < \infty. \tag{4.2.17}$$

Next we use Théorème 6.5 of Chapter IV of Ref. [53], which assumes conditions (4.2.17) and also that the functions $a_i(x, p)$ and $a(x, p)$ of (4.2.16b) lie in $C^{1,\alpha}$ (which is satisfied in our case by the hypothesis on n). The theorem implies that $V \in C^{2,\alpha}_{\text{per}}(Q)$. Finally, we use Théorème 8.10 of Ref. [53] with $k = 1$, viewing Eq.(4.2.2) formally as a linear equation with coefficients

$$a_{ij}(x) = (\epsilon_0 + \epsilon_1 |\nabla V|^2)\delta_{ij}$$

(cf. Eq. (8.1) in Ref. [51]). The hypotheses of Théorème 8.10 are that these coefficients must lie in $C^{1,1}_{\text{per}}(Q)$ and that the right hand side is in $W^{1,2}_{\text{per}}(Q)$. These conditions are satisfied in our situation by the foregoing remarks. The final conclusion is that $V \in W^{3,2}_{\text{per}}(Q)$. □

Lemma 4.2.5 *Let V be a solution of Eq. (4.2.2) (with $n^* = 1$) which lies in $W^{3,2}_{per}(Q)$ and $n \in L^2(Q)$. Then*

$$||\Delta V||_{L^2(Q)} \leq \frac{1}{\epsilon_0}||n-1||_{L^2(Q)}.$$

Proof. Multiply (4.2.2) by $-\Delta V$ and integrate. By applying the assertions of Lemma 4.2.4, we get

$$\begin{aligned}
&-\int \Delta V\,(n-1)\,dx \\
=\;& \sum_{i,j}\int \partial_{x_i}\left[(\epsilon_0+\epsilon_1|\nabla V|^2)\partial_{x_i}V\right]\partial_{x_jx_j}V\,dx \\
=\;& -\sum_{i,j}\int \left[(\epsilon_0+\epsilon_1|\nabla V|^2)\partial_{x_i}V\right]\partial_{x_jx_jx_i}V\,dx \\
=\;& \epsilon_0\int|\Delta V|^2\,dx+\epsilon_1\sum_{i,j}\int\partial_{x_j}\left(|\nabla V|^2\partial_{x_i}V\right)\partial_{x_i}\partial_{x_j}V\,dx \\
=\;& \epsilon_0||\Delta V||^2_{L^2}+\epsilon_1\int|\nabla V|^2\sum_{i,j}\left(\partial_{x_jx_i}V\right)^2dx \\
&+\epsilon_1\sum_{i,j}\int\partial_{x_j}|\nabla V|^2\partial_{x_i}V\;\partial_{x_ix_j}V\,dx \\
=\;& \epsilon_0||\Delta V||^2_{L^2}+\epsilon_1\int|\nabla V|^2\sum_{i,j}\left(\partial_{x_ix_j}V\right)^2\,dx+\frac{\epsilon_1}{2}\int\sum_j\left(\partial_{x_j}|\nabla V|^2\right)^2\,dx \\
&\geq \epsilon_0||\Delta V||^2_{L^2}.
\end{aligned}$$

The assertion now follows by applying the Cauchy-Schwarz inequality to the left-hand side. □

Remark. For the one-dimensional case we can obtain an explicit formula for the unique solution of (4.2.2) as follows. The relevant equation is now

$$((\epsilon_0+\epsilon_1V_x^2)V_x)_x = n-1 =: \hat{n} \tag{4.2.18}$$

or

$$(\epsilon_0+\epsilon_1V_x^2)V_x = \int_0^x \hat{n}(y)\,dy + C_1$$

where C_1 is a constant of integration. Then

$$V_x = h^{-1}\left(\int_0^x \hat{n}(y)\,dy + C_1\right)$$

where h^{-1} is the inverse function of $\epsilon_0 t + \epsilon_1 t^3$. It follows that

$$V(x) = \int_0^x h^{-1}\left(\int_0^y \hat{n}(t)\,dt + C_1\right)\,dy + C_2. \tag{4.2.19}$$

Now we see that $V(0) = V(1) = C_2$, by periodicity. Thus

$$\int_0^1 h^{-1}\left(\int_0^y \hat{n}(t)\,dt + C_1\right)\,dy = 0. \tag{4.2.20}$$

Eq, (4.2.20) is sufficient to determine C_1 uniquely, and then C_2 is also uniquely determined by Eq. (4.2.6).

4.3 The Galerkin sequence

For simplicity of notation, we introduce the assumption previously noted that only one λ_m is non vanishing. We now introduce the Galerkin sequence for (SP) by setting (with $\psi_1^{(N)} = \psi^{(N)}$)

$$\psi^{(N)} = \sum_{|k|<N} d_k^{(N)}(t) h_k \tag{4.3.1}$$

with

$$h_k(x) = e^{2\pi i k x},\ k \in \mathbb{Z}^d, \tag{4.3.2}$$

and

$$\left(\left[i\partial_t \psi^{(N)}(x,t) + \frac{1}{2}\Delta\psi^{(N)} - V^{(N)}(\Psi^{(N)})\psi^{(N)}\right], h_k\right) = 0,\ |k| \leq N. \tag{4.3.3}$$

Also

$$\psi^{(N)}(x,0) = \sum_{|k|\leq N} (\phi, h_k)\, h_k(x) \tag{4.3.4}$$

(here $\phi = \phi_1$). Let

$$n^{(N)}(x,t) = |\psi^{(N)}(x,t)|^2 = \sum_k n_k^{(N)}(t)\ h_k(x). \tag{4.3.5}$$

We see that

$$n_k^{(N)} = \sum_{|l|\leq N, |l-k|\leq N} d_l^{(N)} \bar{d}_{l-k}^{(N)},\ |k| \leq 2N,\ k \neq 0 \tag{4.3.6a}$$

and

$$n_k^{(N)} = 1 \text{ for } k = 0. \tag{4.3.6b}$$

We now define $V^{(N)}$ as the solution of

$$-\nabla \cdot \left(\epsilon_0 + \epsilon_1 |\nabla V^{(N)}|^2\right) \nabla V^{(N)} = n^{(N)} - 1 \tag{4.3.7}$$

in the sense of Lemmata 4.2.2-4.2.5. Let

$$V^{(N)} = \sum_{j \in \mathbb{Z}^d} V_j^{(N)} h_j. \tag{4.3.8}$$

Eq. (4.3.3) is equivalent to a finite system of ordinary differential equations for the coefficients $d_l^{(N)}$ of the Galerkin sequence $(\Psi^{(N)})$ and their complex conjugates $\bar{d}_l^{(N)}$:

$$\dot{d}_l(t) = -2\pi^2 i l^2 d_l(t) - i \sum_{|l| \leq N} V_{k-l}^{(N)} d_l(t) \tag{4.3.9}$$

where we have written d_l instead of $d_l^{(N)}$, and similar equations for the complex conjugates.

We now state

Lemma 4.3.1 *The* $(V_j^{(N)})$, $\quad |j| \leq 2N$, *depend locally Lipschitz-continuously on any set* $D = (d_k)$, *where* $|k| \leq N$.

Proof. From (4.3.6)-(4.3.8) and Lemma 4.2.5, we have for any two sets $D = (d_k)$ and $\tilde{D} = (\tilde{d}_k)$, $\quad |k| \leq N$

$$\begin{aligned} |V_j^{(N)}(D) - V_j^{(N)}(\tilde{D})|^2 \quad & \leq ||\Delta(V^{(N)}(D) - V^{(N)}(\tilde{D}))||_{L^2}^2 \\ & \leq \frac{1}{\epsilon_0^2} \sum_{|l| \leq N} |n_l^{(N)}(D) - n_l^{(N)}(\tilde{D})|^2, \end{aligned}$$

$|j| \leq 2N$. The assertion follows from (4.3.6) since the $n_l^{(N)}$ are given as quadratic polynomials in the $d_l^{(N)}$. □

Lemma 4.3.2 *The differential system (4.3.9) has a unique, global solution*

$(d_k^{(N)})_{|k| \leq N}$ *on* $[0, \infty)$ *for any* N.

Proof. Local existence follows from Lemma 4.3.1 and the usual existence theory for ordinary differential equations. Global existence follows from Lemma 4.4.1 of the next section, namely conservation of the L^2-norm of $\psi^{(N)}$:

$$\sum_{|k| \leq N} |d_k^{(N)}(t)|^2 = ||\psi^{(N)}(\cdot, t)||_{L^2}^2 = ||\psi^{(N)}(\cdot, 0)||_{L^2}^2 = \sum_{|k| \leq N} |d_k(0)|^2 \leq |\phi|^2$$

(using (4.3.4)). □

4.4 Conservation Laws, *a priori* Bounds and Global Existence

We are now ready to prove global existence of strong solutions; we begin with some lemmata on conservation laws.

Lemma 4.4.1 *For any $t \geq 0$ we have for all N*

$$||\psi^{(N)}(\cdot,t)||_{L^2}^2 = ||\psi^{(N)}(\cdot,0)||_{L^2}^2.$$

Proof. We compute

$$\begin{aligned}
\frac{\partial}{\partial t}||\psi^{(N)}(\cdot,t)||_{L^2}^2 &= 2\,Re \int \bar{\psi}^{(N)}\partial_t \psi^{(N)}\,dx \\
&= -2\,Re\, i \int V^{(N)}|\psi^{(N)}|^2\,dx \\
&= 0.
\end{aligned}$$

□

Lemma 4.4.2 *For all $t \geq 0$ and all N,*

$$\int \left\{ |\nabla\psi^{(N)}|^2 + \epsilon_0|\nabla V^{(N)}|^2 + \frac{3}{2}\epsilon_1|\nabla V^{(N)}|^4 \right\} dx = const.$$

Proof. In Eq. (4.3.3), we use $\partial_t\bar{\psi}^{(N)}$ as a multiplier to obtain

$$0 = \int \left\{ i|\partial_t\psi^{(N)}|^2 + \frac{1}{2}\Delta\psi^{(N)}\partial_t\bar{\psi}^{(N)} - V^{(N)}\psi^{(N)}\partial_t\bar{\psi}^{(N)} \right\} dx.$$

Taking the real part gives

$$\begin{aligned}
Re\int \Delta\psi^{(N)}\partial_t\bar{\psi}^{(N)}\,dx &= 2\,Re\int V^{(N)}\psi^{(N)}\partial_t\bar{\psi}^{(N)}\,dx \\
&= \int V^{(N)}\partial_t|\psi^{(N)}|^2\,dx.
\end{aligned}$$

Thus, by partial integration, and using (4.3.7),

$$\begin{aligned}
& -\partial_t \int |\nabla\psi^{(N)}|^2\,dx \\
= \; & 2\int V^{(N)}\partial_t|\psi^{(N)}|^2\,dx \\
= \; & \epsilon_0\partial_t\int |\nabla V^{(N)}|^2\,dx - 2\epsilon_1\int V^{(N)}\partial_t\left[\nabla(|\nabla V^{(N)}|^2\nabla V^{(N)})\right]dx \\
= \; & \epsilon_0\partial_t\int |\nabla V^{(N)}|^2\,dx + 2\epsilon_1\int |\nabla V^{(N)}|^2\partial_t\left(|\nabla V^{(N)}|^2\right)\,dx \\
+ \; & 2\epsilon_1\int |\nabla V^{(N)}|^2\nabla V^{(N)}\cdot\partial_t\nabla V^{(N)}\,dx \\
= \; & \epsilon_0\partial_t\int |\nabla V^{(N)}|^2\,dx + \frac{3}{2}\epsilon_1\partial_t\int |\nabla V^{(N)}|^4\,dx,
\end{aligned}$$

which proves the lemma. □

We now state

Lemma 4.4.3 *Let $\phi \in H^1_{per}(Q)$. Then there is a constant $C > 0$, independent of N and t, such that for all $t \geq 0$ and for all N*

$$\begin{aligned} ||\psi^{(N)}(\cdot,t)||_{H^1_{per}(Q)} &\leq C \\ ||V^{(N)}(\cdot,t)||_{H^2_{per}(Q)} &\leq C \\ ||n^{(N)}(\cdot,t)||_{L^2(Q)} &\leq C \\ ||\nabla V^{(N)}(\cdot,t)||_{L^4(Q)} &\leq C. \end{aligned}$$

Proof. Using Lemma 4.2.1 we have for all $t \geq 0$ and all N, using (4.2.11b) of Lemma 4.2.1 for $\psi^{(N)} - \int_Q \psi^{(N)}\, dx$,

$$||n^{(N)}(\cdot,t) - 1||_{L^2} \leq 1 + C_1 ||\psi^{(N)}(\cdot,t)||^2_{H^1}.$$

Setting $t = 0$ we arrive at

$$||n^{(N)}(\cdot,0) - 1||_{L^2} \leq 1 + C_1 ||\phi||^2_{H^1}. \tag{4.4.1}$$

Using Lemma 4.2.3 with $u = V^{(N)}$ and $v = 0$, we get for all $t \geq 0$

$$\begin{aligned} ||\nabla V^{(N)}||^2_{L^2} &\leq \frac{1}{\epsilon_0} \int |n^{(N)} - 1| \cdot |V^{(N)}|\, dx \\ &\leq \frac{1}{\epsilon_0} ||n^{(N)} - 1||_{L^2} ||V^{(N)}||_{L^2} \\ &\leq C_2 ||n^{(N)} - 1||_{L^2} ||\nabla V^{(N)}||_{L^2}. \end{aligned}$$

In the last step we have used Poincaré's inequality and the fact that

$$\int V^{(N)}\, dx = 0.$$

It follows that for all $t \geq 0$

$$||\nabla V^{(N)}||_{L^2} \leq C_2 ||n^{(N)} - 1||_{L^2}.$$

Taking $t = 0$ in this estimate and using (4.4.1), we see that uniformly in N

$$||\nabla V^{(N)}(\cdot,0)||_{L^2} \leq C. \tag{4.4.2}$$

Using Lemma 4.2.1 again as well as the equivalence of the $H^2(Q)-$ norm with the norm (cf. Ref. [10])

$$\left(||u||^2_{L^2} + ||\nabla u||^2_{L^2} + ||\Delta u||^2_{L^2}\right)^{1/2},$$

we have

$$||\nabla V^{(N)}||_{L^4} \leq C_1 ||V^{(N)}||_{H^2} \leq C_2 \left[||\nabla V^{(N)}||_{L^2} + ||\Delta V^{(N)}||_{L^2} \right], \tag{4.4.3}$$

where we have again used Poincaré's inequality. Setting $t = 0$ in (4.4.3), using Lemma 4.2.5 and Eq. (4.4.2), we get

$$||\nabla V^{(N)}(\cdot, 0)||_{L^4} \leq C. \tag{4.4.4}$$

By Lemmata 4.4.1 and 4.4.2 and Eqs. (4.4.2) and (4.4.3), Lemma 4.4.3 follows, because we have in addition

$$||\psi^{(N)}(\cdot, t)||_{L^2} \leq ||\phi||_{L^2},$$

$$E(t) = ||\nabla \psi^{(N)}(\cdot, t)||^2_{L^2} + \epsilon_0 ||\nabla V^{(N)}(\cdot, t)||^2_{L^2} + \frac{3}{2}\epsilon_1 ||\nabla V^{(N)}(\cdot, t)||^4_{L^4} = E(0).$$

□

Finally, we can state

Lemma 4.4.4. *Let $\phi \in H^2_{per}(Q)$ and $T > 0$. Then there is a constant $C > 0$ depending continuously only on $||\phi||_{H^2}$ and T, such that for all $t \in [0, T]$ and all N we have*

$$||\psi^{(N)}(\cdot, t)||_{H^2_{per}(Q)} \leq C, \qquad ||\psi^{(N)}(\cdot, t)||_{L^\infty_{per}(Q)} \leq C.$$

Proof. Using $\Delta\psi^{(N)}$ as a multiplier in Eq. (4.3.3), one calculates

$$\begin{aligned}
\partial_t \int |\Delta\psi^{(N)}|\, dx &= 2\, Re \int \partial_t \Delta\psi^{(N)} \cdot \Delta\psi^{(N)}\, dx \\
&= 2\, Re \int \Delta^2 \bar{\psi}^{(N)} \partial_t \psi^{(N)}\, dx \\
&= -2\, Re\, i \int \Delta^2 \bar{\psi}^{(N)} V^{(N)} \psi^{(N)}\, dx \\
&= -2\, Re\, i \int \Delta\bar{\psi}^{(N)} \Delta V^{(N)} \psi^{(N)}\, dx \\
&\quad -4\, Re\, i \int \Delta\bar{\psi}^{(N)} \nabla V^{(N)} \cdot \nabla\psi^{(N)}\, dx.
\end{aligned}$$

At this point, we proceed as in Lemma 3.2 of Ref. [10], but the term above involving $\Delta V^{(N)}$ must be treated differently. Instead of replacing $\Delta V^{(N)}$ by $(1 - n^{(N)})$ as in the case of the linear Poisson equation, we estimate $||\Delta V^{(N)}||_{L^2}$ by $||n^{(N)} - 1||_{L^2}$ according to Lemma 4.2.5. The rest of the proof is the same as in Ref. [10]. □

Now we state (reverting to the general case with a sequence (λ_m))

Theorem 4.4.5. *Let $\Phi \in X^2$. Then there is a unique global strong solution (Ψ, V) of the system (4.2.1)-(4.2.4).*

Proof. The idea of the proof is as in [10], Theorem 3.1, using the compact embedding of $H^2_{\text{per}}(Q)$ in $H^1_{\text{per}}(Q)$ and showing that the weak solutions which one gets from the compactness of the Galerkin sequence (following from the a priori bounds and Lemma 4.4.4) are actually strong solutions.

