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EXISTENCE, UNIQUENESS & ASYMPTOTIC
BEHAVIOUR OF THE WIGNER–POISSON SYSTEM
WITH AN EXTERNAL COULOMB FIELD

by

CHRISTOPHER SEAN BOHUN
B.Sc., University of Victoria, 1989
M.Sc., University of Victoria, 1992

A Dissertation Submitted in Partial Fulfillment
of the Requirements for the Degree of

DOCTOR OF PHILOSOPHY

in the Department of Mathematics and Statistics.
We accept this dissertation as conforming
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by photocopying or other means, without the permission of the author.
This dissertation analyzes the Wigner-Poisson system in the presence of an external Coulomb potential. In the first part, the Weyl transform is defined and used to derive an exact quantum mechanical equation for the Weyl transform of the density function $\rho_w$ (the Wigner function) known as the Wigner equation. This equation holds for any Hamiltonian which is a function of the position and momentum operators. The Wigner-Poisson system is then formally derived by imposing various assumptions on the structure of the Hamiltonian. This system describes the behaviour of an effective one-particle distribution in the presence of a large ensemble of particles. Furthermore, it allows the particles to either attract or repel each other as well as attract or repel as a whole from a fixed Coulomb source located at the origin. The second part details the question of existence and uniqueness for the Wigner-Poisson system. It is shown that provided the initial Wigner function is sufficiently regular ($\rho_w, t \in H^2$) and is a valid Wigner distribution, then the Wigner-Poisson system has a unique global mild solution ($\rho_w \in C([0, \infty); H^2)$). This result is independent of both the nature of the external Coulomb potential as well as the interparticle interaction. The proof of this result is accomplished by first transforming the Wigner-Poisson system into a countably infinite set of Schrödinger equations which results in what is referred to as the Schrödinger-Poisson system. Using standard semigroup theory arguments, existence and uniqueness of the Schrödinger-Poisson system is established. The properties of the Wigner-Poisson system are then obtained by reversing the transformation step. Regularity results for both the Schrödinger-Poisson and the Wigner-Poisson systems are compared to the case with no external Coulomb potential. In addition, the known regularity results are extended when there is no
external field. The results illustrate that the introduction of an external Coulomb potential slightly reduces the regularity of the solution. This confirms a conjecture of Brezzi and Markowich. The third part analyzes the asymptotic behaviour of the Wigner–Poisson system. If the configurational energy $E_{a,b}(t)$ is positive for all times then by considering the Schrödinger–Poisson system, solutions will decay in the sense of $L^p$ for $2 < p < 6$. This generalizes a result of Illner, Lange and Zweifel. Moreover, if the total energy is negative then the solutions will not decay in the sense of $L^p$ for any $2 < p \leq \infty$. This generalizes a result of Chadam and Glassey.

Decay estimates for both the Schrödinger–Poisson and the Wigner–Poisson systems are compared to the case with no external Coulomb field. As with the regularity results, the introduction of an external Coulomb field degrades the reported decay rates of the solution.

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Contents

Abstract ii
Contents iv
List of Figures vi
List of Tables vii
Acknowledgements viii
Dedication ix

Chapter 1 Introduction 1

Chapter 2 The Wigner–Poisson System 6
  2.1 Overview ................................................................. 6
  2.2 The Weyl Transformation ........................................... 7
  2.3 The Wigner Function .................................................. 18
  2.4 The Wigner Equation .................................................. 20
  2.5 Derivation of the WP System ...................................... 24

Chapter 3 Global Existence and Uniqueness 33
  3.1 Preliminaries .......................................................... 33
  3.1.1 WP to SP Transformation ..................................... 34
  3.1.2 A Change of Variable .......................................... 37
  3.2 Statement of the Problem ......................................... 39
  3.3 Self-Adjointness on Y .............................................. 42
    3.3.1 Self-Adjointness of $-iA_0$ on $X$ ..................... 43
    3.3.2 Self-Adjointness of $-iA_2$ on $X$ ..................... 45
    3.3.3 An Independent Estimate .................................... 46
    3.3.4 Extension to the Space $Y$ ................................. 48
  3.4 Classes of Solutions .............................................. 52
  3.5 Estimation of $V$ .................................................... 54
  3.6 Local Existence of a Unique Strong Solution ............... 59
  3.7 Global Existence .................................................... 66
Chapter 3

3.7.1 Conservation of Probability .................................................... 70
3.7.2 Conservation of Energy ........................................................... 71
3.7.3 A Crucial Estimate .................................................................. 76
3.8 Regularity Properties ............................................................................ 78
3.9 Global Existence of the WP System .................................................... 84

Chapter 4 Asymptotic Behaviour ................................................................. 89
4.1 An Auxiliary System .............................................................................. 89
4.2 Properties of the Free Propagator ....................................................... 91
4.3 Time Evolution of Operators ............................................................. 95
4.4 An Approximate Conservation Law ................................................... 97
  4.4.1 Preliminary Lemmata .............................................................. 97
  4.4.2 The Notion of Weak Convergence ......................................... 107
  4.4.3 Taking the Limit $\varepsilon \to 0^+$ ......................................................... 109
4.5 Energy Conditions that Ensure Solutions Decay .............................. 118
  4.5.1 Order Relations ......................................................................... 118
  4.5.2 Conditions on the Initial Energy ........................................... 119
4.6 Decay Estimates for the SP System ................................................... 136
4.7 Decay Estimates for the WP System ................................................. 140

Chapter 5 Discussion & Conclusions ............................................................ 144

Bibliography ................................................................................................. 148

Appendix A Notation and Definitions .............................................................. 153

Appendix B Some Classical Analysis ................................................................. 156
  B.1 Useful Inequalities ................................................................................. 156
  B.2 Properties of the Fourier Transform ................................................... 159
  B.3 Results from Classical Analysis ........................................................... 160

Appendix C Additional Proofs ........................................................................ 165

Appendix D A Dirac Notation Primer ............................................................. 167
  D.1 Dirac Formulation ................................................................................. 167
  D.2 Position and Momentum Operators .................................................. 173
# List of Figures

<table>
<thead>
<tr>
<th>Figure</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.1</td>
<td>Variable transformation.</td>
<td>11</td>
</tr>
<tr>
<td>2.2</td>
<td>Potential energies.</td>
<td>27</td>
</tr>
<tr>
<td>2.3</td>
<td>Components of the effective potential.</td>
<td>30</td>
</tr>
<tr>
<td>3.1</td>
<td>Functional dependence of the $L^\infty$ argument.</td>
<td>44</td>
</tr>
<tr>
<td>3.2</td>
<td>Spectrum of the operator $-iA_\beta$.</td>
<td>49</td>
</tr>
<tr>
<td>3.3</td>
<td>A strategy for proving global existence and uniqueness.</td>
<td>53</td>
</tr>
<tr>
<td>3.4</td>
<td>The mapping $F : B_\phi \to B_\phi$.</td>
<td>63</td>
</tr>
<tr>
<td>4.1</td>
<td>Computation of the propagators $G(t)$ and $G(-t)$.</td>
<td>94</td>
</tr>
<tr>
<td>4.2</td>
<td>Behaviour of an explicit ${\theta_n(x)}$ sequence.</td>
<td>100</td>
</tr>
<tr>
<td>4.3</td>
<td>Illustrating that $y(x) = x^2$ is not weak star continuous.</td>
<td>110</td>
</tr>
<tr>
<td>4.4</td>
<td>An analysis of $f(\epsilon, a) = 2(3 + \epsilon)(2 - a)/(4 + 2\epsilon - (3 + \epsilon)a)$.</td>
<td>125</td>
</tr>
<tr>
<td>4.5</td>
<td>Energy densities for $\varphi_1(x)$.</td>
<td>128</td>
</tr>
<tr>
<td>B.1</td>
<td>$\delta_\epsilon(x)$ for various values of $\epsilon$.</td>
<td>163</td>
</tr>
<tr>
<td>B.2</td>
<td>The function $\chi_{[-1,1]} - f_3(x)$.</td>
<td>164</td>
</tr>
</tbody>
</table>
List of Tables

Table 2.1  Possible charge interactions.  ...................................................... 31
Table 3.1  SP regularity for $\beta = 0$ and $\beta \neq 0$.  ............................ 83
Table 4.1  A comparison of SP decay rates.  ............................................... 139
Table 4.2  A comparison of WP decay rates.  ............................................. 142
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To

Mom and Dad
Chapter 1

Introduction

In this dissertation, the Wigner–Poisson (WP) system in the presence of an external Coulomb potential is studied. This system of equations describes the time evolution of the quantum mechanical behaviour of a large ensemble of particles in a vacuum where the long range interactions between the particles can be taken into account. The model also facilitates the introduction of external classical effects. The necessity of studying the behaviour of many-body quantum mechanical models is becoming increasingly important because the characteristic length in many modern VLSI\(^1\) devices is approaching the regime where tunneling effects are becoming more pronounced [49]. Consequently, modern models must be able to bridge the gap between the quantum behaviour and external classical effects such as the applied potential at a bonding site. The WP system is such a model. The model studied in this work has the freedom to allow the states of the system either to attract or repel each other as well as allowing the system as a whole either to attract or repel a Coulomb potential located at the origin.