The uniqueness proof is identical to that of Ref. [10], using $L^\infty-$bounds derived from Lemma 4.2.5 (using Sobolev embedding). $\square$

Corollary 4.4.6. *The strong solution of Theorem 4.4.5 satisfies the conservation laws*

$$||\Psi(\cdot,t)||_X = \text{const.},$$

$$||\nabla\Psi(\cdot,t)||_X^2 + \epsilon_0||\nabla V(\cdot,t)||^2_{L^2(Q)} + \frac{3}{2}\epsilon_1||\nabla V(\cdot,t)||^4_{L^4(Q)} = \text{const.}$$

(all $t \geq 0$).

Proof. The proof is basically the same as the corresponding results for the Galerkin sequence, Lemmata 4.4.1 and 4.4.2, since we know

$$\Psi \in C([0,T],X^2) \cap C^1([0,T],X).$$

$\square$

4.5 Matrix Formulation of the Poisson Equation

In this section we present a matrix formulation of the approximate, quasilinear Poisson equation (4.3.7). This formulation may be useful for numerical purposes.

We begin with Eq. (4.3.8), which was

$$V^{(N)} = \sum V_k^{(N)} h_k,$$

and we use the abbreviation

$$L(V) = -\epsilon_0\Delta V - \epsilon_1\nabla\cdot(|\nabla V|^2\nabla V)$$

(this is the same operator as on the left-hand side of Eq. (4.2.21)). One easily calculates

$$|\nabla V^{(N)}|^2\nabla V^{(N)} = 8\pi^3 i\sum_{k,j,s}(k-j)\cdot k\ (s-j)V_k^{(N)}\bar{V}_{k-j}^{(N)}\,V_{s-j}^{(N)}\,h_s.$$

This gives

$$\begin{aligned} & L(V^{(N)}) \\ = \;\; & 4\pi^2\sum_s\left[\epsilon_0 s^2 V_s^{(N)} + 4\pi^2\epsilon_1\sum_{k,j}(s-j)\cdot(k-j)\,s\cdot k V_k^{(N)}\bar{V}_{k-j}^{(N)}V_{s-j}^{(N)}\right]h_s. \end{aligned}$$

Introducing the vectors

$$\Lambda^{(N)} = \left(V_j^{(N)}\right), \quad \alpha^{(N)} = \left(n_j^{(N)} - \delta_{j0}\right),$$

the terms

$$M(\Lambda^{(N)}) = (M_{kj}), \quad M_{kj} = 2\pi(k-j)kV_{k-j}^{(N)},$$

$$M^*(\Lambda^{(N)}) = (M_{kj}^*), \quad M_{kj}^* = 2\pi(j-k)j\bar{V}_{j-k}^{(N)},$$

and the matrix

$$K^2 := \mathrm{diag}(k^2),$$

we get

Proposition 4.5.1 *The $N-th$ order Galerkin approximate quasilinear Poisson equation is equivalent to the matrix equation*

$$\left[\epsilon_0 K^2 + \epsilon_1 M(\Lambda^{(N)}) \cdot M^*(\Lambda^{(N)})\right] \Lambda^{(N)} = \frac{1}{4\pi^2}\alpha^{(N)}.$$

Remark 1. The product $(M \cdot M^*)_{sk}$ is understood in the following tensor sense:

$$(M \cdot M^*)_{sk} = \sum_j M_{sj} \cdot M_{jk}^* = 4\pi^2 \sum_j (s-j)\cdot(k-j)\, s \cdot k\, V_{s-j}\bar{V}_{k-j}.$$

The dot product used is simply the scalar product in $\mathbb{C}^d$.

Remark 2. Instead of using the sequence $(V^{(N)})$ to approximate the solution of the Poisson equation (4.2.2) we may also use the sequence $(\hat{V}^{(N)})$, where $\hat{V}^{(N)} = P_N V^{(N)}$ and P_N is the projection of $L^2(Q)$ onto the subspace $\mathrm{sp}\{h_k; |k| \leq N\}$. The Fourier series $(\hat{V}^{(N)})$ converges to V in various norms, e.g., in $C_{\mathrm{per}}(Q) \cap L^p(Q) \cap W^{2,2}_{\mathrm{per}}(Q)$, $1 \leq p \leq \infty$. The coefficients of $\hat{V}_N$ may be computed iteratively using Proposition 4.5.1.

Chapter 5

Quantum BGK Modes

5.1 Introduction

In 1957, Bernstein, Greene and Kruskal [31] showed that an infinite family of solutions to the (nonlinear) Vlasov equation could be constructed; specifically, any function of the energy satisfies the stationary equation and this solution, by Galilean transformation, becomes a traveling-wave solution in another frame of reference [58].

More recently, Buchanan [59] has shown that the Wigner transform [33] of any function of the system hamiltonian (assumed time-independent) satisfies the stationary Wigner equation, for either fixed potentials (i.e. the linear equation) or for self-consistent potentials (the nonlinear case). These solutions, or rather our own generalization thereof (cf. Sec. 5.2) will be called "quantum BGK modes" abbreviated QBGK. As in the classical case, these modes can be lifted to traveling-wave solutions by Galilean transformation, but such wave solutions will not be considered in this work.

In Sec. 5.2, a generalization of Buchanan's definition of QBGK modes is considered, and it is shown that every solution of the Wigner equation is such a mode. In particular, the analyses is based on the existence of a complete set of commuting operators [60, 61]. In Sec. 5.3, we use the results of a recent paper [22] to write a spectral formula for a solution of the stationary Wigner-Poisson problem [9] We also give an approximation scheme and prove convergence in various norms. In Sec. 5.4, we comment on some unsolved problems and suggest a possible numerical scheme. We also describe how the classical BGK modes might be generalized.

5.2 The QBGK Modes

We recall that the Wigner equation arises from the Heisenberg equation of motion for the density matrix ρ [33]

$$i\hbar\frac{\partial\rho}{\partial t} = H\rho - \rho H \tag{5.2.1}$$

where H is the system hamiltonian. The Wigner transform of (5.2.1) is the Wigner equation, i.e. the equation which describes the time evolution of the Wigner distribution function which, for an N-particle system in d dimensions, is defined as

$$w(x,p,t) = (\frac{1}{2\pi\hbar})^{Nd}\rho_w(x,p,t) \tag{5.2.2}$$

where ρ_w is the Wigner transform of the density matrix. Again, the formula for the Wigner transform of an operator "A" is given by Eqs. (2.1.2) and (2.1.3).

Evidently, if $\rho = \rho(H)$, a function of the hamiltonian, then $\frac{\partial\rho}{\partial t} = 0$ in Eq. (5.2.1). We point out that ρ should be a density matrix, (i.e., a positive, trace-class operator) with $\frac{d\rho}{dt} = 0$. The solutions of the Wigner equation will be given by

$$w(x,p) = (\frac{1}{2\pi\hbar})^{Nd}[\rho(H)]_w. \tag{5.2.3}$$

We note that in general for any function $g(H), [g(H)]_w \neq g(H_w)$; for example in the case $Nd = 1$ with $g(H) = H^2$, $H = \frac{1}{2}P^2 + V(X)$, we have

$$g(H_w) = (\frac{1}{2}p^2 + V(x))^2 \tag{5.2.4a}$$

but (Ref. [34], Eqs. (25))

$$[g(H)]_w = (\frac{1}{2}p^2 + V(x))^2 + 2\hbar^2\frac{d^2V}{dx^2}. \tag{5.2.4b}$$

(As usual [34, 35], we write operators in capital letters X, P and their Wigner transforms in the lower case x, p.)

These solutions, $[\rho(H)]_w$, are the quantum versions of the classical BGK modes discovered by Buchanan [59]. More generally, let H, A_1, A_2, ..., A_M be a complete set of commuting operators (CSCO) [60, 61]. Then any function $\rho(H, A_1, ..., A_M)$ which is a bounded operator satisfies the stationary Heisenberg equation and its Wigner transform $[\rho(H_1, A_1 ... \mathrm{A}_M)]_w$ satisfies the stationary Wigner equation. We call these solutions QBGK modes whenever $\mathrm{Tr}\rho = 1$. Note that in the one-dimensional case, the CSCO contains only one element, namely the hamiltonian itself. In a pseudo one-dimensional problem, for example a particle in three dimensions moving in a symmetric potential, the components of the angular momentum are additional commuting operators.

Theorem 5.2.1. *Consider the (self-adjoint) hamiltonian $H = \frac{1}{2}P^2 + V(X)$, and its associated stationary Wigner equation* [33]

$$p \cdot \nabla_x w(x,p) - \frac{i}{\hbar}\Theta(V)w(x,p) = 0 \tag{5.2.5a}$$

where $\Theta(V)$ is the pseudo-differential operator

$$(\Theta(V)f)(x,p) = (\frac{1}{2\pi\hbar})^{Nd} \int\limits_{\mathbb{R}^{Nd}\times\mathbb{R}^{Nd}} e^{i(p-p')\cdot\eta/\hbar}[V(x+\frac{\eta}{2}) - V(x-\frac{\eta}{2})]f(x,p')dp'd\eta, \tag{5.2.5b}$$

with V assumed bounded. Then any solution $w(x,p)$ which satisfies the following conditions:

(1) $\iint w(x,p)dx\,dp = 1$

(2) $\iint w(x,p)w[\psi](x,p)dx\,dp \geq 0$

(for every Wigner transform of a pure state ψ) is a QBGK mode.

Remarks. We have not stated the boundary conditions to be imposed on (5.2.5a); whatever they are (e.g. periodic), the solution w is assumed to obey them. The conditions (1) and (2) of Theorem 5.2.1 (see [62]), if satisfied, guarantee that w is a Wigner function, i.e., the Wigner transform of a density matrix. The CSCO constructed from the hamiltonian H is not unique (see below); moreover, the function of the Theorem can be taken as any function of these completions.

Proof. For convenience we set the mass $m = 1$ for every particle in our system, and also take $\hbar = 1$. Then, as is shown by Markowich [3], Eq. (5.2.5a) is equivalent to

$$(H_r - H_s)z(r,s) = 0 \tag{5.2.6a}$$

where

$$H_r = -\frac{1}{2}\Delta_r + V(r) \tag{5.2.6b}$$

and

$$z(r,s) = \hat{w}(x(r,s),\eta(r,s)) \tag{5.2.6c}$$

$$r = x + \frac{\eta}{2}, s = x - \frac{\eta}{2} \tag{5.2.6d}$$

and

$$\hat{w}(x,\eta) = \int_{\mathbb{R}^{Nd}} e^{-ip\cdot\eta} w(x,p)dp. \tag{5.2.6e}$$

We recall the normalization of w, which follows from the condition Trρ=1:

$$\int w(x,p)dp\,dx = 1. \tag{5.2.6f}$$

It follows [3] that $z(r,s)$ is the kernel of a trace-class, positive operator on L^2, call it ρ. Then z can be expanded in terms of its eigenfunctions $(u_i)_{i\in\mathbb{N}}$;

$$z(r,s) = \sum \lambda_i u_i(r)\bar{u}_i(s) \tag{5.2.7}$$

where the λ_i are the (positive) eigenvalue of z and $\sum \lambda_i = 1$.

By the properties of z [9, 3] it follows that ρ is a density matrix, and (5.2.6a) is equivalent to

$$H\rho - \rho H = 0. \tag{5.2.8}$$

Now H can be decomposed as [63]

$$H = H_P + H_C \tag{5.2.9a}$$

where

$$H_P = \sum_j \sum_{k=1}^{r_j} \mu_j E_j^k \tag{5.2.9b}$$

and

$$H_C = \int_{\sigma_c(H)} \mu\, dE_\mu. \tag{5.2.9c}$$

Here the μ_j are eigenvalues of H, and the E_j^k are the spectral projections associated with the point spectrum (each E_j^k is one-dimensional). Similarly, the E_μ are the spectral family for the continuous spectrum. (cf. Ref. [63], Suppl. 1, Th. 1.7. We recall that the quantum-mechanical space of states $\mathcal{H}$ is a separable Hilbert space.) The sum over k is over the r_i degenerate eigenvectors associated with the eigenvalue λ_i.

We now can decompose H

$$\mathcal{H} = \mathcal{H}_P \oplus \mathcal{H}_C \tag{5.2.10}$$

where $\mathcal{H}_P$ and $\mathcal{H}_C$ are reducing subspaces for H (and, of course, for functions of H). Considering $\mathcal{H}_P$ and $\mathcal{H}_C$ as Hilbert spaces in their own right, we can construct an operator H_P^1 such that the set $(H_P,\, H_P^1)$ is a complete set of commuting self-adjoint operators in $\mathcal{H}_P$(see [60, p.56]; note that the operator H_p^1 is not unique.). Let P_P and P_C be the projections onto $\mathcal{H}_P$ and $\mathcal{H}_C$ respectively, and B an arbitrary bounded operator which commutes with every spectral projection of H. (In particular, B commutes with H_P, H_P^1 and H_C.) Then define

$$B_P = P_P B P_P \tag{5.2.11a}$$

$$B_C = P_C B P_C. \tag{5.2.11b}$$

Then by Theorem 17.1, Ref. [60], B_P is a function of H_p and H_P^1;

$$B_P = g(H_P,\, H_P^1). \tag{5.2.12}$$

Now H_C is unitarily equivalent to multiplication by X in $L^2(\mathbb{R}^{Nd}$,d$\mu)$ where

$$d\mu = d(E_\lambda f, f) \tag{5.2.13}$$

and f is a cyclic vector for H in $\mathcal{H}_C$ (Ref. [62], Prop. 1.10).

By Prop. 1.9 of Ref. [63], the image of B_C under the unitary transformation is an operator of multiplication by a measurable, real-valued function on $L^2(\mathbb{R}^{Nd}, d\mu.)$. Therefore there is some function $h \in L^2(\mathbb{R}^{Nd}, d\mu)$ such that

$$B_C = h(H_C). \tag{5.2.14}$$

From (5.2.11) and (5.2.13) we have

$$B = g(H, H_P^1) + h(H_C). \tag{5.2.15}$$

□

5.3 Spectral Representation of QBGK Modes

The Wigner transform of ρ can be computed from Eqs.(2.1.2) and (2.1.3). Choose the (φ_n) in this equation to be the orthonormal set of joint eigenvectors of H and H^1, with eigenvalues μ_m and μ_m^i. Then one can write

$$w(x,p) = (\frac{1}{2\pi})^{Nd} \sum_{m,i} \rho(\mu_m, \mu_m^i) \int e^{ip\cdot\eta} \varphi_m^i(x - \frac{\eta}{2}) \bar{\varphi}_m^i(x + \frac{\eta}{2}) d\mu. \tag{5.3.1}$$

Here $\rho(\mu_m, \mu_m^i)$ is the matrix element of ρ in the state φ_m^i. (Note that $H\varphi_m^i = \mu_m \varphi_m^i \ \forall i$ while $H^1\varphi_m^i = \mu_m^i \varphi_m^i \forall m$). In writing (5.3.1) it has been assumed that the operator valued function $\rho(H, H^1)$ is bounded. In particular, since

$$\int \rho(x,p)\, dx\, dp = 1$$

the function ρ must be chosen so that the sum in Eq. (5.3.1) converges.

A special case of interest is the Wigner-Poisson system with space-periodic boundary conditions on the unit cube $Q \subset \mathbb{R}^d$ [22]. For this system, the potential is given by the solution of the Poisson equation

$$-\Delta V = n - n^* \tag{5.3.2}$$

where

$$n = \int w(x,p) dp$$

and n^* is a given (periodic) background density. Charge neutrality requires

$$\int_Q (n - n^*) dx = 0. \tag{5.3.3}$$

In [22], it is proved that the hamiltonian of this nonlinear system generates a complete, orthonormal set of eigenfunctions (φ_m) with eigenvalues (μ_m). (For $d = 1$, these eigenvalues are necessarily simple.)

One can proceed to define an approximation procedure to calculate the QBGK modes from the spectral formula (5.3.1). Considering the periodic Wigner-Poisson problem on Q^d, $d = 1, 2, 3$, we define

$$w^\nu(x,p) = (\frac{1}{2\pi})^{Nd} \sum_{m=1}^{\nu} \sum_i \rho(\mu_m, \mu_m^i) \int_{Q^d} e^{i\rho\cdot\eta} \varphi_m^i(x - \frac{\eta}{2}) \bar{\varphi}_m^i(x + \frac{\eta}{2}) d\eta. \tag{5.3.4}$$

We now state

Proposition 5.3.1. *Let w be defined by (5.3.1). Then*

$$\lim_{\nu\to\infty} ||w - w^{\nu}||_{L^{\infty}(Q^d,\mathbb{R}^d)} = 0; \tag{5.3.5}$$

if further one has

$$\sum_{m=1}^{\infty}\sum_{i} |\rho(\mu_m, \mu_m^i)|(1 + m^{2/d})^{1/2} < \infty \tag{5.3.6}$$

then also

$$\lim_{v\to\infty} ||w - w^{\nu}||_{w^{1,\infty}(Q^d,\mathbb{R}^d)} = 0. \tag{5.3.7}$$

Proof. (5.3.5) follows from the normalization of the eigenfunctions (φ_m) since

$$|w(x,p) - w^{\nu}(x,p)| \leq C \sum_{m=\nu+1}^{\infty}\sum_{i} |\rho(\mu_m, \mu_m^i)|. \tag{5.3.8}$$

Recall that ρ is positive and trace class, so the right side of (5.3.8) tends to zero as ν tends to infinity.

Using the estimate [22]

$$||\nabla\varphi_m||_{L^2(Q)} \leq (\gamma + Cm^{2/d}) \tag{5.3.9}$$

(with constants $C, \gamma > 0$) we get

$$\int (|\nabla_x w(x,p) - \nabla_x w^{\nu}(x,p)| + |\nabla_p w(x,p) - \nabla_p w^{\nu}(x,p)| dxdp$$

$$\leq C \sum_{m=\nu+1}^{\infty}\sum_{i} \rho(\mu_m, \mu_m^i)[||\nabla_x \varphi_m|| + 1] \tag{5.3.10}$$

which, together with (5.3.8), implies (5.3.7). Let us remark that in this case the eigenvalues satisfy the estimates [22]

$$C^{(1)}m^{2/d} + ||V||_{\infty} \leq \mu_m \leq C^{(2)}m^{2/d} + ||V||_{L^{\infty}}, \ (C^{(1)}, C^{(2)} > 0).$$

5.4 Discussion

The above discussion makes it evident that the classical BGK modes [31] could be generalized to include functions of all constants of the motion. The classic, stationary Vlasov equation is equivalent to

$$\{H_c, f(x,p)\} = 0 \tag{5.4.1}$$

where $\{\ ,\ \}$ is the Poisson bracket and H_c the classical hamiltonian. Since constants of the motion have vanishing Poisson brackets with the hamiltonian, any constants of the motion is a solution of (5.4.1) and, in fact, by the chain rule any joint function of all the constant of the motion is a solution. It is clear that any solution of (5.4.1) must be of this form. This fact has already been noted by Degond [64] and Rein [65].

We also remark that in the representation (5.3.4) different convergence properties might follow from different choice of the operator H^1, since H^1 is quite arbitrary (Ref. [60], p. 56). It could be important to choose a H^1 giving better convergence, particularly in the case of high degeneracy.

The eigenvalues μ_m and the φ_m which appear in Eq. (5.3.4) might be computed by applying minimax principles to the equation [22]

$$-\frac{1}{2}\Delta\varphi_m + (V(\Phi) + \widetilde{V})\varphi_m = \mu_m\varphi_m \tag{5.4.2a}$$

where

$$\Phi = (\varphi_m)_{m\in\mathbb{N}}. \tag{5.4.2b}$$

Here $\widehat{V}$ is a given (periodic) potential and $V(\Phi)$ is the self-consistent potential. In principal, (5.4.2a) could be solved as a finite system of linear equation (after truncation of the set (φ_m)) by iteration−then approximate eigenvalues and eigenfunctions appear in (5.3.4). An interesting, but open, question is whether QBGK modes are stable or ever asymptotically stable. Another unknown is the proper set of boundary conditions (if any) to make the solution unique.

It is not clear how these modes in general might be found from solving the stationary Wigner-Poisson system. (The above analysis indicates one how they might be constructed from solutions of the stationary Schrödinger-Poisson system; this construction might not even be unique, absent a proof of the uniqueness of the potential for the SP-system.)

One case in which a Wigner-type (i.e., pseudo-differential) equation can be constructed for w (at least in the linear case) is for $f(H, H^1; \beta) = exp\,(-\beta H)/Z$; here the partition function $Z = Tr\,exp(-\beta H)$, and β is the inverse temperature. Writing

$$\Omega = exp(-\beta H) \tag{5.4.3}$$

an equation for Ω, called the Bloch equation, can be derived by differentiating with respect to β [34].

$$\frac{\partial \Omega}{\partial \beta} = \frac{1}{2}(H\Omega + \Omega H) \tag{5.4.4a}$$

subject to

$$\Omega(\beta = 0) = 1. \tag{5.4.4b}$$

Applying the Wigner transform for products [33] to Eq. (5.4.4a) leads to a pseudo-differential equation for Ω_w:

$$\frac{\partial \Omega_w}{\partial \beta} = (p^2 - \frac{1}{4}\Delta_x)\Omega_w + B(V)\Omega_w \tag{5.4.5a}$$

where B is the PDO with symbol

$$\frac{1}{2}[V(x + \frac{\eta}{2}) + V(x - \frac{\eta}{2})]. \tag{5.4.5b}$$

This equation has been obtained by Steinrück and Odeh [66]. Using the Schrödinger-Poisson formalism, Arnold et al. [20] have proved existence and uniqueness of solutions to the Bloch equation (this amounts to proving uniqueness of the potential) under periodic boundary conditions, while Markowich [67] has done the same thing for the full space.

There are two problems with this whole approach to the stationary Wigner equation. The first is that, except for the canonical $f = e^{-\beta H}/Z$, in which case the Bloch equation is available, there is no way to calculate w from a given f without first having solved the Schrödinger system (cf. Eq. (5.3.1)), in which case the Wigner solution would be no longer be moot. The second difficulty is the fact that in the nonlinear case, V is a function β, so Eq. (5.4.4a) is not valid.

Chapter 6

The Eigenmatrix Problem

6.1 Introduction

In the present paper we study solutions to the periodic Schrödinger-Poisson (SP) System as treated in Ref. [10], except that we consider stationary states, i.e. solutions of the form ($\hbar = 1$)

$$\Psi(x,t) = e^{-i\boldsymbol{E}t}\Phi(x). \tag{6.1.1}$$

Here Ψ and Φ are vector functions [10], and $\boldsymbol{E}$ is a matrix.

The Schrödinger-Poisson system satisfied by Φ will be time-independent if certain conditions are satisfied by $\boldsymbol{E}$; this matrix is a generalization of the usual energy eigenvalue of elementary quantum mechanics.

This problem with constant $\boldsymbol{E}$ was studied in [68, 69]. The case in which $\boldsymbol{E}$ is a diagonal matrix has been considered in papers by Nier [21] and by Albinus et al.[70]. Nier has proved existence of unique solutions of the (SP) system for both periodic and Dirichlet data. His technique involves studying a variational problem for the potential V; a similar technique is used in [70], where only Dirichlet data are considered. Our technique involves the solution of the nonlinear eigenvalue problem for the Schrödinger equation using a fixed point argument; we restrict our attention to periodic boundary conditions.

We remark that we attach physical significance to the off-diagonal matrix elements of $\boldsymbol{E}$–as transition probabilities which obey a condition of detailed balance [40, p.33]. The eigenvalues of $\boldsymbol{E}$, denoted by μ_m, are taken to be the energies of the various eigenstates.

In this paper we prove that there exists at least one space-periodic solution (Φ,V) of the Schrödinger-Poisson eigenmatrix problem. In Sec. 6.2, the problem is formulated, necessary conditions for the eigenmatrix are derived and a diagonalization procedure is presented. In Sec. 6.3 we prove the existence theorem using a Schauder fixed-point argument, and derive bounds for the eigenvalues μ_m of $\boldsymbol{E}$. We also present an iteration scheme of linear equations for the approximations of the eigenvalues; using minimax principles, it is not necessary to solve for the eigenstates.

As one easily shows, the eigenmatrix does not appear in the stationary Wigner equation, so in this case the usual isomorphism between Schrödinger and Wigner equation [33] no longer holds. In fact, the stationary Wigner equation apparently does not have a unique solution, for example in that any function of the hamiltonian can generate a solution [71]. (These solutions are the analogue of the BGK modes formula in classical Vlasov theory [31].) For this reason, we restrict our attention to (SP).

According to a result of Nier [21], the potential V of (SP) is unique in the space $H^1_{per}(\mathrm{Q})/\mathbb{R}$, where $Q = Q_L$ is the cube $[0, L]^d \subset \mathbb{R}^d$, $d = 1, 2, 3$.

6.2 Formulation of the Problem

The (SP) system describes the time evolution of the vector $\Psi = (\psi_m)_{m\in\mathbb{N}}$. It can be written (see, for example, Refs. [8] and [9]).

$$i\Psi_t = -\frac{1}{2}\triangle\Psi + V(\Psi)\Psi + \tilde{V}\psi \tag{6.2.1a}$$

$$-\triangle V(\Psi) = n_\Psi - n_D \tag{6.2.1b}$$

$$n_\Psi(x,t) = \sum \lambda_m |\psi_m|^2 \tag{6.2.1c}$$

$$0 \le \lambda_m \le 1, \sum \lambda_m = 1. \tag{6.2.1d}$$

We shall denote by Λ the sequence $(\lambda_m)_{m\in\mathbb{N}}$. The system (6.2.1) is to be solved subject to periodic boundary conditions on the cube Q_L; λ_m is the probability of the state λ_m. $\tilde{V}$ is a given external potential depending only on x, while n_D is a given background charge density, also depending only on x. Assumptions on $\tilde{V}$ and n_D are given in Sec. 6.3. This system, or similar systems, has been used to model various semiconductor devices for which quantum effects are important [72, 73, 74].

We study (SP) in the Hilbert spaces Y^3 (see Sec. 6.3) and

$$X^k_\Lambda = \{\Psi = (\psi_m)_{m\in\mathbb{N}} | \psi_m \in H^k_{loc}(\mathbb{R}^d);\ \forall x \in Q_L, \forall m \in \mathbb{N}, \forall \ell \in \mathbb{Z}^d,$$
$$\psi_m(x + \ell L) = \psi_m(x)\} \tag{6.2.2}$$

(The periodicity condition is understood in the L^2 sense.) The inner product in X^k_Λ is

$$(\Psi, \Phi)_{k,\Lambda} = \sum_{m=1}^{\infty} \lambda_m \sum_{|\alpha| \le k} (\partial^\alpha \psi_m, \partial^\alpha \phi_m)_{L^2(Q_L)}. \tag{6.2.3}$$

When we substitute (1.1) into (6.2.1), write $\Phi = (\phi_m)_{m\in\mathbb{N}}$,we should like to recover a stationary equation. Noting Eqs. (6.2.1b) are (6.2.1c), this requires that $\boldsymbol{E}$ be self-adjoint in the Hilbert space

$$\ell^2_\Lambda = \left\{ \xi = (\xi_m)_{m\in\mathbb{N}} | \ \sum_{n=1}^{\infty} \lambda_n |\xi_n|^2 < \infty \right\} \tag{6.2.4a}$$

with inner product

$$(\zeta, \eta)_\Lambda = \sum_{m=1}^{\infty} \lambda_m \zeta_m \bar{\eta}_m. \tag{6.2.4b}$$

Then $e^{i\boldsymbol{E}t}$ will be unitary in ℓ^2_Λ and [cf. (6.2.1c)] $n_\Psi = n_\Phi$, implying $V(\Psi) = V(\Phi)$.

A simple calculation shows that $\boldsymbol{E}$ will be self-adjoint in ℓ^2_n if and only if

$$\lambda_n \bar{\boldsymbol{E}}_{nk} = \lambda_k \boldsymbol{E}_{kn}. \tag{6.2.5}$$

If we interpret $\boldsymbol{E}_{nk}$ as a transition matrix element from the state ϕ_n to the state ϕ_k, then (6.2.5) is the condition of microscopic irreversibility or "detailed balance"[40, 75].

The following set, then, is obtained for Φ:

$$-\frac{1}{2}\triangle\Phi + V(\Phi)\Phi + V\Phi = \boldsymbol{E}\Phi \tag{6.2.6a}$$

$$-\triangle V(\Phi) = n_\Phi - n_D \tag{6.2.6b}$$

where the unitarity of $e^{i\boldsymbol{E}t}$ on ℓ^2_Λ has been used. In addition to the detailed balance condition on $\boldsymbol{E}$, we need to assume that $\boldsymbol{E}$ has a pure point spectrum in ℓ^2_Λ in order to prove existence of solutions.

With these assumptions, $\boldsymbol{E}$ can be diagonalized by a unitary transformation U on ℓ^2_Λ such that

$$U^{-1}\boldsymbol{E}U = M = diag\,(\mu_m)_{m\in\mathbb{N}} \tag{6.2.7a}$$

and

$$\tilde{\Phi} = U^{-1}\Phi \tag{6.2.7b}$$

(so that the solution we seek is $U\,\tilde{\Phi}$). We arrive at the same set of equations (6.2.6) for $\tilde{\Phi}$, but with $\boldsymbol{E}$ replaced by M (noting that V is invariant under U). For convenience we write Φ instead of $\tilde{\Phi}$. Then the equations we wish to solve are

$$-\frac{1}{2}\triangle\phi_m + V(\Phi)\phi_m + \tilde{V}\phi_m = \mu_m\phi_m \tag{6.2.8a}$$

$$-\triangle V(\Phi) = n_\Phi - n_D \tag{6.2.8b}$$

$$n_\Phi = \sum \lambda_m (\mu_m)|\phi_m|^2. \tag{6.2.8c}$$

For the time-dependent problem, the set $\Lambda = (\lambda_m)_{m\in\mathbb{N}}$ is datum [8, 9]. For the eigenproblem, on the other hand, the λ_m are functions of the energy eigenvalues μ_m, for example the Fermi distribution [21, 70, 72, 73]. We always have to enforce the normalization $\sum_{m\in\mathbb{N}} \lambda_m(\mu_m) = 1$. Other distributions beside the Fermi one could be used (for example the Boltzmann distribution $\sim e^{-\mu_m}$). It is merely required that the $\lambda_m(M)$ be strictly monotonically decreasing sufficiently rapidly (plus some other regularity assumptions).

6.3 The Fixed-Point Argument

We begin by defining sequence spaces $\ell(\boldsymbol{F})$ as the set of all sequences $\phi = (\varphi_m)_{m\in\mathbb{N}}$, $\varphi_m \in \boldsymbol{F}$ where $\boldsymbol{F}$ is a Banach space. With the metric

$$d(\phi,\psi) = \sum_{j=1}^{\infty} 2^{-j} \frac{||\varphi_j - \psi_j||_F}{1 + ||\varphi_j - \psi_j||_F}$$

$\ell(\boldsymbol{F})$ is a Fréchet space (i.e., a complete locally convex metric space; cf. [76, p.287], and [77, p.54]; for a Cartesian product of sequence spaces, we impose the Cartesian product metric.)