The quantity \(\rho_w\), known as the Wigner function, was first discovered by Szilard and Wigner [68]. The evolution of this function is governed by the WP system.

\(^1\) VLSI is an abbreviation for the term “very large scale integration”.

The Weyl transform $\rho_w$ of the density matrix $\rho$ allows the quantum dynamics to be cast into a form which allows a direct comparison with the classical analogue. In this description of quantum mechanics, expectation values of quantum mechanical operators are computed by integrating over a phase space rather than through a computation of the trace of the operator.

There are a number of transforms other than the Weyl transform that lead to a similar system. Many of these alternative descriptions have been investigated by Balazs and Jennings [3]. The main advantage of these transformational methods is that one can determine the behaviour of the system by perturbation methods. In addition, the classical behaviour can be extracted by letting $\hbar \to 0$. There is also the advantage of a natural mechanism in which self-consistent field theories appear in the simplest approximation. Some of the resulting equations are the Vlasov equation, time dependent Hartree–Fock equation and the random-phase approximation (linearization of the Hartree approximation). For a statistical mixture of states, the WP system is equivalent to an infinite coupled system of Hartree–Fock equations. This equivalent characterization will be referred to as the Schrödinger–Poisson (SP) system and is demonstrated in this dissertation.

Chapter 2 of this dissertation is primarily concerned with the derivation of the WP system. This is accomplished by using the methods described in [9] with the notation of Leaf [42] to develop in some detail, the Weyl transform of an operator. This procedure allows one to compute the Weyl transform of the $M$-body Hamiltonian with some arbitrary external potential. The result is an exact kinetic equation for $\rho_w$, known as the Wigner equation, which holds for any Hamiltonian that is a function of the position and momentum operators. An explanation of the intuitive meaning of the Wigner function can be found in [3]. It is then shown that making various assumptions on the form of the $M$-body Hamiltonian for a system of $M$ particles leads to a set of equations that are the quantum equivalent of the BBGKY
hierarchy [13]. Further assumptions on the Hamiltonian result in an equation for the Weyl transform of an effective one-particle density function. The WP system is obtained by specifying that the internal potential arises from a Coulomb interaction.

The Wigner–Poisson system without an external Coulomb potential has been studied previously [10, 37]. Brezzi and Markowich [10] proved that if the states of the system repel each other then the Wigner–Poisson system has a unique global solution. This result was extended by Illner, Lange and Zweifel [37] in which an alternative approach was used to show that if the states attracted each other then there still exists a unique global solution. Their method also simplified the analysis of the repulsive case. Reference [37] also obtained decay estimates (in time), a topic not dealt with in [10].

In chapter 3 the question of existence and uniqueness is considered. It is proved that the WP system, with the addition of an external Coulomb potential, has a unique global solution irrespective of the sign of this external field. The technique used is essentially a variation of the method used in [37]. First, the WP system is reduced to a SP system in a fashion analogous to that described by Markowich [10, 48]. A set of necessary and sufficient conditions for a phase space function to be a Wigner distribution [51] is also required in this reduction procedure. The resulting SP system is then shown to have a unique global solution by combining the methods described in [37] with the technique of treating the external Coulomb potential as part of the unperturbed operator as prescribed in the work of Chadam and Glassey [14]. The existence and uniqueness results are presented and compared to the results where there is no external potential [37]. This chapter concludes by lifting the SP system results to the WP system as in [10, 37] at which point the results are again compared to the case with no external potential. As predicted in [10], there is some loss of regularity with the introduction of an external field.

Asymptotic behaviour is discussed in chapter 4. In this analysis the SP system
is considered once again in detail. However, the external potential is no longer treated as part of the unperturbed operator since it is advantageous to use the asymptotic properties of the evolution of the free Schrödinger operator. Because of this, the Coulomb potential is regularized and a pseudoconformal conservation law is developed for all values of the regularization parameter. A weak compactness argument, which uses the regularity results produced in chapter 3, is then used to obtain the pseudoconformal conservation law in the limit as the regularization is removed. The phrase pseudoconformal was introduced by Ginibre and Velo [27] to refer to the nonrelativistic version of conformal invariance. Recently [35, 36] it has come to refer to any approximate conservation law that involves the time dependent position operator.

It is shown in chapter 4 that the total energy $E_{tot}$ of the system is a conserved quantity and can be decomposed into a kinetic ($\|\nabla \Psi(\cdot, t)\|_{L^2}^2/2$) and a configurational ($E_{a,\beta}(t) = 1/2 \int Vn \, dx + \beta \int V_0 n \, dx$) component. If the configurational energy $E_{a,\beta}(t)$ is positive for all $t \geq 0$ then it is proved that this energy decays as $O(t^{-1})$. Moreover, this condition is shown, by a variation of a method described by Dias and Figueira [19], to be equivalent to the decay of the SP system in the sense of $L^p$ for $2 < p < 6$. This generalizes the results found in [19, 37]. This chapter also yields the result that if the total energy $E_{tot}$ is negative, then the SP system cannot decay in the sense of $L^p$ for any $2 < p \leq \infty$. This statement generalizes an observation first made by Chadam and Glassey [14]. An explicit initial wave function is given with the property that when the external potential is repulsive, the solution to the corresponding SP system is guaranteed to decay in time whereas when the external potential is attractive, the solution cannot decay and consequently the SP system must attain some nontrivial asymptotic configuration. Decay estimates for the SP system are compared to the case where there is no external potential [37]. The decay results reported in [37] are typically stronger than those reported for a nonvanishing
Coulomb potential. This is due to the fact that if there is no external potential and the particles repel each other then the conclusion that the configurational energy $E_{\alpha,\beta}(t)$ decays as $O(t^{-1})$ is equivalent to the conclusion that $\|V(\cdot, t)\|_2 = O(t^{-1/2})$. In the presence of an external Coulomb potential such a conclusion cannot be inferred. The last section of this chapter lifts the decay estimates for the SP system to the WP system and again makes a comparison to the case without an external potential. For the SP system, there is a reduction in the rate of decay between the cases with and without the Coulomb potential. However for the corresponding WP system, the reported rate of decay of $\rho_w$ is the same irrespective of the external potential. The consequences of having a nonvanishing external potential manifests itself in a much restricted admissible range of $L^p$ spaces where the decay results of $\|\Theta(V_{\text{eff}})\rho_w(\cdot, t)\|_p$ and $\|n(\cdot, t)\|_q$ are applicable. Specifically, $p = 2$ versus $2 \leq p \leq \infty$ and $1 \leq q \leq 3$ versus $1 \leq q \leq \infty$ for the case with and without the external Coulomb potential respectively.
Chapter 2

The Wigner-Poisson System

2.1 Overview

The objective of this chapter is the formal derivation of the Wigner-Poisson system henceforth referred to as the WP system. A WP system describes the quantum mechanical behaviour of a large ensemble of particles in a vacuum under the influence of an exterior potential field taking into account weak, long range interactions of the particles. This system is the quantum analogue of the Vlasov-Poisson system [29] and as such it is occasionally referred to as the quantum Vlasov-Poisson equation.

In an attempt to make this work as self contained as possible, the WP system is formally developed though a number of stages. The first stage is the definition of the Weyl transform of an operator and the formulation of a number of its properties. Following this is the examination of the the Weyl transform of the density matrix of a quantum mechanical system. Because of its important role in the computation of the expectation value of a given operator, this phase space function is widely referred to as the Wigner function. One may think of the Wigner function as the quantum equivalent of the classical particle distribution function [9].

In the next section, an exact kinetic equation for the Wigner function known as the Wigner or quantum Liouville equation is developed by utilizing the properties
of the Weyl transform. This equation was originally derived in 1932 by Wigner and Szilard [68] as the quantum interpretation of the classical Liouville equation. Together the Weyl transform and the Wigner function describe a quantum mechanical system in terms of phase space functions. The state of the system is described by the Wigner function whose evolution is given by the Wigner equation. Statistical averages of observable quantities of the system are obtained by integrating over the phase space variables [9].

However, as with the classical Liouville equation, there are a number of inherent drawbacks when using the Wigner equation. Although it is exact, a many-body potential that incorporates both short and long range effects is not available for the Hamiltonian. In addition, the dimension of the phase space on which an \(M\)-body Wigner equation is posed is \(6M\), excluding any hope for a numerical solution except for small numbers of particles.

A tractable many-body problem is obtained by considering single particle approximations of the Wigner equation which contain a self-consistent potential to account for many-body effects. This approximation is known as the WP system or quantum Vlasov equation [49]. It is analogous to the classical Vlasov equation in that it arises by developing the quantum mechanical equivalent of the BBGKY hierarchy [13]. The chapter concludes by formally developing this hierarchy in the last section. Sections 2.2 and 2.3 make extensive use of Dirac notation and the reader is referred to appendix D.1 for a summary of its properties.

### 2.2 The Weyl Transformation

In the accepted statistical interpretation of quantum theory, the possible values of a dynamical variable \(A\) are the eigenvalues \(a_\alpha\) of the corresponding (observable)
2.2: The Weyl Transformation

linear Hermitian\(^1\) operator \(A\) in the Hilbert space of state vectors. The probability of observing some state \(|\psi(t)\rangle\) with the particular value \(a_\alpha\) is equal to \(|\langle \phi_\alpha, \psi \rangle|^2\), the square of the modulus of the projection of \(|\psi(t)\rangle\) on the corresponding eigenvector \(|\phi_\alpha\rangle\). A complete or irreducible representation for the given quantum mechanical system is given by a set of commuting observables \(A\) such that their eigenvectors \(|\phi_\alpha\rangle\) span the whole space, i.e. such that any \(|\psi(t)\rangle = \sum_\alpha \langle \phi_\alpha, \psi(t) \rangle \phi_\alpha\).

However, different formulations\(^2\) are possible in which functions in a phase space are associated to both the states and the observed quantities. One example of such a formulation consists in employing for these functions the Weyl transform of the density function (known as the Wigner function) and the Weyl transform of the operator under consideration. This formulation will be subsequently demonstrated for a general \(M\)-particle system. Much of this material has been presented by Leaf [42]. We proceed formally using the properties of the underlying Hilbert space.

In the analysis that follows it will be assumed that all the integrals are convergent and that changes in the order of integration are justified. Under these circumstances, consider the Hilbert space \(\mathcal{H}\) of a quantum mechanical system with \(M\) degrees of freedom. For a system containing \(M\) particles, one may think of \(\mathcal{H} = L^2(\mathbb{R}^{3M})\). Let \(X = \{X_1, X_2, \ldots, X_M\}\) be the Cartesian coordinate operator and \(P = 2\pi \hbar K = 2\pi \hbar \{K_1, K_2, \ldots, K_M\}\) be the conjugate momentum operator, so that the space \(\mathcal{H}\) is spanned by the eigenvectors \(|x\rangle\) of \(X\) or \(|k\rangle\) of \(K\). This notation has the dual advantage of avoiding normalization factors which depend upon \(M\) and having a phase space element \(dx\,dk\) which is independent of \(\hbar\) (\(\hbar := \hbar/2\pi\) where \(\hbar\) is Planck's constant).

\(^1\) To ensure that the eigenvalues of a physical observable are real valued, the corresponding operator must be a Hermitian operator.

\(^2\) Cohen [15], Groenewold [32], Leaf [42], Margenan and Hill [47], Moyal [50], Shirokov [60], Weyl [67], Wigner [68].
2.2: The Weyl Transformation

The commutation rules of the operators $K$ and $X$ read

$$
[K,K] = 0, \quad [X,X] = 0, \quad [K,X] = -\frac{i}{2\pi} U,
$$

(2.1)

where $U$ is the unit Cartesian tensor with components $(i,j = 1,2,\ldots,M)$. Alternatively, the commutation rules may be expressed with the compact expression

$$
x_i k_j - k_j x_i = i/(2\pi) \delta_{ij}.
$$

The sets of eigenvectors $|k\rangle$ and $|x\rangle$ of the momentum and coordinate operators $K$ and $X$ form complete sets for $\mathcal{H}$. The orthogonality relations for these vectors are

$$
<k',k> = \delta(<k'-k>), \quad <x',x> = \delta(<x'-x>)
$$

(2.2.a)

and the unity operators are

$$
\int_{\mathbb{R}^M} |k\rangle \langle k| dk = I = \int_{\mathbb{R}^M} |x\rangle \langle x| dx,
$$

(2.2.b)

with $I$ the unit operator in the Hilbert space. The notation for the Fourier transform is introduced next.

**Definition 2.1** Let $f = f(x)$ be an element of $L^2(\mathbb{R}^M)$. Then

$$
\mathcal{F}f(k) := \int_{\mathbb{R}^M} e^{-2\pi ik \cdot x} f(x) dx
$$

(2.3.a)

denotes the Fourier transform of $f$ and for $g = g(k) \in L^2(\mathbb{R}^M)$,

$$
\mathcal{F}^{-1}g(x) := \int_{\mathbb{R}^M} e^{2\pi ik \cdot x} g(k) dk.
$$

(2.3.b)

is its corresponding inverse.

The connection between the $|x\rangle$ and $|k\rangle$ representations is illustrated by using the transfer matrix

$$
<x,k> = e^{2\pi ik \cdot x}.
$$

(2.4)

---

3 See equation (D.18) of appendix D.
This indicates that

\[
\langle k, \psi(t) \rangle = \int_{\mathbb{R}^3M} \langle k, x \rangle \langle x, \psi(t) \rangle \, dx
\]

\[
= \int_{\mathbb{R}^3M} e^{-2\pi i k \cdot x} \langle x, \psi(t) \rangle \, dx.
\]

Consequently, the momentum basis can be expressed as the Fourier integral representation of the coordinate basis [9].

Consider the identity for a linear operator \( A \) of the Hilbert space

\[
A = \int_{(\mathbb{R}^3M)^4} |x''\rangle \langle x'', k''\rangle \langle k'', Ak'\rangle \langle k', x'\rangle \langle x' | \, dx' \, dx'' \, dk' \, dk''
\]

which can be verified by using the unit operators (2.2.b). Introducing the vector transformation,

\[
\begin{align*}
\text{Position} & \quad \text{Wave number} \\
x'' = x + \eta/2, & \quad k'' = k + \xi/2, \\
x' = x - \eta/2, & \quad k' = k - \xi/2,
\end{align*}
\]

for each of the \( M \) particles, the independent position vectors \( x' \) and \( x'' \) are converted into the centre and relative position vectors, \( x \) and \( \eta \). Simultaneously, the wave number vectors \( k' \) and \( k'' \) are exchanged with \( k \), the centre and \( \xi \), the relative wave number vectors. This transformation is depicted in figure 2.1.

With the use of (2.4) and (2.2.a-b), identity (2.5) decouples under this change of variable into

\[
A = \int_{\mathbb{R}^3M \times \mathbb{R}^3M} A_w(x, k) \Delta(x, k) \, dx \, dk.
\]

The function

\[
A_w(x, k) := \int_{\mathbb{R}^3M} e^{2\pi i k \cdot x} \langle k + \xi/2 | A | k - \xi/2 \rangle \, d\xi
\]

\footnote{See Leaf, B. [42], upon which most of the material in this section is based.}
2.2: The Weyl Transformation

Figure 2.1: Variable transformation.
Graphical representation of the position and wave number transformations for one of the $M$ particles. The left hand side shows the transformation to the centre and relative position coordinates while the right hand side depicts the transformation to the centre and relative wave number coordinates. $P_j(x')$ denotes particle $j$ at position $x'$ whereas $P_j(k')$ denotes particle $j$ at wave number $k'$.

is called the Weyl transformation\(^5\) of the quantum operator $A$ with respect to the coordinate operators $K$ and $X$. If $A$ is Hermitian, the function $A_w(x, k)$ is real, as follows from equation (2.7). The Hermitian operator

$$
\Delta(x, k) := \int_{\mathbb{R}^M} e^{2\pi i k \cdot x} (x + \eta/2) (x - \eta/2) d\eta
$$

is independent of $A$ and does not treat the variables $k$ and $x$ in a symmetric fashion.