Let

$$Y^k = \ell(H^k_{per}(Q_L)) \times \ell(\mathbb{R}), \qquad k \in \mathbb{N}_0 = \mathbb{N} \cup \{0\}.$$

To define the operator T whose fixed point we seek in Y^1, some technical assumptions are necessary on the functions $\lambda_m(t)$ for dimensions $d = 1, 2, 3$: Let

$$\lambda_m(t) = \frac{\tilde{\lambda}_m(t)}{\Lambda(t)} \tag{6.3.1a}$$

where

$$\Lambda(\mu) := \sum_{m\in\mathbb{N}} \tilde{\lambda}_m(\mu_m), \tag{6.3.1b}$$

with $t \in \mathbb{R}$, $\mu = (\mu_m)_{m\in\mathbb{N}}$. Then we assume

(Λ_1): For each $m \in \mathbb{N}$, $\tilde{\lambda}_m(t)$ is a continuous, positive, decreasing function of t;

(Λ_2): $0 < c^* := \sum_{m\in\mathbb{N}} \tilde{\lambda}_m(t)\,(\frac{c^{(1)}}{2L^2}m^{2/d})m^{1/2} < \infty$ where $c^{(1)} > 0$ is a universal constant to be specified later (Lemma 6.3.2); let us define $\mu^{(j)}(\gamma)$, $j = 1, 2$, by $\mu_m^{(1)}(\gamma) = \frac{c^{(1)}}{L^2}m^{2/d} - \gamma$, $\mu_m^{(2)}(\gamma) = \frac{c^{(2)}}{L^2}m^{2/d} + \gamma$, where $c^{(2)} > 0$ is another universal constant also introduced in Lemma 6.3.2;

(Λ_3): $n_D \in L^2_{per}(Q_L)$, $\tilde{V}$ real,and $\tilde{V} \in L^\infty_{per}(Q_2)$.

Let us note some consequences of (Λ_1) and (Λ_2). First, we have

$$0 < \tilde{c} := \Lambda(\tilde{\mu}) \leq c^* < \infty \tag{6.3.2a}$$

for $\tilde{\mu} = (\tilde{\mu}_m)$, $\tilde{\mu}_m := \frac{c^{(1)}}{2L^2}m^{2/d}$. Also, for all $\gamma > 0$

$$0 < \Lambda(\mu^{(1)}(\gamma)) < \infty \tag{6.3.2b}$$

since, with $N(\gamma) := [\frac{2L^2}{c^{(1)}}\gamma]^{d/2}$

$$\sum_{m\geq N(\gamma)} \tilde{\lambda}_m(\mu_m^{(1)}(\gamma)) \leq \sum_{m\geq N(\gamma)} \tilde{\lambda}_m\,(\frac{c^{(1)}}{2L^2}m^{2/d}) \leq \tilde{c}\,,$$

so that

$$0 < \Lambda(\mu) < \infty \tag{6.3.2c}$$

for any sequence $\mu = (\mu_m)$ s.t. $\mu_m \geq \mu_m^{(1)}(\gamma)$. (Furthermore, let us mention that (Λ_1) could be weakened to include cases where $\tilde{\lambda}_m(t)$ are non-negative, but we do not consider this here.)

The most important special case where (Λ_1), (Λ_2) are satisfied is that of the Fermi function:

$$\tilde{\lambda}_m(t) = \frac{c_m}{e^{\alpha(t-\mu_F)} + 1}$$

with a bounded, strictly positive sequence (c_m) which contains physical parameters such as mass, temperature, Boltzmann and Planck constants, etc. α is the inverse temperature and μ_F is the so-called Fermi level.

Lemma 6.3.1. *Let $(\Phi, \mu) \in Y^1$ and $||\Phi||^2_{L^4} := \sum_{m\in\mathbb{N}} \lambda_m(\mu_m)||\phi_m||^2_{L^4(Q)} < \infty$. Then the Poisson equation (6.2.8b) has a solution $V \in H^2_{per}(Q_L)/\mathbb{R}$ s.t.*

$$||V||_{L^\infty} \leq V_0 + CL^2\{||n_0||_{L^2} + ||\Phi||^2_{L^4}\} \tag{6.3.3}$$

with a generic constant $C > 0$ and an arbitrary constant $V_0 \geq 0$.

Proof. Let $\tilde{n} = n_\Phi - n_D$ [cf. (6.2.1b)]. Then introducing the Fourier basis $\{h_k\}_{k\in\mathbb{Z}^d}$ with $h_k(x) = L^{-d/2} \exp\left(\frac{2\pi i}{L} k \cdot x\right)$, the Fourier coefficients of $\tilde{n} = n_\Phi - n_D$ are

$$\tilde{n}_k = (\tilde{n}, h_k) = \int_0^L \tilde{n}_k(x)\bar{h}_k(x)dx.$$

Then

$$V = V_0 + \frac{L^2}{4\pi^2} \sum_{k\in\mathbb{Z}^d\setminus\{0\}} \frac{\tilde{n}_k}{k^2} h_k \quad (V_0 \in \mathbb{R})$$

is a solution of (6.2.8b) in $H^2_{per}(Q_L)$. (Note that the charge neutrality condition implies $\tilde{n}_0 = 0$.) The L^∞ estimates follows from

$$||V||_{L^\infty} \leq ||V_0||_{L^\infty} + \frac{L^2}{4\pi^2}\{\sum_{k\in\mathbb{Z}^d\setminus\{0\}} \frac{1}{k^4}\}^{1/2}\{\sum_{k\in\mathbb{Z}^d} |\tilde{n}_k|^2\}^{1/2}$$

and

$$\{\sum_{k\in\mathbb{Z}^d} |\tilde{n}_k|^2\}^{1/2} = ||\tilde{n}||_{L^2} \leq ||n_D||_{L^2} + ||n_\Phi||_{L^2}$$

$$\leq ||n_D||_{L^2} + \sum \lambda_m(\mu_m)||\phi_m||^2_{L^4}.$$

Lemma 6.3.2. *Let $V \in L^\infty_{per}(Q_L)$ and real. Then the linear eigenvalue system*

$$-\frac{1}{2}\Delta\varphi_m + V\varphi_m = \mu_m\varphi_m,\ m \in \mathbb{N} \tag{6.3.4}$$

has a solution sequence $(\Phi,\mu) \in Y^2$ where $\Phi = (\varphi_m)_{m\in\mathbb{N}}$ is an orthonormal system in $L^2_{per}(Q)$; the eigenvalues $\mu = (\mu_m)_{m\in\mathbb{N}}$ are real, arranged in increasing order and fulfill $\mu_m \to \infty$ for $m \to \infty$. Furthermore, there are positive generic constants $c^{(1)}$, $c^{(2)} > 0$ such that the estimate

$$-||V||_\infty + \frac{c^{(1)}}{L^2} m^{2/d} \leq \mu_m \leq \frac{c^{(2)}}{L^2} m^{2/d} + ||V||_\infty \tag{6.3.5}$$

is valid.

Proof. The existence follows from well-known results of the theory of elliptic differential equations [79] and the minimax characterization of eigenvalues of self-adjoint linear operators (see [79, p.446 ff.] or [80]). In the proof of (6.3.5), we first consider the case V= 0 and $L = 2\pi$. Then the proof of the lower bound in (6.3.5) can be found in Ref. [79] (Appendix, Prop. 4.1). Using similar notation and counting the eigenvalues according to multiplicity we have (still for $V = 0$)

$$0 \le \mu_1 \le \mu_2 \le ... \le \mu_m \le, ..., \mu_m \to \infty \, for \; m \to \infty. \tag{6.3.6}$$

We define for $p \in \mathbb{N}_0 = \mathbb{N} \cup \{0\}$

$$\mathcal{E}_p = \Big\{ \ell \in \mathbb{N}_0^d | \sum_{\substack{\alpha \in \mathbb{N}_0^d \\ |\alpha|=1}} \ell_1^{2\alpha_1} + ... + \ell_d^{2\alpha_d} \le p \Big\} \tag{6.3.7}$$

(for $d = 1, 2, 3$); let N_p be the cardinality of $\mathcal{E}_p$. By definition $\mathcal{E}_p$ consist of μ_1,...,μ_{N_p}, thus $\mu_{N_p} \le N_p$. We now prove the inequality

$$N_p \ge c^* p^{d/2} \tag{6.3.8}$$

with a finite constant $c^* > 0$ (depending only on d). Let Q^* be the largest cube with center at zero inscribed in the ball with center at zero and radius $\sqrt{p}$. The side L^* of this cube is proportional to $\sqrt{p}$. This implies that there are at least $([L^*] + 1)$ eigenvalues in the ball. This proves (6.3.8).

Now let m be given and let q be the smallest integer $\ge (\frac{m}{c^*})^{2/d}$; further, set $q_1 = [c^* q^{d/2}]$. Then $m \le q_1$ and by monotonicity we arrive at

$$\mu_m \le \mu_{q_1} \le \mu_{N_q} \le q < (\frac{m}{c^*})^{2/d} + 1 \le cm^{2/d}.$$

Here we have used $q_1 \le N_q$ together with (6.3.7) for the case $V = 0$.

Applying both the minimax method and the comparison principle for eigenvalues [79],[80], we see that (6.3.5) follows for any bounded potential V, the constants depending only on d (for the case $L = 2\pi$). For arbitrary L, (6.3.5) is obtained by a simple scaling argument.

Remark. We may write (6.3.5) also in the form

$$-||V||_\infty + c^{(1)}(\frac{m}{|Q_L|})^{2/d} \le \mu_m \le ||V||_\infty + c^{(2)}(\frac{m}{|Q_L|})^{2/d}.$$

We now introduce the fixed point operator T and the set $S \subset Y^1$ s.t.
$T : S \to S$ has a fixed point in S. Let $\gamma \ge \gamma_0$ be a positive constant to be specified later and $c^{(1)}$, $c^{(2)}$ be the constants from Lemma 6.3.2; $\mu^{(1)}(\gamma) = (\mu_m^{(1)}(\gamma))$ as defined in (Λ_2). Then set

$$\begin{aligned} S = S_\gamma = \{(\Phi, \mu) \in Y^1 | \Phi = (\varphi_m)_{m\in\mathbb{N}},\, \mu = (\mu_m)_{m\in\mathbb{N}},\, ||\varphi_m||_{L^2} \le 1; \\ ||\nabla\varphi_m||_{L^2} \le K_m(\gamma) = (\gamma + \frac{2c^{(2)}}{L^2} m^{2/d})^{1/2},\, \mu_m^{(1)}(\gamma) \le \mu_m,\, \forall m \in \mathbb{N}\}. \end{aligned} \tag{6.3.9}$$

Evidently S is a convex subset of Y^1. For $(\Phi, \mu) \in S$, let

$$T(\Phi, \mu) = (\tilde{\Phi}, \tilde{\mu})$$

where $\tilde{\Phi} = (\pm\tilde{\varphi}_m)_{m\in\mathbb{N}}$, $\tilde{\mu} = (\tilde{\mu}_m)_{m\in\mathbb{N}}$ with $\tilde{\varphi}_m$ and $-\tilde{\varphi}_m$ associated with the same $\tilde{\mu}_m$ $(\forall_m \in \mathbb{N})$; the (φ_m, μ_m) are the orthonormal solutions of the linear eigenvalue problem

$$-\frac{1}{2}\Delta\tilde{\varphi}_m + (V(\Phi) + \tilde{V})\tilde{\varphi}_m = \tilde{\mu}_m\tilde{\varphi}_m \tag{6.3.10}$$

$(\forall m \in \mathbb{N})$ with L-periodic boundary conditions on Q where $V(\Phi)$ is given by Poisson's equation (6.2.8b). Later, in proving continuity of T, we are confronted with the fact that both $\tilde{\varphi}_m$ are normalized eigenfunctions with the same eigenvalue $\tilde{\mu}_m$, a fact which must be incorporated into the definition of T, but in proving the other properties of Lemma 6.3.3 we will ignore it (since S_γ is invariant under the transformation $\varphi_m \to -\varphi_m$). From Lemmata 6.3.1 and 6.3.2 it follows that T is well-defined on S.

Lemma 6.3.3. *Let conditions* (Λ_1)–(Λ_3) *hold. Then there is a constant* $\gamma > 0$ *s.t.* $T(S_\gamma) \subset S_\gamma$. *Further,* T *is continuous on* S_γ *and* $T(S_\gamma)$ *is relatively compact on* Y^1.

For the proof of the crucial Lemma 6.3.3 we need the technical

Lemma 6.3.4. *There exists a generic constant* $C > 0$ *(not depending on* L*) such that for any* $\varphi \in H^1_{per}(Q_L)$

$$||\varphi||_{L^4_{(Q_L)}} \leq C\Big\{L^{d/4}||\varphi||_{L^2_{(Q_L)}} + ||\nabla\varphi||^{d/4}_{L^2(Q_L)}||\varphi||^{1-d/4}_{L^2(Q_L)}\Big\}. \tag{6.3.11}$$

Proof. The result follows from the Gagliardo–Nirenberg inequality [10] [78] for functions with mean value zero. The independence of C on L follows from a scaling argument.

Proof *(of Lemma 6.3.3).* Let $(\Phi, \mu) \in S_\gamma$ with $\gamma > \gamma_0$ [cf. (Λ_1)–(Λ_3)]. Choosing $V_0 = 0$ in Lemma 6.3.1, using the definition of S_γ and Eq. (6.3.2) we get that $\sum_{m\in\mathbb{N}}\tilde{\lambda}_m(\mu_m)$ converges (since $\mu_m \geq \mu^{(1)}_m(\gamma)$). Thus $\sum_{m\in\mathbb{N}}\lambda_m(\mu_m) = 1$ and furthermore

$$\begin{aligned}4||V(\Phi)||_{L^\infty} &\leq 4CL^2\{||n_D||_{L^2} + C^2\sum_{m\in\mathbb{N}}\lambda_m(\mu_m)[L^{d/4} + K^{d/4}_m]^2\}\\ &\leq 4CL^2||n_D||_{L^2} + 8C^3L^2\sum_{m\in\mathbb{N}}\lambda_m(\mu_m)(\gamma + \frac{2c^{(2)}}{L^2}m^{2/d})^{d/4}. \end{aligned}\tag{6.3.12}$$

If we denote the last term in (6.3.12) by J we have $J = J_1 + J_2$, where J_1 is the sum over all $m \leq N(\gamma)$ and J_2 the remainder. [See (6.3.2b) for the definition of $N(\gamma)$.]

Now we arrive at

$$J_1 \leq \sum_{m \leq N(\gamma)} \lambda_m(\mu_m)[1 + \frac{4c^{(2)}}{c^{(1)}}]^{d/4} \gamma^{d/4} \leq \tilde{c}_1 \gamma^{d/4} \tag{6.3.13}$$

(with $\tilde{c}_1 := (1 + \frac{4c^{(2)}}{c^{(1)}})^{d/4}$),

$$J_2 \leq \sum_{m \geq N(\gamma)} \lambda_m(\mu_m)[\frac{c^{(1)}}{L^2} + \frac{2c^{(2)}}{L^2}]^{d/4} m^{1/2}$$

$$\leq \frac{\tilde{c}_2 \sum_{m \geq N(\gamma)} \tilde{\lambda}_m(\frac{c^{(1)}}{2L^2} m^{2/d}) m^{1/2}}{\sum_{m \leq N(\gamma)} \tilde{\lambda}_m(\frac{c^{(1)}}{2L^2} m^{2/d})}, \tag{6.3.14}$$

(where $\tilde{c}_2 := [c^{(1)} + 2c^{(2)}]^{d/4} L^{-d/2}$).

By (6.3.2a) we can choose an appropriate $\gamma_0 > 0$ s.t. for $\gamma \geq \gamma_0$ the sum in the denominator of (6.3.14) is $\geq \tilde{c}/2$; then using (Λ_2) we get

$$J_2 \leq 2\tilde{c}_2 \frac{c^*}{\tilde{c}}$$

which finally implies that for all $\gamma \geq \gamma_1 \geq \gamma_0$ (with an appropriate γ_1)

$$4||V(\Phi)||_{L^\infty} + 4||\tilde{V}||_{L^\infty} \leq 4||\tilde{V}||_{L^\infty} + 4CL^2||n_D||_{L^2}$$
$$+ 8C^3 L^{d/2+2} + C^3 L^2 \tilde{c}_2 \frac{c^*}{\tilde{c}} + 8C^3 L^2 \tilde{c}_1 \gamma^{d/4} \leq \gamma \tag{6.3.15}$$

From Lemma 6.3.2, we get, for all $m \in \mathbb{N}$

$$\frac{1}{2} \int_Q |\nabla \varphi_m|^2 dx = -\int_Q (V(\Phi) + \tilde{V})|\varphi_m|^2 dx + \tilde{\mu}_m. \tag{6.3.16}$$

Since by Lemma 6.3.2 we have also

$$\tilde{\mu}_m \leq \frac{c^{(2)}}{L^2} m^{2/d} + ||\tilde{V}||_{L^\infty} + ||V(\Phi)||_{L^\infty}$$

we obtain from (6.3.16) and (6.3.15) for all $m \in \mathbb{N}$

$$||\nabla \tilde{\varphi}_m||^2_{L^2} \leq 4||V(\Phi)||_{L^\infty} + 4||\tilde{V}||_{L^\infty} + \frac{2c^{(2)}}{L^2} m^{2/d}$$
$$\leq \gamma + \frac{2c^{(2)}}{L^2} m^{2/d} \leq K_m^2.$$

Thus, we have again by Lemma 6.3.2 and Eq. (6.3.15) that $||\tilde{\varphi}_m||_{L^2} = 1$ and

$$\tilde{\mu}_m \geq \frac{c^{(1)}}{L^2} m^{2/d} - ||V(\Phi) + \tilde{V}||_{L^\infty}$$
$$\geq \frac{c^{(1)}}{L^2} m^{2/d} - (||V(\Phi)||_{L^\infty} + ||\tilde{V}||_{L^\infty}) \geq \frac{c^{(1)}}{L^2} m^{2/d} - \gamma = \mu_m^{(1)}(\gamma);$$

similarly, $\tilde{\mu}_m \leq \mu_m^{(2)}(\gamma)$. Thus $T(S_\gamma) \subset S_\gamma$.