**Definition 2.2** The Weyl transformation of the operator $A : \mathcal{H} \rightarrow \mathcal{H}$ is

$$
A_w(x, k) := \int_{\mathbb{R}^M} e^{2\pi i \xi \cdot x} (k + \xi/2|A|k - \xi/2) d\xi.
$$

Two lemmas are required in order to develop a symmetric expression for $\Delta(k, x)$.

---

\(^5\) Some authors [9, 10, 37] refer to this operation as the Wigner transformation.
Lemma 2.3 If $|x\rangle$ is an eigenvector of the Cartesian coordinate operator $X$ in the Hilbert space $\mathcal{H}$ then formally

$$|x + \eta/2\rangle = e^{-2\pi i \eta \cdot K} |x - \eta/2\rangle$$

where $K$ is the momentum operator defined in equation (2.1).

Proof. Using the expression (2.4) and expanding over momentum eigenstates using (2.2.b) allows the momentum operator to act directly on the momentum states. That is,

$$e^{-2\pi i \eta \cdot K} |x - \eta/2\rangle = \int_{\mathbb{R}^3} e^{-2\pi i \eta \cdot K} |k\rangle \langle k, x - \eta/2| \text{dk}$$

$$= \int_{\mathbb{R}^3} e^{-2\pi i \eta \cdot k} e^{-2\pi i k \cdot (x - \eta/2)} |k\rangle \text{dk}.$$ 

Completing the integration gives the left hand side. □

Lemma 2.4 If $|x\rangle$ is an eigenvector of the Cartesian coordinate operator $X$ in the Hilbert space $\mathcal{H}$ then formally

$$|x\rangle \langle x| = \delta(X - x) := \int_{\mathbb{R}^3} e^{2\pi i \xi \cdot (X - x)} d\xi.$$  

(2.11)

Proof. For any $|x'\rangle$ in the complete set of eigenvectors corresponding to the $X$ operator

$$|x\rangle \langle x, x'| = \delta(x - x') |x\rangle$$

$$= \int_{\mathbb{R}^3} e^{2\pi i \xi \cdot (x - x')} |x\rangle d\xi$$

$$= \int_{\mathbb{R}^3} e^{2\pi i \xi \cdot (X - x')} |x\rangle d\xi$$

where the $\delta$ function representation on $\mathbb{R}^3$

$$\delta(x - x') = \int_{\mathbb{R}^3} e^{2\pi i \xi \cdot (x - x')} d\xi = \delta(x' - x)$$

has been utilized. □
Continuing with the symmetric construction of $\Delta(x, k)$, equation (2.10) is substituted into (2.8) to yield the projection operator

$$|x - \eta/2\rangle\langle x - \eta/2|.$$ 

Using expression (2.11) of lemma 2.4, equation (2.8) becomes

$$\Delta(x, k) = \int_{\mathbb{R}^3} e^{2\pi i \eta (k - K)} e^{-2\pi i \xi (x + \eta/2 - z)} d\xi d\eta. \tag{2.12}$$

Utilizing the commutation rules (2.1) one finds the commutator

$$[2\pi i \eta \cdot (k - K), 2\pi i \xi \cdot (x - \eta/2 - X)] = [2\pi i \eta \cdot K, 2\pi i \xi \cdot X] = 2\pi i \xi \cdot \eta.$$

Since this is a scalar, both operators $2\pi i \eta \cdot (k - K)$ and $2\pi i \xi \cdot (x - \eta/2 - X)$ commute with their commutator which validates the use of the operator identity

$$e^A e^B = e^{A+B+\frac{1}{2}[A,B]}.$$

Hence, equation (2.12) can be expressed in the symmetric form

$$\Delta(x, k) = \int_{\mathbb{R}^3} e^{2\pi i \xi \cdot (x - X) + \eta \cdot (k - K)} d\xi d\eta. \tag{2.13}$$

If the roles of $x$ and $k$ are reversed and the steps in the above argument retraced, this symmetric form yields additional expressions. This procedure yields an expression for $\Delta(x, k)$ which is the counterpart of equation (2.8):

$$\Delta(x, k) = \int_{\mathbb{R}^3} e^{2\pi i \xi \cdot x} |k - \xi/2\rangle\langle k + \xi/2| d\xi. \tag{2.14}$$

To summarize, there are three equivalent expressions for the Hermitian operator $\Delta(x, k)$. The initial expression (2.8) involves an integration over the spatial variable $x$. The fact that $\delta(x) = \delta(-x)$ has been used.

---

6 The fact that $\delta(x) = \delta(-x)$ has been used.

7 Valid for any operators $A$ and $B$ that commute with their commutator [3].
2.2: The Weyl Transformation

\[ \eta. \] This was transformed to the relation (2.13) which treats the \( k \) and \( z \) variables in a symmetric fashion. Using the symmetry of the \( k \) and \( z \) and retracing though the argument that generated relation (2.13), revealed expression (2.14) which involves an integration over the momentum variable \( \xi \). As a result, relation (2.14) is considered the counterpart of expression (2.8).

These various expressions for \( \Delta(x, k) \) allow \( A_w(x, k) \), the Weyl transform of the operator \( A \), to be expressed in different forms, all of which revolve around the expression for the trace of an operator. Since the trace of the operator \( A \) may be written in terms of the complete set \( |k\rangle \) as

\[ \text{Tr } A = \int_{\mathbb{R}^{2M}} \langle k, Ak \rangle dk, \]

one has the identity

\[ \text{Tr } (A|k''\rangle\langle k'|) = \int_{\mathbb{R}^{2M}} \langle k, Ak'' \rangle \langle k', k \rangle dk = \langle k', Ak'' \rangle. \]  \hspace{1cm} (2.15)

The identity (2.15) illustrates the connection between expression (2.7) for \( A_w(x, k) \) and expression (2.14) for \( \Delta(x, k) \) as the concise formula

\[ A_w(x, k) = \text{Tr } [\Delta(x, k)]. \] \hspace{1cm} (2.16)

With (2.8) for \( \Delta(x, k) \), the alternative form for the trace

\[ \text{Tr } A = \int_{\mathbb{R}^{2M}} \langle x, Ax \rangle dx \] \hspace{1cm} (2.17)

and an application of expression (2.16), one finds the counterpart of (2.7):

\[ A_w(x, k) = \int_{\mathbb{R}^{2M}} e^{2\pi i \eta k} \langle x - \eta/2, A|x + \eta/2\rangle d\eta. \] \hspace{1cm} (2.18)

By letting \( \{u_j\}_{j \in \mathbb{N}} \) be an orthonormal basis for \( \mathcal{H} \), expression (2.18) becomes

\[ A_w(x, k) = \int_{\mathbb{R}^{2M}} e^{2\pi i \eta k} \sum_{l, m} u_l(x - \eta/2) \bar{u}_m(x + \eta/2) \langle u_l, A u_m \rangle d\eta. \]
2.2: The Weyl Transformation

This form of the Weyl transform coincides with the definition used in [9].

The expressions (2.9) and (2.18) show that the set of operators in Hilbert space may be mapped onto their Weyl transforms \( A_w(x, k) \). By using the various representations of the operator \( \Delta(x, k) \) given by expressions (2.8), (2.13) and (2.14) a given function \( A_w(x, k) \) can be used to generate an operator \( A \).

An interesting example is obtained if one uses the symmetric expression (2.13) for \( \Delta(x, k) \) and makes the replacement \( \xi \to -\xi \), \( \eta \to -\eta \), so that expression (2.6) becomes

\[
A = \int_{(R^3)^4} A_w(x, k) e^{2\pi i [\xi (x-x) + \eta (K-k)]} \, dk \, dx \, d\xi \, d\eta. \tag{2.19}
\]

By defining the Fourier transform \( \mathcal{F}A_w(\xi, \eta) \) of \( A_w(x, k) \) as

\[
\mathcal{F}A_w(\xi, \eta) = \int_{R^3 \times R^3} e^{-2\pi i [\xi x + \eta \eta]} A_w(x, k) \, dk \, dx \tag{2.20.a}
\]

with inverse

\[
A_w(x, k) = \int_{R^3 \times R^3} e^{2\pi i [\xi x + \eta \eta]} \mathcal{F}A_w(\xi, \eta) \, d\xi \, d\eta, \tag{2.20.b}
\]

relation (2.19) may be written as

\[
A = \int_{R^3 \times R^3} e^{2\pi i [\xi X + \eta K]} \mathcal{F}A_w(\xi, \eta) \, d\xi \, d\eta. \tag{2.21}
\]

Accordingly, the prescription for obtaining the quantum operator \( A(X, K) \) corresponding to a Weyl transform \( A_w(x, k) \) is to replace \( k \) and \( x \) in the Fourier representation (2.20.b) by the operators \( K \) and \( X \). This is the same prescription originally proposed by Weyl [67] for obtaining the quantum operator from a function of the classical Cartesian coordinates and momenta. This prescription is incorrect [61] since the Weyl transform defined in equation (2.7) is not the same as the classical function. The latter is obtained by taking the classical limit \( \hbar \to 0 \) of the Weyl transform. To extract the classical limit with the notation used here requires that one first replace the wave number operator \( K \) with the scaled momentum operator \( P/2\pi\hbar \).
There are a number of desirable properties enjoyed by the Weyl transform of various operators which will be detailed in the propositions that follow. Most of this subsequent analysis has appeared in the joint paper [9] as well as various other publications [3, 50, 51, 64]. The main reason for the interest in the Weyl transform is the computation of the trace of various operators.