We now show that $T(S_\gamma)$ is relatively compact in Y^1. Since Y^1 is a metric space, it is sufficient to show sequential compactness of $T(\Phi^{(N)}, \mu^{(N)}) = (\tilde{\Phi}^{(N)}, \tilde{\mu}^{(N)})$ for a sequence $(\Phi^{(N)}, \mu^{(N)})_{N\in\mathbb{N}} \subset S_\gamma$. Let $\Phi^{(N)} = (\varphi_m^{(N)})$, $\mu^{(N)} = (\mu_m^{(N)})$ and similarly for $\tilde{\Phi}^{(N)}$ and $\tilde{\mu}^{(N)}$. We show that the H^2–norm of each component sequence $(\tilde{\varphi}_m^{(N)})$, m fixed, is bounded. This follows from Lemma 6.3.2 and the definition of S_γ since

$$||\tilde{\varphi}_m^{(N)}||_{L^2} = 1, \quad ||\nabla \tilde{\varphi}_m^{(N)}||_{L^2} \leq K_m(\gamma).$$

From

$$-\frac{1}{2}\Delta\tilde{\varphi}_m^{(N)} + (V(\Phi^{(N)}) + \tilde{V})\tilde{\varphi}_m^{(N)} = \tilde{\mu}_m^{(N)}\tilde{\varphi}_m^{(N)}$$

we obtain

$$||\Delta\tilde{\varphi}_m^{(N)}||_{L^2} \leq 2(||V(\Phi^{(N)})||_{L^\infty} + ||\tilde{V}||_{L^\infty}) + 2\,\tilde{\mu}_m^{(N)}$$
$$\leq \frac{\gamma}{2} + \frac{2c^{(2)}}{L^2} m^{2/d} + 2\gamma = 2K_m^2(\gamma) + \frac{\gamma}{2}. \tag{6.3.17}$$

Since H^2_{per} is compactly embedded in H^1_{per}, each component-sequence $(\tilde{\varphi}_m^{(N)})$ has a subsequence which converges in $H^1_{per}(Q_L)$; the same is true of the component-sequence $(\tilde{\mu}_m^{(N)})_{N\in\mathbb{N}}$, since by Lemma 6.3.2 we have an estimate of the type $|\tilde{\mu}_m^{(N)}| \leq \alpha_m$ ($\forall m \in \mathbb{N}$). By the definition of the topology of Y^1, a diagonalization procedure gives a subsequence of $(\tilde{\Phi}^{(N)}, \tilde{\mu}^{(N)})$ which converges in the topology of Y^1.

To prove continuity of T on S_γ, again it is enough to deal with sequences. Thus, let $(\Phi^{(N)}, \mu^{(N)}) \to (\Phi, \mu) \in S_\gamma$ on Y^1. We first show that

$$V(\Phi^{(N)}) \to V(\Phi) \tag{6.3.18}$$

in $L^\infty(Q)$; we have

$$-\Delta(V(\Phi^{(N)}) - V(\Phi)) = n_{\Phi^{(N)}} - n_\Phi$$

and by Lemma 6.3.1

$$||V(\Phi^{(N)}) - V(\Phi)||_{L^\infty} \leq C_L \sum_{m\in\mathbb{N}} \lambda_m(\mu_m^{(N)})|| \, |\varphi_m^{(N)}|^2 - |\varphi_m|^2||_{L^2}$$
$$+ C_L \sum_{m\in\mathbb{N}} |\lambda_m(\mu_m^{(N)}) - \lambda_m(\mu_m)| \, ||\varphi_m||_{L^4}^2 =: R_1^{(N)} + R_2^{(N)}.$$

We first see that

$$\Lambda(\mu^{(N)}) \to \Lambda(\mu), \; N \to \infty \tag{6.3.19}$$

because for any $\epsilon > 0$ there is an integer N_1 (which depends on ϵ) s.t. [cf. Eq. (6.3.2)]

$$2 \sum_{m\geq N_1+1} \tilde{\lambda}_m(\mu_m^{(1)}(\gamma)) < \epsilon/2;$$

now choose N_2 (depending on ϵ) s.t. for $m = 1, ..., N_1$

$$|\tilde{\lambda}_m(\mu_m^{(N)}) - \tilde{\lambda}_m(\mu_m)| < \frac{\epsilon}{2N_1} \text{ for all N } \geq N_2;$$

this gives

$$|\Lambda(\mu^{(N)}) - \Lambda(\mu)| \leq \sum_{m\leq N_1(\epsilon)} |\tilde{\lambda}_m(\mu_m^{(N)}) - \tilde{\lambda}_m(\mu_m)|$$
$$+ 2 \sum_{m\geq N_1(\epsilon)+1} \tilde{\lambda}_m(\mu_m^{(1)}(\gamma)) < \epsilon,$$

for $N \geq N_2$. This implies (6.3.19).

Using the definition of S_γ and Lemma 6.3.4 we get analogously (with same notation for N_1 and N_2 as above)

$$R_1^{(N)} \leq 2 \sum_{m\leq N_1} ||\varphi_m^{(N)} - \varphi_m||_{L^2}$$
$$+ C(\gamma) \frac{\sum_{m\geq N_1+1} \tilde{\lambda}_m(\mu_m^{(1)}(\gamma))}{\tilde{\lambda}_1(\mu_1^{(2)}(\gamma))} < \epsilon$$

for $N \geq N_2$. Also

$$
\begin{aligned}
R_2^{(N)} \leq C(\gamma) \sum_{m\in\mathbb{N}} & \frac{|\tilde{\lambda}_m(\mu_m^{(N)}) - \tilde{\lambda}_m(\mu_m)|}{|\Lambda(\mu^{(N)})|} \\
& + C(\gamma) \frac{|\Lambda(\mu^{(N)}) - \Lambda(\mu)|}{\Lambda(\mu^{(N)}) \cdot \Lambda(\mu)} \sum_{m\in\mathbb{N}} \tilde{\lambda}_m(\mu_m) \\
\leq & \frac{C(\gamma)}{\tilde{\lambda}_1(\mu_1^{(2)}(\gamma))} \Big\{ \sum_{m\leq N_1} + \sum_{m\geq N_1+1} \Big\} |\tilde{\lambda}_m(\mu_m^{(N)}) - \tilde{\lambda}_m(\mu_m)| \\
& + \tilde{c}(\gamma)|\Lambda(\mu^{(N)}) - \Lambda(\mu)| < \epsilon
\end{aligned}
$$

for $N \geq N_2$. This implies (6.3.18).

Let us now assume that there is a subsequence of $(\tilde{\Phi}^{(N)}, \tilde{\mu}^{(N)})_{N\in\mathbb{N}}$ which does not converge to $(\tilde{\Phi}, \tilde{\mu})$ in Y^1. (We denote the subsequence with the same notation as the sequence.)

By the compactness of $T(S_\gamma)$ we may assume that $(\tilde{\Phi}^{(N)}, \tilde{\mu}^{(N)}) \to (\Psi, \nu) \in S_\gamma$ in Y^1 for $N \to \infty$. Since $V(\Phi^{(N)}) \to V(\Phi)$ in $L^\infty(Q_L)$ for $N \to \infty$ [using (6.3.22)], the (ψ_m, ν_m) are weak solutions of the normalized eigenvalue problem for the Schrödinger operator $-\frac{1}{2}\Delta + (V(\Phi)+\tilde{V})$, (with L-periodic boundary conditions on Q, and then by elliptic regularity theory are also strong solutions in $H^2_{per}(Q_L)$(cf. Ref. [78]). This implies that up to a possible reordering, the $(\pm\psi_m, \nu_m)$ are equal to the $(\pm\tilde{\varphi}_m, \tilde{\mu}_m)$, that is $(\tilde{\Phi}^{(N)}, \tilde{\mu}^{(N)}) \to (\tilde{\Phi}, \tilde{\mu})$ which is a contradiction. This concludes the proof of the Lemma.

Using the Schauder-Tychonov fixed-point theorem for locally convex topological vector spaces (see [81, p.230]) we conclude from Lemma 6.3.3

Theorem 6.3.5. *Let $(\Lambda_1) - (\Lambda_3)$ hold, and let $d = 1, 2, 3$. Then the Schrödinger-Poisson eigenvalue problem (6.2.8) has a solution (Φ, μ) in Y^2.*

From the Theorem, the definition of S_γ and (6.3.17) follows

Corollary 6.3.6. *Let the assumptions of Theorem 6.3.5 be true, and assume furthermore that*

$$\sum_{m\in\mathbb{N}} \tilde{\lambda}_m(\tilde{\mu}_m) m^{\frac{2k}{d}} < \infty,\ k = 1, 2 \tag{6.3.20}$$

with and $\tilde{\mu}$ as in (6.3.2a). Then the solution (Φ, μ) satisfies $\Phi \in X^k_\Lambda$ (cf. Definition (6.2.2)-(6.2.3)) and the same is true for any solution of the (SP) eigenmatrix problem (6.2.6) which is derived from Φ by a unitary transformation of the type (6.2.7b).

Remarks. Property (6.3.20) holds for the Fermi function for all $k \in \mathbb{N}$; this gives higher-order regularity of the eigensolution Φ if the data $\tilde{V}$ and n_0 are sufficiently regular.

Theorem 6.3.5 is true also for $d \geq 4$ under certain smallness assumptions on the data (e.g., the period L or n_{D} or $\tilde{V}$).

Chapter 7

Inflow Boundary Conditions

7.1 Introduction.

In the development of various types of semiconductor devices, the crucial information needed by the design engineer is the $I-V$ curve, i.e. the current flowing through the device as a function of the applied voltage. Typically, such devices are non-ohmic and can, in fact, exhibit negative differential resistance, i.e. as the voltage increases through a certain range, the current can decrease (cf. Fig. 1, Ref. [82])

During the past decade, interest in quantum semiconductors has been particularly intense due to the development of devices which depend upon quantum phenomena for their operation (e.g. resonance-tunneling diodes) [82, 83] as well as to the emergence of microscopic devices (e.g. "quantum dots") [84] in which quantum mechanics enters due to the omnipresence of boundaries.

To deal with quantum semiconductors a popular approach has been the Wigner equation (WE) or, more generally, the Wigner-Poisson (WP) system of equations [33]. (WE) refers to a linear system, i.e., with a given potential, while (WP) involves a self-consistent Coulomb force. These systems may be considered quantum versions of the classical Vlasov transport equation (or Vlasov-Poisson system in the nonlinear case).

Many studies of (WP) have been carried out for the whole space [8, 9]. But for modeling semiconductors, one must deal with finite geometry, and hence the problem of boundary conditions must be faced. Periodic boundary conditions were considered in Ref. [10]. (See the bibliography there for further references.)

Since the Wigner equation is supposed to be simply a reformulation of quantum mechanics as expressed by the Schrödinger equation [33], one would expect that the appropriate boundary conditions for the former should be those induced, through the definition of the Wigner function, by self-adjoint boundary conditions on the quantum hamiltonian. Examples of such boundary conditions are Floquet ($\psi(x+1) = e^{i\alpha}\psi(x), \alpha \in \mathbb{R}$); Neumann and Dirichlet. (Note $\alpha = 0$ in the Floquet case corresponds to the periodic boundary conditions mentioned earlier.)

None of these conditions, for one reason or another, can be lifted satisfactorily to the Wigner equation (see Ref. [85] for a complete discussion); thus something else must be sought, for example the inflow conditions used in Refs. [82] and [83]. A modified version of the inflow conditions, so-called absorbing boundary conditions [40, 26, 1] are sometimes used to avoid spurious reflections at boundaries, but such conditions will not be considered here. To try to understand the (non-quantum) origin of inflow conditions, recall [33] the formula connecting the Wigner function $w(x, v, t)$ with the Schrödinger wave-function ψ (in the one-dimensional case):

$$w(x, v, t) = \frac{1}{2\pi} \int_{\mathbb{R}} e^{i\eta v} \overline{\psi}(x + \frac{\eta}{2}, t)\psi(x - \frac{\eta}{2}, t)\, d\eta.$$

Inflow conditions at $x = 0$ (specification of $w(0, v, t)$ for $v > 0$) arise from a pure incoming wave

$$\int w_+(v) e^{ivx}\, dv, \;\; v > 0$$

for *all* x, not solely for $x < 0$. So inflow conditions are definitely non-quantum.

Nonetheless we have decided to use the inflow conditions [40]. These, common in transport theory, specify the incoming distribution of particles at free surfaces. We take the point of view that the Wigner equation is an entity unto itself separately from its origin in the Schrödinger equation, and seek to determine whether or not it is well-posed with inflow conditions. In Ref. [4] this problem was treated for the time-dependent case, with homogeneous inflow conditions, while in Ref. [86] the existence of unique mild solutions for the time-dependent nonlinear equation with inhomogeneous inflow data was proved for a crystal lattice with the velocity restricted to the first Brillouin Zone. In this paper, we consider the linear time-dependent and stationary equations (with emphasis on the latter) for both bounded and unbounded velocity domains.

In order to help clarify the situation for (WE), we begin (in Sec. 7.2) with a brief discussion of the classical linear Vlasov equation (VE), and continue with the non-stationary (WE) in Sec. 7.3. Adopting a relaxation-time model [14, 15] for the time-dependent equation, we are able to show exponential decay to a solution of the stationary equation. In Sec. 7.3, we discuss solutions of the stationary (WE); they are known to exist, and they are called BGK modes [31] in the case of (VE), and QBGK modes for (WE) [87]. They are not unique. In fact, the non-uniqueness corresponds to "trapped particles" in the classical case [88] and the analogue thereof in the quantum case (bound states). We have been able to prove the existence of a weak solution for the stationary equation with inflow boundary conditions, but the current may not be defined unless the solution possesses sufficient additional regularity in which case the current exists and is constant. If we restrict our attention to the first Brillouin Zone, as in Ref. [86], we obtain strong solutions and unique existence of the current. In the

Appendix we discuss some deficiencies of the relaxation time model and discuss a better model. We hope eventually to detail results for (VP) and (WP) similar to those presented here. In fact, it is not even obvious that the linear Wigner equation has any advantage over the ordinary Schrödinger theory, so this work might be considered a first step toward dealing with the (nonlinear) (WP) system.

7.2 Remarks on the linear Vlasov Equation.

Henceforth we restrict our attention to one-dimensional systems as representing reasonable models of most semiconductor devices. Our remarks on the (VE) problem are motivated by the fact that we use some similar ideas for the Wigner equation. The relevant equation, with a relaxation-time scattering model, can be written (with the electron charge $= -1$)

$$\frac{\partial f}{\partial t} + v\frac{\partial f}{\partial v} - V'(x)\frac{\partial f}{\partial v} + \frac{f}{\tau} = \frac{f_0}{\tau}. \tag{7.2.1}$$

Here $f = f(x,v,t), x \in [0,1], v \in \mathbb{R}, t \in \mathbb{R}^+; \tau$ is the relaxation time. The relaxation distribution, $f_0(x,v)$ is assumed to obey the corresponding stationary equation.

$$v\frac{\partial f_0}{\partial x}(x,v) - V'(x)\frac{\partial f_0}{\partial v} = 0, \tag{7.2.2}$$

with $f_0 \in L^2([0,1] \times \mathbb{R}_v)$.

Arnold [14, 15] has already noted that f_0 should be position-dependent. In the solid-state physics literature [89] (and in Ref. [40]) f_0 is taken constant in space. Eq. (7.2.1) is to be solved subject to the conditions

$$f(x,v,0) = f_I(x,v) \tag{7.2.3}$$
$$f(0,v,t) = f_I(0,v) = f_+(v) \qquad v > 0 \tag{7.2.4}$$
$$f(1,v,t) = f_I(1,v) = f_-(v) \qquad v < 0 \tag{7.2.5}$$

with $f_I \in X, f_+, f_- \in L^2(\mathbb{R}_v)$ where solutions are sought in the space

$$X = L^2([0,1] \times \mathbb{R}_v)\,. \tag{7.2.6}$$

Assuming sufficient regularity, for instance strong solutions which lie in the domain of the linear operator

$$A = v\frac{\partial}{\partial x} - V'(x)\frac{\partial}{\partial v}\ , \tag{7.2.7}$$

one proves without too much difficulty

Proposition 7.2.1. *There exists a unique strong solution of Eq. (7.2.1) subject to (7.2.3)-(7.2.5).*

Proposition 7.2.2. *There exist classical solutions $f_0 \in D(A)$ to the stationary equation (7.2.2) subject to (7.2.4) and (7.2.5).*

The proof of Prop.7.2.2 involves the introduction of the BGK modes [87], i.e., arbitrary functions of the energy. (All solutions of (7.2.2) are BGK modes.) The energy, in turn, generates a set of characteristics to (7.2.2) which determine the solution uniquely on the non-periodic orbits originating from the inflow data. On the periodic characteristics, any function of the energy with sufficient regularity and compact support is a solution. These periodic solutions represent "trapped particles" [88] and are independent of the inflow. The solution is unique modulo these trapped particle solutions.

Proposition 7.2.3. *If $f, f_I, f_0 \in D(A)$ then $f(\cdot,\cdot,t) \to f_0$ in X as $t \to \infty$ where f is a strong solution to (7.2.1) and f_0 a classical solution to (7.2.2).*

Proposition 7.2.4. *Let $vf_0 \in L^1(\mathbb{R}_v)$. Then the stationary current calculated from the f_0 of Prop. 7.2.2 is unique.*

Proof. We have already pointed out that the solution is unique modulo trapped particles which obviously cannot contribute to the current, so the result is intuitively correct. It can be proved by integrating Eq.(7.2.2) over v; then since the current is given by

$$I(x) = -\int_{\mathbb{R}_v} v f_0(x,v)dv \tag{7.2.8}$$

it follows that

$$\frac{\partial I(x)}{\partial x} = 0; \tag{7.2.9}$$

the current is constant. Now take two different solutions with the same inflow data, $f_0^{(1)}$ and $f_0^{(2)}$. Then

$$f_0 = f_0^{(1)} - f_0^{(2)}$$

satisfies (7.2.2) with zero inflow. Multiply by f_0 and integrate to obtain

$$\int_{\mathbb{R}_v} v[f_0^2(1,v) - f_0^2(0,v)]dv = 0.$$

Since both terms are non-negative (by the zero inflow condition) both vanish. Thus, for example,

$$f_0^{(1)}(1,v) = f_0^{(2)}(1,v)$$

or from (7.2.8)

$$I^{(1)}(1) = I^{(2)}(1)$$

and since the current is constant, the proposition follows.

The above proof makes it clear that the current can be calculated from the solution for $v > 0$). (We obtain a similar result for the Wigner equation in Sec. 7.4.) In fact, in the classical case, the inflow data alone determines the current:

$$I = -\int_{\sqrt{2V_{max}}}^{\infty} v f_+(v)dv - \int_{-\sqrt{2V_{max}}}^{-\infty} v f_-(v)dv \tag{7.2.10}$$

for $V_{max} > 0$, where V_{max} is the maximum of the potential on [0,1]. This equation can sometimes be used as a figure of merit for the degree of "quantumness" of a semiconductor system; Eq.(7.2.10) does not hold for quantum systems due to tunneling and quantum reflection.

7.3 The Wigner Equation.

The equation we deal with is [33, 8, 9]

$$\frac{\partial w}{\partial t}(x,v,t) + v\frac{\partial w}{\partial x} - i\Theta(V)w(x,v,t) + \frac{w}{\tau} = \frac{w_0}{\tau}, \quad x \in [0,1]. \tag{7.3.1}$$

The velocity variable $v \in \mathbb{R}$ (Case 1) or $v \in B$, the first Brillouin zone (Case 2). As is pointed out in Ref. [86], defining the density (and, we should mention, the current) in Case 1 is "a major problem since L^1 estimate is usually not available." While this statement refers to the nonlinear problem, it appears to be equally valid for the linear case.

The definition of the pseudo-differential operator $\Theta(V)$ is, for Case 1,

$$(\Theta(V)w)(x,v,t) = \frac{1}{2\pi}\int_{\mathbb{R}_{v'}\times\mathbb{R}_k} e^{ik(v-v'}[V(x+\frac{k}{2}) - V(x-\frac{k}{2})]w(x,v',t)dv'dk \tag{7.3.2}$$

while for Case 2 it is defined as in Eq.(1.10) of Ref. [86]. Note that the potential must be extended beyond the interval $[0,1]$ for (7.3.2) to make sense.

Analogously to Sec. 7.2, in (7.3.1) w_0 is taken to be a solution of the stationary Wigner equation

$$v\frac{\partial w_0(x,v)}{\partial x} - i\Theta(V)w_0 = 0. \tag{7.3.3}$$

Eq. (7.3.1) is subject to conditions (7.2.3)-(7.2.5) and Eq. (7.3.3) is subject to (7.2.4) and (7.2.5).

In Ref. [10], the momentum was quantized due to the periodic boundary conditions. In the present, inflow, case no quantization is indicated, again verifying that our model, which does not derive from self-adjoint boundary conditions on a quantum hamiltonian, is at best quasi-classical [85]. The following results are formulated for Case 1, but are equally valid for Case 2, with $\mathbb{R}_v$ replaced by B.

Lemma 7.3.1. *$\Theta(V)$ is a bounded skew-adjoint operator on X. If $\Theta w(x,\cdot,t) \in L^1(\mathbb{R}_v)$, then*

$$\int (\Theta w)(x,v,t)dv = 0 \tag{7.3.4}$$

Proof. See lemmata 1 and 2 of Ref. [4] for the first statement. The second follows directly from integration of (7.3.3) an after obvious variable transformation.
Remark. The skew-adjoint property of Θ implies

$$\int w(x,v,t)(\Theta w)(x,v,t)dv = 0. \tag{7.3.5}$$

Introduce the operator Ω defined by

$$\Omega w = v\frac{\partial w}{\partial x} - i\Theta(V)w \tag{7.3.6}$$

defined on

$$D(\Omega) = \{w \in X \,|\, v\frac{\partial w}{\partial x} \in X,\ \text{w satisfies homogeneous inflow conditions}\} \tag{7.3.7}$$

Then

Proposition 7.3.2. *Ω generates a continuous semigroup of contractions $T(t)$ on X.*

Proof. It is proved in Lemma 6 of Ref. [4] that $-v\frac{\partial}{\partial x}$ generates a contraction semigroup on X. Since (Lemma 7.3.1) $i\Theta(V)$ is a bounded perturbation to $-v\frac{\partial}{\partial x}$, the result follows (see Ref. [46]).

Introduce the operator

$$Cw = v\frac{\partial w}{\partial x}, \quad D(C) = \{w \in X \,|\, Cw \in X\}. \tag{7.3.8}$$

We define a strong solution of (7.3.1) to be a function $w \in C([0,T];D(C)) \cap C^1([0,T];X)]$, where $D(C)$ is equipped with the graph norm, such that w obeys Eqs.(7.2.3)-(7.2.5). Then

Proposition 7.3.3. *A strong solution of (7.3.1) is unique.*

Proof. Assume, by way of contradiction, that there are two solutions w_1 and w_2 with the same data, and set $w = w_1 - w_2$. Then w obeys

$$\frac{\partial w}{\partial t} + v\frac{\partial w}{\partial x} - i\Theta(V)w + \frac{w}{\tau} = 0 \tag{7.3.9}$$

subject to zero initial and homogeneous inflow data. Multiply (7.3.9) by w and integrate over x, v, t to obtain

$$\frac{1}{2}||w(\cdot,\cdot,T)||_X^2 + \int_0^T \int_{\mathbb{R}_v} v[w^2(1,v,t) - w^2(0,v,t)]dvdt$$

$$+\frac{1}{\tau}\int_0^T ||w^2(\cdot,\cdot,t)||_X dt = 0. \tag{7.3.10}$$

(All operations used in obtaining (7.3.10) are allowed by the definition of strong solutions and by the fact that $vw(x,v,t)$ is a continuous function in X as is implied by Sobolev imbedding of vw.)

Since in (7.3.10) all terms are non-negative, it follows that $w = 0$, proving the result.

We seek solutions of (7.3.1) in the form

$$w(x,v,t) = w_h(x,v,t)e^{-t/\tau} + w_p(x,v) \tag{7.3.11}$$

where w_h is a strong solution of the homogeneous equation

$$\frac{\partial w_h}{\partial t}(x,v,t) + v\frac{\partial w_h}{\partial x} - i\Theta(V)w_h = 0 \tag{7.3.12}$$

with

$$w_h(x,v,0) = w_I(x,v) - w_p(x,v) \tag{7.3.13}$$

and homogeneous inflow data

$$w_h(0,v,t) = 0, \qquad v > 0 \tag{7.3.14}$$

$$w_h(1,v,t) = 0, \qquad v < 0. \tag{7.3.15}$$

Substituting into (7.3.1) gives the following equation for w_p :

$$v\frac{\partial w_p}{\partial x}(x,v) - i\Theta(V)w_p = \frac{w_0(x,v) - w_p(x,v)}{\tau}, \tag{7.3.16}$$

with boundary conditions

$$w_p(0,v) = w_+(v), \qquad v > 0 \tag{7.3.17}$$

$$w_p(1,v) = w_-(v), \qquad v < 0 \tag{7.3.18}$$

with $v\frac{\partial w_p}{\partial x} \in X$. We note that $w_p = w_0$ solves (7.3.16)-(7.3.18).

Proposition 7.3.4. *Let $w_I - w_p \in D(\Omega)$. Then there exists a unique global strong solution w_h to the system (7.3.12)-(7.3.15) such that $e^{-t/\tau}w_h(\cdot,\cdot,t) \to 0$ in X as $t \to \infty$.*

Proof. The global existence and uniqueness follow from Prop. 7.3.3; uniform boundedness of w_h in t on X is implied by the following argument. Multiply Eq. (7.3.12) by w_h and integrate over x, v, t to obtain

$$||w_h(\cdot,\cdot,t)||_X^2 + \int_0^t \int_{R_v} v[w_h^2(1,v,s) - w_h^2(0,v,s)]\, ds\, dv = ||w_I - w_p||_X^2. \tag{7.3.19}$$

The boundedness follows from the fact that the right hand side of this equation is independent of t, and that the second term on the left side is non-negative. This immediately implies the asymptotic result.

The above propositions have verified the following.

Theorem 7.3.5. *Assume $w_I - w_0 \in D(\Omega)$ where $w_I \in X$ with $w_0 \in X$ a given solution of Eq. (7.3.3) such that $v\frac{\partial w_0}{\partial x} \in X$ and w_0 satisfies the boundary conditions (7.2.4) and (7.2.5).*

Then Eq.(7.3.1) has a unique, global strong solution of the form (7.3.11) with $w_p = w_0$. Further, $w(\cdot,\cdot,t) \to w_0$ in X as $t \to \infty$. As pointed out earlier, these results all hold also in the (Brillouin) Case 2, if X is replaced by $X_B = L^2([0,1] \times B)$ in which case the current and density also exist.

7.4 The Stationary Wigner Equation

Theorem 7.3.5 assumes the existence of a solution w_0 of the stationary Wigner equation with inflow boundary conditions such $w_0 \in X$ and $v\frac{\partial w_0}{\partial x} \in X$. We recall that for simplicity we are considering potentials which are polynomials of degree N on $[0,1]$ with arbitrary extension to the exterior. Without loss of generality we may assume $V(0) = 0$.

The equation we consider is (7.3.3) subject to inflow boundary data, i.e.

$$w_0(0,v) = w_+(v), \qquad v > 0 \tag{7.4.1}$$

$$w_0(1,v) = w_-(v), \qquad v > 0, \tag{7.4.2}$$

with $w_\pm \in L^2(\mathbb{R}_v)$. As already noted, there are infinitely many formal solutions of this problem, all of which may be constructed as the Wigner transform [33] of a function of the hamilitonian

$$H = -\frac{1}{2}\frac{d^2}{dx^2} + V(x). \tag{7.4.3}$$

(See Ref. [87]). This means that

$$w_0 = [g(H)]_w(x,v) \tag{7.4.4}$$

for some real function g; the subscript w means "Wigner transform." Note that $[g(H)]_w \neq g(H_w)$ in general.

If $g(H)$ is expanded in a formal power series, then a formal solution would be

$$w_0(x,v) = \sum_{n\in\mathbb{N}_0} \alpha_n [H^n]_w(x,v) \tag{7.4.5}$$

with real coefficients α_n. To obtain a solution to our problem, it is necessary to find coefficients α_n such that the series converges (in X) and the inflow boundary conditions are fulfilled.

We begin by computing $[H^n]_w$. This is done as follows. We first recall the formula [34] for the Wigner transform of the product of two operators AB in terms of A_w and B_w:

$$[AB]_w = A_w e^{\frac{\Lambda}{2i}} B_w \tag{7.4.6}$$

where Λ is the Poisson bracket operator

$$\Lambda = \overleftarrow{\partial_v}\,\overrightarrow{\partial_x} - \overleftarrow{\partial_x}\,\overrightarrow{\partial_v}. \tag{7.4.7}$$

The arrows indicate the direction in which the derivatives operate. For example

$$A_w \Lambda B_w = \{A_w, B_w\}_{PB} = \partial_v A_w \partial_x B_w - \partial_x A_w \partial_v B_w.$$

Then

$$[H^n]_w = H_w e^{\frac{\Lambda}{2i}} [H^{n-1}]_w = [H^{n-1}]_w e^{\frac{\Lambda}{2i}} H_w$$

$$= H_w e^{-\frac{\Lambda}{2i}} [H^{n-1}]_w; \tag{7.4.8}$$

note [33] [34]

$$H_w = \frac{1}{2}v^2 + V(x). \tag{7.4.9}$$

This leads to the crucial formula

$$[H^n]_w = H_w cos\frac{\Lambda}{2}[H_w^{n-1}] = [H_w]^{n-1} cos\frac{\Lambda}{2} H_w. \tag{7.4.10}$$

Because of the form of $H, [H^n]_w$ is a finite sum, so the cosine and the exponentials in the above formulas are well defined.

Lemma 7.4.1. *Eq. (7.4.8) is equivalent to*

$$[H^n]_w = [H^{n-1}]_w H_w - \frac{1}{8}\frac{\partial^2}{\partial x^2}[H^{n-1}]_w + R_{M_1}$$

with

$$R_{M_1} = \sum_{k=1}^{M_1} \frac{(-1)^k}{(2k)!2^{2k}} \frac{\partial^{2k} V}{\partial x^{2k}} \frac{\partial^{2k}}{\partial v^{2k}} [H^{n-1}]_w$$

where

$$M_1 = min(n-1, [\frac{N}{2}]).$$

Remark. Recall the potential is a polynomial of degree N.
Proof. The proof is a simple process of differentiating, using the power series expansion of cosine and noting that in powers of Λ cross terms do not contribute by virtue of Eq. (7.4.9).

Corollary 7.4.2. *We have*

$$[H^n]_w = \sum_{j=0}^{n} C_{nj}(x) v^{2j} \tag{7.4.11}$$

where the C_{nj} are C^∞ on $[0, 1]$.

Remark. The C^∞ property follows from the fact that V is a polynomial. The same result would follow for any C^∞ potential.

Lemma 7.4.3. *(Recursion formula.)*

$$C_{nl} = (V - \frac{1}{8}\frac{\partial^2}{\partial x^2})C_{n-1,l} + \frac{1}{2}C_{n-1,l-1} +$$

$$+\sum_{k=1}^{M_{l+1}} \frac{(-1)^k}{(2k)!2^{2k}}(2l+2k)(2l+2k-1)\dots(2l+1)V^{(2k)}C_{n-1,k+l} \tag{7.4.12}$$

$$0 \leq l \leq n$$

with

$$M_l = min(n-l,[\frac{N}{2}]).$$

In particular

$$\begin{aligned} C_{nn} &= 2^{-n} \\ C_{n,n-1} &= \frac{V}{2^{n-1}} + \frac{1}{2}C_{n-1,n-2}, \quad n \geq 2 \\ C_{10} &= V \\ C_{nL} &= 0, \quad l > n. \end{aligned} \tag{7.4.13}$$

Proof. The proof of (7.4.12) follows by induction using Lemma 7.4.1 and Corollary 7.4.2, collecting coefficients of powers of v^2. Note $C_{00} = 1$ because $[H^0]_w = 1$.