**Proposition 2.5** For every trace class operator $A$,

$$\text{Tr } A = \int_{\mathbb{R}^M \times \mathbb{R}^M} A_w(x, k) \, dk \, dx.$$  \hfill (2.22)

*(If $A$ is not trace class, the integral is unbounded.)*

**Proof.** The simple proof is based on the fact that the $dk$ integral of (2.18) gives $\delta(\eta)$ which leaves us with the expression (2.17) for the trace of an operator. \hfill \Box

A similar proof gives the result:

**Proposition 2.6** Let $A, B$ be trace class operators in $\mathcal{H}$ such that $AB$ is trace class. Then

$$\text{Tr } AB = \int_{\mathbb{R}^M \times \mathbb{R}^M} A_w(x, k)B_w(x, k) \, dk \, dx.$$  \hfill (2.23)

This result explains one of the main advantages with using the Weyl representation. Typically when computing traces, there is a sum over intermediate states which is not the case in the Weyl representation.

The real variables $x$ and $k$ may be thought of as the classical position and momentum variables, as is now explained.

**Proposition 2.7** Let the operator $A$ be a function of $X$ alone; $A = A(X)$. Then $A_w(x, k) = A(x)$. Similarly if the operator $B = B(K)$, then $B_w(x, k) = B(k)$.

**Proof.** Since $A(X)$ is a multiplication operator in the $x$-representation [43, 65], the inner product in equation (2.18) can be written as

$$\langle x - \eta/2 | A(X) | x + \eta/2 \rangle = \langle x - \eta/2 | A(x + \eta/2) | x + \eta/2 \rangle$$
\[ = A(x + \eta/2)(x - \eta/2, x + \eta/2) \]
\[ = A(x + \eta/2)\delta(\eta). \]

As a result,
\[ A_w(x, k) = \int_{\mathbb{R}^{3M}} e^{2\pi i \eta \cdot k} A(x + \eta/2)\delta(\eta) \, d\eta = A(x) \]
as required.

The proof of the second half of proposition 2.7, concerning \( B(K) \) is similar, except that one uses expression (2.7) for the Weyl transform and the fact that in momentum space, \( B(K) \) becomes the multiplication operator \( B(k) \). □

We consider this proposition sufficient justification for viewing the real variables \( x \) and \( k \) as the classical position and momentum \((3M)\) vectors of the system. In the same way, the Weyl transform of the density matrix \( \rho \) will be shown to have some similarity to the classical distribution function of statistical mechanics.

The last result of this section will prove to be useful in the derivation of the Wigner equation. It determines how to compute the Weyl transform of the commutator of two operators. It is stated without proof.

**Proposition 2.8** If \( A \) and \( B \) are both operators in the Hilbert space \( \mathcal{H} \) then the Weyl transform of their commutator \( C = [A, B] = AB - BA \) is given by
\[ [A, B]_w(x, k) = \left[ A_w \left( x + \frac{i}{4\pi} \nabla_k, k - \frac{i}{4\pi} \nabla_x \right) - A_w \left( x - \frac{i}{4\pi} \nabla_k, k + \frac{i}{4\pi} \nabla_x \right) \right] B_w(x, k). \]
The proof can be found in any of the standard references [3, 32, 42].

The computation of the Weyl transform of various operators and specialized techniques for their evaluation can be found in various texts on electrodynamics [17] or the paper by Groenewold [32]. The definition of the Weyl transform has been studied by many authors [3, 51, 64]. Unfortunately, different authors use various definitions for the momentum as well as differing on the definition of the Fourier
transform. This accounts for the seemingly different formulae seen throughout the literature.

2.3 The Wigner Function

Quantum averages, or expectation values, are computed according to

$$\langle A \rangle = \text{Tr} \ \rho A. \quad (2.24)$$

Proposition 2.6 explains how to compute such averages by integrating over the phase space $\mathbb{R}^M_k \times \mathbb{R}^M_k$, in analogy with statistical mechanics. For this reason, one defines the Wigner function $\rho_w(x, k)$, as the Weyl transform of the density matrix $\rho$ [65]. If the wave function of a system is indeterminate, it may still be described as the projection sum over the states of the ensemble [8]. Specifically, if the states $|\Psi\rangle = \{|\psi_j\rangle\}_{j \in \mathbb{N}}$ of the ensemble systems are distributed with probabilities $\{\lambda_j\}_{j \in \mathbb{N}}$ then the density operator may be written as [43, 65]

$$\rho = \sum_j \lambda_j \rho_j, \quad 0 \leq \lambda_j \leq 1, \quad \sum_j \lambda_j = 1 \quad (2.25)$$

where $\rho_j = |\psi_j\rangle\langle\psi_j|$ is the orthogonal projection onto the state vector $|\psi_j\rangle$. For a system in a pure state, $|\psi_j\rangle$ say, $\lambda_j = \delta_{j,j_0}$. The $|\psi_j\rangle$ obey the time-dependent Schrödinger equation

$$i\hbar \frac{\partial |\psi_j\rangle}{\partial t} = H|\psi_j\rangle, \quad |\psi_j(t = 0)\rangle = |\varphi_j\rangle, \quad \forall j \quad (2.26)$$

where $H$ is the Hamiltonian of the $M$-body system.

Equation (2.18) (the definition of the Weyl transform) and expression (2.25) for the density operator yield

$$\rho_w(x, k) = \sum_j \lambda_j \int_{\mathbb{R}^M_k} e^{2\pi i k \cdot \eta} \overline{\psi}_j(x + \eta/2) \psi_j(x - \eta/2) \, d\eta. \quad (2.27)$$
2.3: The Wigner Function

Except for the sum over \( j \), this is the formula with which Wigner [68] began his treatment. It is also the formula which Markowich [48] derived as a solution of the Wigner equation.

Since \( \text{Tr } \rho = \sum_j \lambda_j = 1 < \infty \), \( \rho \) is trace class. Therefore, using proposition 2.5, the normalization \( \text{Tr } \rho = 1 \) implies that

\[
\int_{\mathbb{R}^3 M \times \mathbb{R}^3 M} \rho_w(x, k) \, dk \, dx = 1.
\]

This Wigner function cannot be a true distribution, because it is not positive; it is real because \( \rho \) is self-adjoint. It is important to note that the Weyl transform of a general operator is not necessarily real [51]. However, the spatial density \( n(x) \) is positive

\[
n(x) := \int_{\mathbb{R}^3 M} \rho_w(x, k) \, dk = \sum_j \lambda_j |\psi_j(x)|^2.
\]

In fact, (2.28) is the usual expression for the spatial density in standard quantum mechanics [65]. Similarly, the density in momentum space is readily seen, by integrating \( \rho_w \) over \( x \) and using relation (2.9) for the Weyl transform, to be

\[
h(k) := \int_{\mathbb{R}^3 M} \rho_w(x, k) \, dx = \sum_j \lambda_j \int_{\mathbb{R}^3 M} \int_{\mathbb{R}^3 M} e^{2\pi i x \cdot \xi} \overline{\psi_j(k - \xi/2)} \psi_j(k + \xi/2) \, d\xi \, dx
\]

\[
= \sum_j \lambda_j \int_{\mathbb{R}^3 M} \delta(\xi) \overline{\psi_j(k - \xi/2)} \psi_j(k + \xi/2) \, d\xi
\]

\[
= \sum_j \lambda_j |\psi_j(k)|^2
\]

which is also standard. As with a classical distribution function [13], integrating \( \rho_w \) over momentum space yields the spatial density and integrating over space gives the momentum density. The spatial and momentum densities can also be used to
calculate expectation values. Equation (2.24), proposition 2.6 and proposition 2.7 with \( A = A(X) \) gives

\[
\langle A \rangle = \text{Tr} \rho A = \int_{\mathbb{R}^4} A_w(x, k) \rho_w(x, k) \, dk \, dx
\]

\[
= \int_{\mathbb{R}^4} A(x) \rho_w(x, k) \, dk \, dx
\]

\[
= \int_{\mathbb{R}^4} A(x) \rho(x) \, dx
\]

(2.30.a)

while if \( B = B(K) \)

\[
\langle B \rangle = \int_{\mathbb{R}^4} B(k) \rho(k) \, dk.
\]

(2.30.b)

More generally, for any operator \( C \)

\[
\langle C \rangle = \int_{\mathbb{R}^4} C_w(x, k) \rho_w(x, k) \, dk \, dx.
\]

(2.30.c)

### 2.4 The Wigner Equation

A kinetic equation for \( \rho_w \) can be derived by using the fact that, in the Schrödinger picture, \( \rho(x, k, t) \) is the solution of the von Neumann equation [62]

\[
i\hbar \frac{\partial \rho}{\partial t} = [H, \rho],
\]

with \( H = H(X, K) \) the Hamiltonian of the system under consideration. By taking the Weyl transform of this equation and using proposition 2.8 the exact quantum mechanical equation

\[
i\hbar \frac{\partial \rho_w}{\partial t} = \left[ H_w\left( x + \frac{i}{4\pi} \nabla_k, k - \frac{i}{4\pi} \nabla_x \right), H_w\left( x - \frac{i}{4\pi} \nabla_k, k + \frac{i}{4\pi} \nabla_x \right) \right] \rho_w
\]

(2.31)

is obtained. It should be emphasized that this equation holds for any Hamiltonian which is a function of the position and momentum operators.

As an application of the material in the previous sections assume for the moment that the Hamiltonian is of the form

\[
H = \frac{p^2}{2m} + V(X, t)
\]

(2.32)
where \( V(X,t) \) is any real valued potential energy function. By defining a kinetic energy operator \( T(K) \) which depends only on the momentum operator \( K \) one has
\[
H(X, K, t) = \frac{4\pi^2 \hbar^2}{2m} K^2 + V(X, t) = T(K) + V(X, t). \tag{2.33}
\]
Proposition 2.7 indicates that \( T_w(x, k) = T(k) \) and \( V_w(x, k, t) = V(x, t) \) so that
\[
\begin{align*}
T_w \left( x + \frac{i}{4\pi} \nabla_k, k - \frac{i}{4\pi} \nabla_x \right) - T_w \left( x - \frac{i}{4\pi} \nabla_k, k + \frac{i}{4\pi} \nabla_x \right) & = T \left( k - \frac{i}{4\pi} \nabla_x \right) - T \left( k + \frac{i}{4\pi} \nabla_x \right) \\
& = \frac{4\pi^2 \hbar^2}{2m} \left[ \left( k - \frac{i}{4\pi} \nabla_x \right)^2 - \left( k + \frac{i}{4\pi} \nabla_x \right)^2 \right] \\
& = -i\hbar \frac{2\pi \hbar k}{m} \cdot \nabla_x \tag{2.34}
\end{align*}
\]
and
\[
\begin{align*}
V_w \left( x + \frac{i}{4\pi} \nabla_k, k - \frac{i}{4\pi} \nabla_x, t \right) - V_w \left( x - \frac{i}{4\pi} \nabla_k, k + \frac{i}{4\pi} \nabla_x, t \right) & = V \left( x + \frac{i}{4\pi} \nabla_k, t \right) - V \left( x - \frac{i}{4\pi} \nabla_k, t \right). \tag{2.35}
\end{align*}
\]
Combining equations (2.31), (2.33), (2.34) and (2.35) and dividing by a factor of \( i\hbar \) yield
\[
\frac{\partial \rho_w}{\partial t} + \frac{2\pi \hbar k}{m} \cdot \nabla_x \rho_w + \frac{i}{\hbar} \left[ V \left( x + \frac{i}{4\pi} \nabla_k, t \right) - V \left( x - \frac{i}{4\pi} \nabla_k, t \right) \right] \rho_w = 0. \tag{2.36}
\]
The last term of the left hand side can be simplified as follows. Consider the expression (2.27) for the Wigner function\(^8\) which is repeated here for convenience
\[
\rho_w(x, k, t) = \sum_j \lambda_j \int_{\mathbb{R}^3} e^{2\pi i \eta \cdot k} \overline{\psi}_j(x + \eta/2, t) \psi_j(x - \eta/2, t) \, d\eta.
\]
This expression implies that the Fourier transform with respect to the wave number \( u(x, \eta, t) = \mathcal{F}\rho_w(x, k, t) \) is given by
\[
u(x, \eta, t) = \sum_j \lambda_j \psi_j(x - \eta/2, t) \overline{\psi}_j(x + \eta/2, t). \tag{2.37}
\]
\(^8\) The time dependence is shown explicitly.
Equation (2.27) implies that
\[
\left[ V\left(x + \frac{i}{4\pi} \nabla_k, t\right) - V\left(x - \frac{i}{4\pi} \nabla_k, t\right) \right] \rho_w = \sum_j \lambda_j \int_{\mathbb{R}^3} e^{2\pi i q \cdot k} \left[ V(x - \eta/2, t) - V(x + \eta/2, t) \right] \psi_j(x - \eta/2, t) \overline{\psi}_j(x + \eta/2, t) d\eta. \tag{2.38}
\]
Thus, equation (2.38) can be written as
\[
-\mathcal{F}^{-1} \delta V \mathcal{F} \rho_w \quad \text{with} \quad \delta V = V\left(x + \frac{\eta}{2}, t\right) - V\left(x - \frac{\eta}{2}, t\right). \tag{2.39}
\]
Accordingly, the last term on the left hand side of the expression (2.36) may be expressed as
\[
\left[ V\left(x + \frac{i}{4\pi} \nabla_k, t\right) - V\left(x - \frac{i}{4\pi} \nabla_k, t\right) \right] \rho_w(x, k, t) = -\Theta(V) \rho_w(x, k, t) \tag{2.40}
\]
where \(\Theta(V) = \mathcal{F}^{-1} \delta V \mathcal{F}\) is the pseudo-differential operator with symbol given by the expression (2.39). Introducing the velocity vector \(v\) with components
\[
p_j/m = 2\pi \hbar k_j/m
\]
and putting together equations (2.40) and (2.36) leads to the Wigner equation
\[
\frac{\partial \rho_w}{\partial t} + v \cdot \nabla x \rho_w - \frac{i}{\hbar} \Theta(V) \rho_w = 0. \tag{2.41}
\]
Notice that this equation bears considerable resemblance to the classical Liouville equation [13]
\[
\frac{\partial f}{\partial t} + \frac{p}{m} \cdot \nabla_x f - \nabla_x V \cdot \nabla_p f = 0. \tag{2.42}
\]
To attempt a direct comparison, we start with equation (2.36) rather than the above relation (2.41). Starting at this point allows us to transform to the classical momentum variable \(p = 2\pi \hbar k\). Taking the Fourier transform of equation (2.36) with respect to the wave number variable \(k\) gives
\[
\frac{\partial \hat{\rho}_w}{\partial t} + \frac{2\pi \hbar}{m} \frac{i}{2\pi} \nabla \cdot \nabla \hat{\rho}_w - \frac{i}{\hbar} \left[ V\left(x + \frac{\eta}{2}, t\right) - V\left(x - \frac{\eta}{2}, t\right) \right] \hat{\rho}_w = 0
\]
2.4: The Wigner Equation

with \( \hat{\rho}_w = \hat{\rho}_w(x, \eta, t) \) since \( \mathcal{F}(2\pi ku) = i\nabla_\eta(\mathcal{F}u) \). Next this expression is rewritten in terms of a conjugate momentum \( \zeta = \eta/\hbar \). This transformation is required since \( \eta \) has the dimensions of length whereas \( \zeta \) has the dimensions of a conjugate momentum. This procedure results in the expression

\[
\frac{\partial \hat{\rho}_w}{\partial t} + \frac{i}{m}\nabla_\zeta \cdot \nabla_x \hat{\rho}_w - \frac{i}{\hbar} \left[ V\left(x + \frac{\hbar \zeta}{2}, t\right) - V\left(x - \frac{\hbar \zeta}{2}, t\right) \right] \hat{\rho}_w = 0.
\]

This is to be compared to the Fourier transform of the classical Liouville equation (2.42) with respect to momentum [48]

\[
\frac{\partial \hat{f}}{\partial t} + \frac{i}{m}\nabla_\zeta \cdot \nabla_x \hat{f} - i\nabla_x V \cdot \zeta \hat{f} = 0.
\]

The Fourier transform of the classical particle density \( f = f(x, p, t) \) with respect to momentum has been denoted as \( \hat{f}(x, \zeta, t) \). Letting \( \hbar \to 0 \), formally

\[
\frac{i}{\hbar} \left[ V\left(x + \frac{\hbar \zeta}{2}, t\right) - V\left(x - \frac{\hbar \zeta}{2}, t\right) \right] \to i\zeta \cdot \nabla_x V
\]

and the Wigner equation (2.41) turns into the classical Liouville equation (2.42).