Corollary 7.4.4. *The matrix C with elements C_{nl} is invertible; denoting $\gamma_{nl} = (C^{-1})_{nl}$ we have $\gamma_{nn} = 2^n$ and $\gamma_{n_j} = 0, j > n$.*

Lemma 7.4.5. *There is a constant K, depending only on V and its (finite number of) derivatives such that for any n*

$$|C_{nl}| \leq K^n, \quad l = 0,\dots,n. \tag{7.4.14}$$

Proof. We use induction on n, starting with $C_{00} = 1$. Let K_1 be the supremum of $C_{n-1,l}$ over $[0,1]$ and over all indices n, l and k appearing on the right hand side of (7.4.12) as coefficients (including the coefficients which appear in the second derivative term). There are only a finite number of such coefficients because V is a polynomial and the maximum number of terms appearing in the sum is in (7.4.12) is uniformly bounded in n. Then $K = MK_1$ where M is the maximum number of coefficients appearing in this process, which is also uniformly bounded in n.

Now assume that

$$|\frac{\partial^{2j} C_{n-1,l}}{\partial x^{2j}}| \leq K^{n-1}, \quad 0 \leq 2j \leq N.$$

Then it is clear by the definition in (7.4.12) that

$$|C_{nl}| \leq K^n, \quad 0 \leq 2j \leq N.$$

We now choose $K_0 > \min\,(K, 2^6.)$ Then it is clear by the definition in (7.4.12) that

Lemma 7.4.6. *The elements γ_{nj} of the matrix C^{-1} satisfy the bound*

$$|\gamma_{nj}| \leq \frac{K_0^{n^2+\frac{1}{2}}}{(\frac{1}{2}K_0^6)^n}, \quad j = 0, 1, \ldots n.$$

Proof. We observe that since C is triangular, C^{-1} can be computed by inverting the main minor matrices successively. Let A_n be the inverse of the $(n+1)st$ main minor matrix whose determinant is $2^{-\frac{(n+1)(n+2)}{2}}$. Each γ_{nj} contains $(n+1)!$ products of the type

$$C_{0i_0}C_{1i_1}C_{2i_2}\ldots C_{ni_n}, \quad i_j \leq j$$

where the sequence $(i_0, i_1, \ldots i_n)$ is a permutation of the integers 0 to n. Using Lemma 7.4.5 this implies

$$|\gamma_{nj}| \leq (n+1)!2^{\frac{(n+1)(n+2)}{2}}K^{n\frac{(n+1)}{2}}. \tag{7.4.15}$$

Using the elementary estimate

$$K_1^j \geq j\, logK_1 \qquad (\forall K_1 > 1)\,.$$

We get from (7.4.13)

$$|\gamma_{nj}| \leq \frac{(2K_1)^{\frac{(n+1)(n+2)}{2}}K^{\frac{n(n+1)}{2}}}{(logK_1)^n}. \tag{7.4.16}$$

The result is implied by (7.4.16) with the choice $K_1 = \frac{1}{2}\, K_0^{\frac{1}{6}}$.

Proposition 7.4.7. *Choose $a > 0$ and let $w_+ \in L^2(\mathbb{R}_v)$ be the restriction to $v > 0$ of a real analytic function of v^2 with expansion*

$$w_+(v) = \sum_{n=0}^{\infty} p_n v^{2n}$$

where the p_n are such that

$$\sum_{n=0}^{\infty} |p_n| K_p^{2n^2} < \infty \tag{7.4.17}$$

with $K_p = K_0$ (Lemma 7.4.6) if $a > 4$ and $K_p = \max(K_0,\, e^{\sqrt{2/a}})$ if $a \leq 4$. Then there exists a sequence $(\alpha_n)_{n\in\mathbb{N}_0}$ of real numbers such that

$$w_0(x,v) = \sum_{n=0}^{\infty} \alpha_n \sum_{j=0}^{n} C_{nj}(x) v^{2j} \tag{7.4.18}$$

is a weak solution of (7.3.3) for $v > 0$ satisfying the inflow boundary condition (7.3.17) at $x = 0$, with the $C_{nj}(x)$ given by Lemmata 7.4.2, 7.4.3. Furthermore $w_0 \in C^\infty([0,1] \times \mathbb{R}_v^+) \cap L^p([0,1] \times \mathbb{R}_v^+; e^{-av^2})$ and $w_0 \in L^p_{loc}([0,1] \times \mathbb{R}_v)$, $\quad 1 \leq p \leq \infty$.

Proof. Noting Eqs. (7.4.4) and (7.4.5), we see that (7.4.18) represents a formal solution of (7.3.3). To prove the proposition it is necessary to choose the α_n such that (7.4.18) converges to a function in $L^p([0,1] \times \mathbb{R}_v; e^{-av^2})$ and satisfies the inflow condition at $x = 0$. This condition requires

$$w_+(v) = \sum_{n=0}^{\infty} \alpha_n \sum_{j=0}^{n} C_{nj}(0) v^{2j}, \quad v > 0. \tag{7.4.19}$$

Introduce the vector notation

$$\tilde{\alpha} = (\alpha_n)_{n \in \mathbb{N}_0}$$

$$\tilde{v} = (v^{2n})_{n \in \mathbb{N}_0}$$

$$\tilde{p} = (p_n)_{n \in \mathbb{N}_0}.$$

Then

$$w_+(v) = \tilde{p}^T \tilde{v}$$

and the boundary condition is expressed as

$$\tilde{p}^T \tilde{v} = \tilde{\alpha}^T C(0) \tilde{v}$$

which implies

$$\tilde{\alpha}^T = \tilde{p}^T C(0)^{-1}.$$

Substituting into (7.4.18) gives

$$w_0(x,v) = \tilde{p}^T C(0)^{-1} C(x) \tilde{v}.$$

To prove the result, it is sufficient to show that the function $w_1(x,0)$ defined by

$$w_1(x,v) := \tilde{p}^T C(0)^{-1} C(x) \tilde{v} e^{-\frac{a}{2}v^2} \tag{7.4.20}$$

is bounded, since the other factor $e^{-\frac{a}{2}v^2}$ gives the asserted L^p properties. We use Stirling's formula in the form

$$\frac{n^{n+\frac{1}{2}}e^{-n}}{n!} = \frac{1}{2\pi}(1+w_n), \quad \lim_{n\to\infty} w_n = 0. \tag{7.4.21}$$

We consider the case $a > 4 (a < 4$ is similar). Denoting the elements of the matrix $C(0)^{-1}C(x)$ by

$$M_{nj} = \sum_{l=0}^{n} \gamma_{nl}(0)C_{lj}, \qquad j \leq n$$

We get, by Lemmata 7.4.5 and 7.4.6, taking the appropriate supremum over $x \in [0,1]$

$$|M_{nj}| \leq \frac{(n+1)K_0^{n^2+n+\frac{1}{2}}}{(log(\frac{1}{2}K_0^6))^n}.$$

Substituting this estimate into (7.4.20) and using (7.4.21) twice, we find

$$w_1(x,v) \leq D\sum_{n=0}^{\infty} \frac{|p_n|}{\sqrt{n}} \frac{K_0^{2n^2}}{(logK_0)^{2n}(\frac{a}{2})^n}$$

which is finite by hypothesis. Here D is a constant depending only on K_0, i.e. on the supremum of all the (finite number of) derivatives of $V(x), x \in [0,1]$. The C^∞ property is obvious. The L^P_{loc} property follows from the above calculations without the weight function by restricting v to a compact subset of $\mathbb{R}_0$.

Theorem 7.4.8. *With w_+ as in Prop.7.4.7 and with similar assumptions on w_-, there exists weak solution $w_0(x,v)$ of Eq. (7.3.3) (which is classical pointwise) satisfying the inflow boundary conditions*

$$w_0(0,v) = w_+(v), \qquad v > 0 \tag{7.4.22}$$

$$w_0(1,v) = w_-(v), \qquad v < 0 \tag{7.4.23}$$

with

$$w_0 \in C^\infty([0,1]\times\mathbb{R}_v\backslash\{0\}) \cap L^P([0,1]\times\mathbb{R}_v; e^{-av^2})$$

for all $a > 0$, and $1 \leq p \leq \infty$.

Proof. The proof proceeds as in Prop.7.4.7 for the boundary at $x = 1$. Then w_0 is constructed by joining the two solutions. We denote by $B^\pm$ the sets of $\{v \in B \,|\, v > 0\}$ and $\{v \in B \,|\, v < 0\}$, we recall B is the first Brillouin zone. The following theorems apply to Case 2 only.

Theorem 7.4.9. *Let $w_\pm \in L^2(B^\pm)$ be the restriction to $v > 0$ and $v < 0$ of a real analytic function of v^2 with expansion*

$$w_\pm(v) = \sum_{n=0}^{\infty} p_n^\pm v^{2n}$$

where the $p_n^\pm$ are such that

$$\sum_{n=0}^{\infty} |p_n^\pm| K^{2n^2} < \infty$$

with k_0 from Lemma 7.4.6. Then there exist sequences of real numbers $(\alpha_n^\pm)_{n\in\mathbb{N}_0}$ such that

$$w_0^\pm(x,v) = \sum_{n=0}^{\infty} \alpha_n^\pm \sum_{j=0}^{n} C_{nj}(x) v^{2j}, \; v \in B^\pm$$

is a weak solution of (7.3.3) (which is classical pointwise) subject to the boundary conditions

$$w^+(0,v) = w_+(v)$$

$$w^-(1,0) = w_-(v)$$

and $[0,1] \times B^\pm$, and $w_0^\pm \in L^p([0,1] \times B^\pm), 1 \le p \le \infty$. The solution defined by $w_0 = w^+, v \in B^+$, $w_0 = w^-, v \in B^-$ is a classical solution of (7.3.3) with $v \in B$ subject to the inflow conditions (7.4.22) and (7.4.23) on $[0,1] \times B\backslash\{0\}$ and $w_0 \in L^p([0,1] \times B), 1 \le p \le \infty$. Furthermore vw_0, $v\frac{\partial w_0}{\partial x}$ and $\Theta w_0 \in L^p([0,1] \times B), 1 \le p \le \infty$.

The proof follows from the L^p results of Theorem 7.4.8.

Theorem 7.4.10. *Define the current by*

$$I = -\int_B v w_0(x,v) dv.$$

Then

1. *I is constant*
2. *I is unique*
3. *$I = -\int_{B^-} v w_0^+(1,v) - \int_{B^-} v w_-(1,v)\, dv$.*

Proof.

1. This follows from integration of Eq. (7.3.3) and noting $\int \Theta w dv = 0$ (in both cases 1 and 2). See Eq. (1.10) of Ref. [86].

2. The proof is analogous to that of Prop. 7.2.4.

3. This follows from the definition of the current and (1)

Remarks.

1. Result of (3) of the above theorem indicates that the current could be calculated from w^+ (or w^-) alone if these could be constructed independently .

2. The results of Theorem 7.4.10 also holds for Case 1 if appropriate regularity holds. Note that the density

$$n = \int_B w_B(x,v)dv$$

   always exists in Case 2, but the analogous quantify in Case 1, involving an integration over $\mathbb{R}_v$, may not [86].

3. In principle, if v is restricted to a bounded set (Case 2) the x variable should be discrete. The hybrid limit used here, with x continuous, is used also in Ref. [86], and some justification for it is given in [40, p.56-57]. Case 1 is also a regularization and for small a computations for Cases 1 and 2 would agree closely, with Case 1 current

$$I_a = \int_{\mathbb{R}_v} v w_0(x,v) e^{av^2} dv$$

   obeying an analogue of Theorem 7.4.10. The limit $a \to 0$ (or $B \to \mathbb{R}_v$) have not been shown to exist.

4. It is well known that weight functions like $\exp(-v^2/2)$ appear in transport theory quite often, e.g. in the theory of the semi-classical Boltzmann equation with measure-valued scattering rates in the collision operator $Q(F)$; it may happen that Q has eigenvalues (e.g. zero) of infinite multiplicity with eigenspaces generated by functions of type $\exp(-v^2/2)P(v^2/2)$ for any polynomial P satisfying some periodicity property (see Ref. [90]).

7.5 The Relaxation-Time Approximation

The relaxation-time model adopted in this chapter does not conserve charge. This can be seen by integrating Eq. (7.3.1) over velocity (assuming appropriate regularity) to obtain

$$\frac{\partial n}{\partial t} + \frac{\partial I}{\partial x} = \frac{n_0 - n}{\tau} \tag{7.5.1}$$

where n is the density and n_0 is the density corresponding to w_0. Charge conservation would require the right-hand side of (7.5.1) to be equal to zero. A model which does conserve charge is given in [40, p.34]:

$$\frac{\partial w}{\partial t}(x,v,t) + v\frac{\partial w}{\partial x} - i\Theta(V)w = \frac{1}{\tau}(w_0(x,v)\int w(x,v,t)\,dv - w(x,v,t)\int w_0(x,v)\,dv). \tag{7.5.2}$$

(Actually, in Ref. [86] w_0 is taken independent of x. This model clearly does conserve charge, but the results obtained in the present paper for the simpler relaxation-time model have not been proved for this more general model. Perhaps this will be the subject of a future paper.

The rational for a non-charge-conserving model is the following intuitive model. At time t, an electron is "absorbed" from the ambient distribution, held in captivity for a time τ, after which it is re-emitted. Since the ambient density is different at time t and $t+\tau$, the number of electrons absorbed are not balanced by the number re-emitted, which were absorbed at an earlier time.

Chapter 8

Conclusion and Discussion

This concludes our discussion of the (WP)-(SP) system. Recapping we have seen the following results. As a possible model for time dependent dissipation in the (WP)-(SP) system, chapter three shows that there exists a global, unique solution to the derived system. In chapter four, a “quasilinear” (SP) system was considered which modeled the effects of a nonlinear dependence of the dielectric constant on the self-consistent electric field. Here too we showed that there exists a global unique solution to the system. In chapter five, a definition of quantum BGK modes was put forth which facilitated an understanding of the time independent (WP) system and its connections to the time independent (SP) problem. Moreover, in chapter five we considered an “eigenmatrix” solution to the time independent (SP) problem with periodic boundary conditions. There we showed the existence of a set of (non-unique) eigenfunctions along with a unique self-consistent potential. Regularity of solutions was also shown assuming the smoothness of the given statistical distribution functions. Lastly, in chapter seven “inflow” boundary conditions were introduced and considered on a linear (given potential) Wigner equation. It was hoped that by their introduction that inflow boundary conditions would lead to a “physically” acceptable model for carrying out numerical studies on the (WP) system. There we showed that the derived current was in fact unique, thereby bolstering the plausibility of the model. Finally, in appendix A a numerical scheme was put forth which will hopefully model the self-consistent effects of the (SP) system. Moreover, it is hoped that the models previously considered will be able to be integrated into this scheme and that the results will be comparable to simulations found in the literature.

Last but not least, there are a few considerations left still “open” concerning the models from chapters six and seven. The first question to arise is whether the eigenmatrix problem be extended to the full space problem. Here, of course, one would not just expect energy eigenvalues but also continuous spectrum. Hence the analysis would have to be suitable extended. An answer to this question would lead to a better understanding of the stationary (WP) problem since as chapter five implies every stationary solution must be the Wigner transform of a function of this "solution" hamiltonian (i.e., a solution of the full space case implies the existence of a self-consistent potential and hence its hamiltonian.) This, in turn, would shed light on the study of "self-consistent" scattering; see [92] for current research on this topic. The second question raised is whether inflow boundary conditions be used in conjunction with the stationary (WP) problem. By the nature of the (WP) problem we have no *a priori* knowledge of the existence of the self-consistent potential. This knowledge of the potential was integral to the expansion used in the analysis in chapter seven and it would be interesting how one might extend this work. It is clear that these two problems alone will lead to some interesting mathematical analysis.

Appendix A

Numerical scheme for the (SP) system

A.1 Matrix Evolution Equations for Steady State Problems

In this appendix we shall propose a method to investigate both the analytic and numerical aspects of the self-consistent Bloch evolution equation (i.e., the Bloch equation where the hamiltonian depends upon the solution through a Poisson equation). For this problem one could consider the same domains and physical boundary conditions usually used for the time dependent cases. Here we shall derive a system of evolution equations for the general case and then present an explicit scheme in the one dimensional case with periodic boundary conditions.