It has already been previously mentioned that the Wigner equation (2.41) is an exact equation for the \( M \)-body system with the given Hamiltonian (2.32). Unfortunately, a functional form for the potential energy \( V(x) \) that incorporates both the long range and short range effects is not available. This problem is alleviated by making various assumptions on the density matrix and integrating out the effects of all the \( M \) particles except one. The resulting equation, known as the WP system, is a Wigner equation for the one remaining body with an additional self-consistent expression for the potential energy.
2.5 Derivation of the WP System

Consider $M$ particles all with mass $m$ where each particle has its motion governed by the Schrödinger equation

$$i\hbar\frac{\partial\psi_j}{\partial t} = H\psi_j, \quad j \in \{1, 2, \ldots, M\} \quad (2.43)$$

with the $M$-body Hamiltonian

$$H = \frac{p^2}{2m} + V(x_1, \ldots, x_M, t).$$

Except for explicitly indicating the position vectors for the $M$ particles, this expression for the Hamiltonian is the same as that used in the previous section. The kernel of the ensemble density matrix is then given by the expression

$$\rho(r_1, \ldots, r_M, s_1, \ldots, s_M, t) = \bar{\psi}(r_1, \ldots, r_M, t)\psi(s_1, \ldots, s_M, t), \quad r_j, s_j \in \mathbb{R}^3$$

with $\psi$ the wave function of the ensemble. The $\{r_j\}$ and $\{s_j\}$ values are simply coordinates for each of the $M$ particles. Using the Schrödinger equation (2.43) one can verify that $\rho$ satisfies the Heisenberg equation

$$i\hbar\frac{\partial\rho}{\partial t} = (H_s - H_r)\rho \quad (2.44)$$

with the subscript on the Hamiltonian indicating the spatial dependence.

The first assumption is that the $M$ particles are indistinguishable. If two particles are truly indistinguishable, the Hamiltonian $H$ must be symmetric under arbitrary exchanges of these particles [43]. Hence, this condition is reflected in the density matrix as

$$\rho(r_1, \ldots, r_M, s_1, \ldots, s_M, t) = \rho(r_{\pi(1)}, \ldots, r_{\pi(M)}, s_{\pi(1)}, \ldots, s_{\pi(M)}, t) \quad (2.45)$$

$^9$ The spin coordinates of the particles have been suppressed.
holds for any permutation \( \pi \) of the set \( \{1, \ldots, M\} \) and for all \( r_j, s_j \in \mathbb{R}^3, t \geq 0 \). This condition on the density matrix will hold if the wave function \( \psi \) is antisymmetric

\[
\psi(x_1, \ldots, x_M, t) = \text{sgn}(\pi)\psi(x_{\pi(1)}, \ldots, x_{\pi(M)}, t), \quad \forall \pi, \forall x_j, t \geq 0, \quad (2.46)
\]

or if it is symmetric

\[
\psi(x_1, \ldots, x_M, t) = \psi(x_{\pi(1)}, \ldots, x_{\pi(M)}, t), \quad \forall \pi, \forall x_j, t \geq 0. \quad (2.47)
\]

The choice of symmetry for the spatial portion of the wave function is usually prescribed as a property of the particles involved in the quantum mechanical system rather than a property of the wave function itself. A system of particles that obey (2.46) are called fermions whereas a system of particles that satisfy (2.47) are called bosons.

The characteristic which determines to which of these categories a particle belongs is given by the spin of the particle\(^{10}\). Bosons have integral spin whereas fermions have half-integral spin. Examples of fermions include electrons and neutrons. Photons, \( \pi \) and \( K \) mesons are examples of bosons.

In either case, condition (2.46) or (2.47) imply the condition (2.45) on the density matrix. The Heisenberg equation for the density matrix (2.44) then gives the condition

\[
V(x_1, \ldots, x_M, t) = V(x_{\pi(1)}, \ldots, x_{\pi(M)}, t), \quad \forall \pi, \forall x_j, t \geq 0. \quad (2.48)
\]

Given this condition on the potential energy, it is easy to see that (2.45) is conserved in the evolutionary process.

To model the motion of subensembles, one introduces subensemble density matrices. The density matrix corresponding to \( d \) particles is obtained by evaluating

\(^{10}\) For a more detailed explanation see Gasiorowicz [25].
the density matrix \( \rho \) at \( r_j = s_j \) for \( j = d + 1, \ldots, M \) and by integrating with respect to these coordinates:

\[
\rho^{(d)}(r_1, \ldots, r_d, s_1, \ldots, s_d; t) := \int_{\mathbb{R}^{3(M-d)}} \rho(r_1, \ldots, r_d, u_{d+1}, \ldots, u_M, s_1, \ldots, s_d, u_{d+1}, \ldots, u_M; t) \, du_{d+1} \ldots du_M. \tag{2.49}
\]

As with the density matrix for the \( M \) particles, the trace of the subensemble \( \rho^{(d)} \) represents the position density of the \( d \)-particle ensemble

\[
n^{(d)}(x_1, \ldots, x_d; t) = \rho^{(d)}(x_1, \ldots, x_d, x_1, \ldots, x_d; t).
\]

As well, the subensemble inherits the indistinguishability property

\[
\rho^{(d)}(r_1, \ldots, r_d, s_1, \ldots, s_d; t) = \rho^{(d)}(r_{\pi(1)}, \ldots, r_{\pi(d)}, s_{\pi(1)}, \ldots, s_{\pi(d)}; t)
\]

for all permutations of \( \{1, \ldots, d\} \) and all \( r_j, s_j \in \mathbb{R}^3, t \geq 0 \).

Our second assumption, illustrated in figure 2.2, is that the potential \( V \) is the sum of an external potential energy \( V_e \) and an internal potential energy \( V_i \) stemming from two-particle interactions

\[
V(x_1, \ldots, x_M; t) = \sum_{j=1}^{M} V_e(x_j; t) + \frac{1}{2} \sum_{j=1}^{M} \sum_{k \neq j}^{M} V_i(x_j, x_k)
\]

with

\[
V_i(x_j, x_k) = V_i(x_k, x_j), \quad j, k = 1, \ldots, M.
\]

This gives the Heisenberg equation for \( \rho \) as\(^{11}\)

\[
is \hbar \frac{\partial \rho}{\partial t} = -\frac{\hbar^2}{2m} \sum_{j=1}^{M} (\Delta_{s_j} \rho - \Delta_{r_j} \rho) + \sum_{j=1}^{M} [V_e(s_j, t) - V_e(r_j, t)] \, \rho \\
+ \frac{1}{2} \sum_{j=1}^{M} \sum_{k \neq j}^{M} [V_i(s_j, s_k) - V_i(r_j, r_k)] \, \rho. \tag{2.50}
\]