The evolution equation for this problem is derived from the specific form of the density operator ($\rho = \Omega/Z(\beta)$) for canonical distributions from quantum statistical theory. This Bloch equation has, in part, already been considered for a given potential in [66]. Moreover, an approximate result where the dependence of the potential on β was neglected was studied both for existence and uniqueness in [20], and numerical solvability [25]. However, a full description of the self-consistent problem is currently an active area of research.

One abstract result [71] gives insight to the connection between stationary solutions of the Wigner-Poisson system and the spectral properties of H. It states that for a given (WP) system any solution to the stationary (WP) equation is the Wigner transform of a function of a complete set of commuting observables (CSCO) generated by the hamiltonian. Conversely, it shows that any bounded real valued function of this (CSCO) is a solution to the stationary Wigner system. This result implies that an uncountable infinity of stationary solutions exist for a given (WP) system. In fact, this proposed study is a subset of this result for a specified form of this "real bounded function" of the (CSCO) and is given by the relevant physics involved.

The physically relevant density matrices for our problem is given by the following. For an ensemble obeying Boltzmann statistics Ω is given by

$$\Omega = exp(-\beta H)\,, \tag{A.1.1}$$

so that $\rho = \Omega/Z(\beta)$. Here $H = \frac{1}{2}P^2 + V(x)$ is the hamiltonian operator for a given system, and we define the partition function to be $Z(\beta) = Tr(\Omega)$. Consequently at $\beta = 0$ this operator is $\Omega(0) = id$. Now differentiating with respect to β we find that the evolution equations for the problem to be:

$$\partial_\beta \Omega = (-H + \beta\partial_\beta V)\Omega \tag{A.1.2}$$

subject to the initial condition $\Omega(0) = id$. From this equation one can derive the evolution of $\Omega(\beta)$ in a specific or known representation.

Let $\{\phi_n\}_{n\in\mathbb{N}}$ be a basis for the Hilbert space for which one poses the problem. Now expand Ω with respect to the projections P_n of this basis to obtain

$$\Omega(\beta) = \sum_{n,m} \Omega_{nm}(\beta) P_{nm} \tag{A.1.3}$$

Where $\Omega_{nm}(\beta) =< \phi_n, \Omega\phi_m >$ and $P_{nm} =< \phi_m, \cdot > \phi_n$. After taking the Wigner transform of Eq.(A.1.3) one finds

$$\Omega_w(x,p,\beta) = \sum_{n,m} \Omega_{nm}(\beta) \int e^{ip\eta}\overline{\phi}_n(x+\frac{\eta}{2})\phi_m(x-\frac{\eta}{2})\,d\eta. \tag{A.1.4}$$

The evolution of the matrix element of Ω is given by the following "Master" equations.

$$\frac{\partial\Omega_{nm}}{\partial\beta} = -\sum_k \Omega_{km}[\langle\phi_n, H\phi_k\rangle - \beta\cdot\langle\phi_n, \frac{\partial V}{\partial\beta}\phi_k\rangle] \tag{A.1.5a}$$

$$\triangle V(x) = n(x,\beta) = 1 - \frac{1}{Z}\sum_{i,j}\Omega_{ij}\overline{\phi}_i(x)\phi_j(x) \tag{A.1.5b}$$

$$\frac{\partial V}{\partial\beta} = -\frac{1}{Z}\sum_{i,j}\alpha_{ij}(x)[\frac{\partial\Omega_{ij}}{\partial\beta} - \frac{Z'}{Z}\Omega_{ij}] \tag{A.1.5c}$$

$$\alpha_{ij}(x) = \int_0^x\int_0^y \overline{\phi}_i(y')\phi_j(y')dy'dy\;; \tag{A.1.5d}$$

Again, the matrix equations are subject to the initial condition $\Omega_{nm}(0) = \delta_{nm}$.

Note here and in the sequel we shall consider the (1D) problem on $[0,1]$, more complicated geometries could be studied with further knowledge of the relevant Green's functions. In Sec. A.2 we shall consider this space-domain with periodic boundary conditions. Consequently we make full use of the explicit integration of Eq.(A.1.5b) to determine that

$$V(x,\beta) = \int_0^x\int_0^y n(y',\beta)dy'\,dy + C_1 x + C_2 \tag{A.1.6}$$

where the number density "$n(x,\beta)$" is given by the right hand side of Eq.(A.1.5b) and satisfies the charge neutrality condition $\int n(x,\beta)dx = 0$.

Clearly, the existence and uniqueness analysis is a non-trivial matter. However, it is felt that these equations are still simpler than solving the corresponding operator equations using spectral methods. Once the matrix elements for the hamiltonian are calculated, it is a matter of solving a system of ordinary differential equations. Of course one difficulty is that the matrix elements are β dependent due to their coupling with the β dependent hamiltonian. Hence, the development of a "self-consistent" scheme to calculate the solution at some final β^* is necessary.

A.2 Numerical Scheme for Steady State Solutions

We shall investigate the following procedure to determine Ω and V at some specified inverse temperature "β^*". Starting at $\beta = 0$ one solves Eq.(A.1.5b) for the potential "$V(x,0)$" using the initial condition $\Omega_{nm}(0) = \delta_{nm}$ (truncating the number of n, m terms at some fixed positive integer N). This in turn specifies the value of H at $\beta = 0$; denote this operator by $H(0)$. Now depending on the problem, one determines $\Omega_{nm}(\Delta\beta)$ ($\Delta\beta = \beta^*/M$, M some fixed positive integer) from the corresponding evolution equation. Taking Eq.(A.1.5a) and integrating with respect to β one obtains

$$\Omega_{nm}(\Delta\beta) = \delta_{nm} - \sum \int_0^{\Delta\beta} \Omega_{km}[\langle\phi_n, H\phi_k\rangle - \beta'\langle\phi_n, \frac{\partial V}{\partial\beta'}\phi_k\rangle]d\beta' \ . \tag{A.2.1}$$

For the moment, we shall investigate the explicit scheme defined by approximating this integral by the value at the left end point. It is not clear at this point if an implicit scheme may be necessary for stability. A possible implicit scheme will be introduced in a later section. Proceeding, one now determines $\Omega_{nm}(\Delta\beta)$ to be

$$\Omega_{nm}(\Delta\beta) = \delta_{nm} - \Delta\beta \cdot \langle\phi_n, H(0)\phi_m\rangle \ . \tag{A.2.2}$$

This in turn allows us to find:

$$\begin{aligned} Z(\Delta\beta) &= \mathrm{Tr}(\delta_{nm}) - \Delta\beta\langle\phi_n, H(0)\phi_n\rangle && \text{(A.2.3a)} \\ Z'(\Delta\beta) &= -\langle\phi_n, H(0)\phi_n\rangle && \text{(A.2.3b)} \\ \frac{\partial\Omega_{nm}}{\partial\beta}(\Delta\beta) &= -\langle\phi_n, H(0)\phi_m\rangle \ . && \text{(A.2.3c)} \end{aligned}$$

These quantities are used to determine $V(x,\Delta\beta)$ using Eq.(A.1.6). This in turn specifies $H(\Delta\beta)$ and using Eq.(A.1.5c) one finds $\partial V/\partial\beta(\Delta\beta)$. We now calculate the next step $\Omega_{nm}(2\Delta\beta)$ and this is found to be

$$\begin{aligned} \Omega_{nm}(2\Delta\beta) = \delta_{nm} &- \Delta\beta \cdot \langle\phi_n, H(0) + H(\Delta\beta)\phi_m\rangle + (\Delta\beta)^2\langle\phi_n V'(\Delta\beta)\phi_m\rangle && \text{(A.2.4)} \\ &+ (\Delta\beta)\sum_k \langle\phi_k, H(0)\phi_m\rangle[\langle\phi_n, \{H(\Delta\beta) - \Delta\beta \cdot V'(\Delta\beta)\}\phi_k\rangle] \ . \end{aligned}$$

This process is thus continued to the final step β^*. Having done this one repeats the process a $N, M \to \infty$ $(\Delta\beta \to 0)$. Clearly, two aspects of this scheme must be investigated. First, one needs to prove that the quantity $(\Omega_{nm}(\beta^*), V(x, \beta^*))$ does indeed converge in this limit to the self-consistent solution at β^*. Second, one should determine error estimates for the quantities involving N, M and $\Delta\beta$.

This scheme is reminiscent of the operator splitting method used in [23] to determine the time evolution for the self-consistent (WP) problem. Here β serves as the time parameter, but just as in [23] one investigates the convergence of the approximate solution to the self-consistent one in the limit as the "time" step goes to zero.

A.3 Solutions for Periodic Boundary Conditions on $[0, 1]$

In this section we explicitly determine the values of Ω_{nm} and V for the first three β steps using the periodic basis $\{e^{2\pi inx}\}_{n\in\mathbb{Z}}$ on the Hilbert space $L^2_{per}[0, 1]$. As in Sec. A.1 we approximate all sums, here they are taken from $(-N + 1,..,0,...,N + 1)$, unless specified otherwise. Here $\Omega_{nm}(0) = \delta_{nm}$ as in Sec. A.1, because of the different sum $Z(0) = \mathrm{Tr}(\delta_{nm}) = 2N$.

Starting with the calculation of $V(x, 0)$, from Eq.(A.1.5b) we see that $n(x, 0) = 0$. Consequently, it follows that $V(x, 0) = C_1x + C_2$. We can always chose $C_2 = 0$ since V is a potential; moreover from periodicity of V at every β step we determine that $C_1 = 0$ also holds. Now $H(0) = \frac{1}{2}P^2$ and one easily calculates $\langle\phi_n, H(0)\phi_n\rangle = 2\pi^2m^2\delta_{nm}$. It follows that $\Omega(\Delta\beta)$ is given by Eq.(A.2.2)

$$\Omega_{nm}(\Delta\beta) = (1 - 2\pi^2m^2 \cdot \Delta\beta)\delta_{nm}\,; \tag{A.3.1}$$

and $Z(\Delta\beta)$ given by

$$Z(\Delta\beta) = 2N - 2\pi^2(\Delta\beta)\sum n^2\ . \tag{A.3.2}$$

From Eq.(A.1.5a) we find that

$$\frac{\partial\Omega_{nm}}{\partial\beta} = -2\pi^2m^2\delta_{nm} \tag{A.3.3}$$

For future convenience we define $\sigma_1(N) = -2\pi^2\sum n^2$, hence $Z'(\Delta\beta) = \sigma_1$. We demand that the Ω_{nm} remain positive operators for all β steps; an immediate consequence of this fact is a "smallness" estimate on the step size "$\Delta\beta$" namely that

$$\Delta\beta < \frac{2N}{|\sigma_1|} \tag{A.3.4}$$

We are now ready to use Eq.(A.1.5b) again to find $V(x, \Delta\beta)$. Since $\Omega_{nm}(\Delta\beta)$ is diagonal it follows immediately that $n(x, \Delta\beta) = 0$ and as in the $V(x, 0)$ case $V'(0, \Delta\beta)$ and $V(0, \Delta\beta)$

are found to be zero. Continuing from Eq.(A.1.5c) we have that

$$\frac{\partial V}{\partial \beta}(x, \Delta\beta) = \frac{1}{2N + \sigma_1 \Delta\beta} \sum_n [\frac{\sigma_1}{2N + \sigma_1 \Delta\beta}(1 - 2\pi^2 n^2 \Delta\beta) + 2\pi^2 n^2]\alpha_{nn}(x) \tag{A.3.5}$$

where $\alpha_{nn}(x) = \frac{1}{2}x^2$ from Eq.(A.1.5d).

Finally, we have all the quantities needed to determine $\Omega_{nm}(2\Delta\beta)$. From Eq.(A.2.4) we determine it to be

$$\begin{aligned}
\Omega_{nm}(2\Delta\beta) &= (1 - 2\pi^2 m^2 \cdot \Delta\beta)\delta_{nm} \\
&- (\Delta\beta) \sum_k (1 - 2\pi^2 m^2 \cdot \Delta\beta)\delta_{km}[2\pi^2 n^2 \delta_{nk} - (\Delta\beta)\langle\phi_n, \frac{\partial V}{\partial \beta}\phi_k\rangle] \\
&= (1 - 2\pi^2 m^2 \cdot \Delta\beta)\delta_{nm} \\
&- (\Delta\beta)(1 - 2\pi^2 m^2 \cdot \Delta\beta)[2\pi^2 n^2 \delta_{nm} - (\Delta\beta)\langle\phi_n, \frac{\partial V}{\partial \beta}\phi_k\rangle] && \text{(A.3.6a)} \\
\langle\phi_n, \frac{\partial V}{\partial \beta}(\Delta\beta)\phi_k\rangle &= \langle\phi_n, \frac{1}{2}x^2\phi_k\rangle\gamma(1-\gamma) && \text{(A.3.6b)} \\
\gamma &= \frac{\sigma_1}{2N + \sigma_1 \Delta\beta} && \text{(A.3.6c)} \\
\langle\phi_n, \frac{1}{2}x^2\phi_k\rangle &= \frac{1}{3}\delta_{nm} + a_{nm}(1 - \delta_{nm}) && \text{(A.3.6d)} \\
a_{nm} &= \frac{1}{4\pi i(m-n)}[1 - \frac{2}{2\pi i(m-n)}] \,. && \text{(A.3.6e)}
\end{aligned}$$

$\Omega_{nm}(2\Delta\beta)$ can be simplified to

$$\begin{aligned}
\Omega_{nm}(2\Delta\beta) &= [(1 - 2\pi^2 m^2 \cdot \Delta\beta)^2 + \frac{\gamma(1-\gamma)(\Delta\beta)^2}{3}(1 - 2\pi^2 m^2 \cdot \Delta\beta)]\delta_{nm} \\
&+ (\Delta\beta)^2\gamma(1-\gamma)(1 - 2\pi^2 m^2 \cdot \Delta\beta)a_{nm}(1 - \delta_{nm}) && \text{(A.3.7)}
\end{aligned}$$

The value $Z(2\Delta\beta)$ is found to be

$$\begin{aligned}
Z(2\Delta\beta) &= 2N + 2\sigma_1\Delta\beta + (\Delta\beta)^2[\sigma_2 + \frac{\gamma(1-\gamma)}{3}(\sigma_1\Delta\beta + 2N)] && \text{(A.3.8)} \\
\sigma_2(N) &= \sum 4\pi^4 n^4 && \text{(A.3.9)}
\end{aligned}$$

One can now calculate $V(x, 2\Delta\beta)$ from Eq.(A.1.5b):

$$V(x, 2\Delta\beta) = \frac{(\Delta\beta)^2\gamma(1-\gamma)}{Z(2\Delta\beta)} \sum_{n,m} \frac{(1 - 2\pi^2 m^2 \cdot \Delta\beta)a_{nm}(1 - \delta_{nm})}{[2\pi i(m-n)]^2}[1 - e^{2\pi i(m-n)x}] \tag{A.3.10}$$

Here the diagonal terms of $\Omega_{nm}(2\Delta\beta)$ cancel with the constant term in the density $n(x, 2\Delta\beta)$; moreover one must choose

$$V'(0, 2\Delta\beta) = \frac{(\Delta\beta)^2\gamma(1-\gamma)}{Z(2\Delta\beta)} \sum_{n,m} \frac{(1 - 2\pi^2 m^2 \cdot \Delta\beta)a_{nm}(1 - \delta_{nm})}{[2\pi i(m-n)]} \tag{A.3.11}$$

so that $V(x+1, 2\Delta\beta) = V(x, 2\Delta\beta)$. One can determine $Z'(2\Delta\beta)$ and $\frac{\partial\Omega_{nm}}{\partial\beta}(x, 2\Delta\beta)$ they are given by:

$$
\begin{aligned}
Z'(2\Delta\beta) &= 2\sigma_1(N) + (\Delta\beta)[\sigma_2(N) + \frac{\gamma(1-\gamma)}{3}(\sigma_1 + 2N)] && \text{(A.3.12a)} \\
\frac{\partial\Omega_{nm}}{\partial\beta}(2\Delta\beta) &= [\frac{\gamma(1-\gamma)(\Delta\beta)}{3} - (2\pi^2 n^2)](1 - 2\pi^2 m^2 \cdot \Delta\beta)]\delta_{nm} \\
&+ (\Delta\beta)\gamma(1-\gamma)(1 - 2\pi^2 m^2 \cdot \Delta\beta)a_{nm}(1 - \delta_{nm})\,. && \text{(A.3.12b)}
\end{aligned}
$$

Finally, one can determine $\frac{\partial V}{\partial\beta}(x, 2\Delta\beta)$ using Eq.(A.1.5c) along with Eq.(A.3.5), Eqs.(A.3.6), and Eqs.(A.3.11)-(A.3.12).

As a final note, it is hoped that by a closer examination of this method that convergence could be shown. This will be the subject of future research.

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