\(^{11}\) \( \Delta_{s_j} := \frac{\partial^2}{\partial s_{1,j}^2} + \frac{\partial^2}{\partial s_{2,j}^2} + \frac{\partial^2}{\partial s_{3,j}^2} \) is the Laplacian operator with respect to the coordinates \( (s_1, s_2, s_3) \in \mathbb{R}^3 \) of the \( j^{th} \) particle. This is not the Hermitian operator \( \Delta(x, k) \) defined by equation (2.8).
To obtain the equation of motion for $\rho^{(d)}$ one sets $u_j = s_j = r_j$ for $j = d + 1, \ldots, M$ in relation (2.50) and integrates over $\mathbb{R}^{3d+1} \times \cdots \times \mathbb{R}^{3M}$. Assuming that $\rho \to 0$ sufficiently fast as $|s_j| \to \infty, |r_j| \to \infty$, yields the expression

$$i\hbar \frac{\partial \rho^{(d)}}{\partial t} = -\frac{i\hbar^2}{2m} \sum_{j=1}^{d} (\Delta s_j \rho^{(d)} - \Delta r_j \rho^{(d)}) + \sum_{j=1}^{d} [V_0(s_j, t) - V_0(r_j, t)] \rho^{(d)}$$

$$+(M - d) \sum_{j=1}^{d} \int_{\mathbb{R}^3} [V_1(s_j, u_s) - V_1(r_j, u_s)] \rho^{(d+1)}(r_1, \ldots, r_d, u_s, \ldots, u_s, u_s, t)$$

for $1 \leq d \leq M - 1$, with

$$\rho^{(d+1)} = \rho^{(d+1)}(r_1, \ldots, r_d, u_s, \ldots, s_1, \ldots, s_d, u_s, t).$$

The system of equations (2.51.a) constitutes the quantum equivalent of the BBGKY hierarchy [49]. While it is not possible to solve this system exactly for finite $M$, one can extract a particular solution in the limit of arbitrarily large $M$. At this point, suppose that the internal potential energy is of the order $1/M$ so that the total
potential energy generated by each particle

\[ V_{j,t}(x_1, \ldots, x_M, t) = V_e(x_j, t) + \sum_{k=1}^{M} V_i(x_j, x_k) \]

remains finite as the total number of particles \( M \) becomes arbitrarily large. Under this assumption, for fixed \( d \) with \( M \to \infty \), (2.51.a) becomes

\[
i \hbar \frac{\partial \rho^{(d)}}{\partial t} = -\hbar^2 \sum_{j=1}^{d} (\Delta_s \rho^{(d)} - \Delta_r \rho^{(d)}) + \sum_{j=1}^{d} [V_e(s_j, t) - V_e(r_j, t)] \rho^{(d)}
\]

\[ + \sum_{j=1}^{d} \int_{\mathbb{R}^3} [V_i(s_j, u) - V_i(r_j, u)] M \rho^{(d+1)}_{u} \, du. \quad (2.52) \]

The third and final assumption is that the subensembles move independently from each other which is reasonable for small subensembles. This condition is reflected in the so-called Hartree ansatz [25]

\[
\rho^{(d)}(r_1, \ldots, r_d, s_1, \ldots, s_d, t) = \prod_{j=1}^{d} \rho^{(1)}(r_j, s_j, t). \quad (2.53)\]

An equation for the one-particle density matrix \( \rho^{(1)} \) can now be obtained by setting \( d = 1 \) in equation (2.52) and by using the ansatz (2.53) for \( d = 2 \):

\[
i \hbar \frac{\partial \rho^{(1)}}{\partial t} = -\hbar^2 (\Delta_s \rho^{(1)} - \Delta_r \rho^{(1)}) + [V_{\text{eff}}(s, t) - V_{\text{eff}}(r, t)] \rho^{(1)}, \quad r, s \in \mathbb{R}^3, t > 0 \quad (2.54.a)\]

with the effective potential energy given by the equation

\[
V_{\text{eff}}(x, t) = V_e(x, t) + \int_{\mathbb{R}^3} V_i(x, y) M \rho^{(1)}(y, y, t) \, dy. \quad (2.54.b)\]

The difference of the Laplacian operators in (2.54.a) suggests the transformation to the centre of mass and relative position coordinates \((x, \eta)\) defined via

\[
x = \frac{r + s}{2}, \quad \eta = r - s, \quad x, \eta \in \mathbb{R}^3.\]
Multiplying (2.54.a) by $M$ and applying the transformation gives the expression for
\[ u(x(r,s), \eta(r,s), t) = M \rho^{(1)}(r,s,t): \]
\[
\frac{\partial u}{\partial t} + \frac{i \hbar}{m} \nabla_\eta \cdot (\nabla_x u) - \frac{i}{\hbar} \left[ V_{\text{eff}} \left( x + \frac{\eta}{2}, t \right) - V_{\text{eff}} \left( x - \frac{\eta}{2}, t \right) \right] u = 0, \quad x, \eta \in \mathbb{R}^3, t > 0. \tag{2.55}
\]
\[
\text{Taking the inverse Fourier transform with respect to } \eta \text{ results in the expression for } \]
\[ w(x, k, t) = \mathcal{F}^{-1} u(x, \eta, t) \]
\[
\frac{\partial w}{\partial t} + v \cdot \nabla_x w - \frac{i}{\hbar} \Theta (V_{\text{eff}}) w = 0 \tag{2.56.a}
\]
with $v = 2\pi \hbar k / m$. The self-consistent potential energy can also be transformed by noting
\[ M \rho^{(1)}(y,y,t) = u(y, \eta = 0, t) = \int_{\mathbb{R}^3} w(x, k, t) \, dk = n(x, t) \]
which is the number density so that expression (2.54.b) becomes
\[ V_{\text{eff}}(x, t) = V_c(x, t) + \int_{\mathbb{R}^3} V_i(x, y)n(y, t) \, dy, \quad x \in \mathbb{R}^3, t > 0, \tag{2.56.b} \]
where the number density is given as
\[ n(x, t) = \int_{\mathbb{R}^3} w(x, k, t) \, dk. \tag{2.56.c} \]
Equation (2.56.a) is a Wigner equation similar to expression (2.41) which was derived in section 2.4. Expression (2.56.a) with (2.56.b) is called the quantum (or nuclear) Vlasov equation.

The WP system is obtained by specifying that the internal potential energy arises from a Coulomb interaction. For this reason the effective potential energy is chosen to be given as
\[ V_{\text{eff}}(x, t) = \frac{\beta}{4\pi|x|} + \frac{\alpha}{4\pi} \int_{\mathbb{R}^3} \frac{n(y, t)}{|y - x|} \, dy \tag{2.57} \]
with $\alpha, \beta \in \mathbb{R}$. The energy comes from an external point charge of strength $\beta$ at the origin and an extended body of strength $\alpha$ and number density $n(x, t)$. This
The effective potential at the point $x$ is a combination of the fields from the point charge of strength $\beta$ at the origin and the extended charge distribution defined by $n(y, t)$ and having a strength of $\alpha$.

is illustrated in figure 2.3. This addition of an external Coulomb field (attractive or repulsive) of arbitrary strength is considered to be the first step in looking at a periodic lattice of external potentials as one might find in a crystal.

Combining the Wigner equation (2.56.a) with expression (2.57) for the potential energy gives the WP system for $w(x, k, t)$ with an external Coulomb potential. The system (2.56.a), (2.57) with $n(x, t)$ given by (2.56.c) is to be solved subject to the initial condition

$$w(x, k, t = 0) = w_f(x, k).$$

Depending upon the choice of signs for $\alpha$ and $\beta$ the external Coulomb field will either attract ($\beta < 0$) or repel ($\beta > 0$) the particle distribution. As well, the particle distribution as a whole will either tend to coalesce ($\alpha < 0$) or disperse ($\alpha > 0$). Table 2.1 details the four possibilities.
Table 2.1: Possible charge interactions.

Listed are the four possible tendencies of the system. The "Origin" column refers to whether the Coulomb field at the origin either attracts or repels the particle distribution as a whole.

Rather than exhibiting the existence and uniqueness of this WP system directly, the next chapter begins by showing how to convert the quantum Liouville equation into a countable collection of Schrödinger equations all coupled through a self-consistent potential \( V \). This countable collection of Schrödinger equations is referred to as the Schrödinger–Poisson (SP) system. By first proving existence and uniqueness results for the SP system and then reconstructing the WP system, one can obtain existence and uniqueness results for the initial WP system.

We conclude by summarizing below the equations that define the WP system.

One seeks a solution \( w = w(x, k, t), x \in \mathbb{R}^3, k \in \mathbb{R}^3, t \in \mathbb{R} \) of the system of equations

\[
\frac{\partial w}{\partial t} + v \cdot \nabla_x w - \frac{i}{\hbar} \Theta(V_{\text{eff}})w = 0 \tag{2.59.a}
\]

\[
V_{\text{eff}}(x, t) = \frac{\beta}{4\pi|x|} + \frac{\alpha}{4\pi} \int_{\mathbb{R}^3} \frac{n(y, t)}{|y - x|} dy \tag{2.59.b}
\]

where \( \alpha, \beta \in \mathbb{R}, v = 2\pi k/m \) and

\[
n(x, t) = \int_{\mathbb{R}^3} w(x, k, t) dk \tag{2.59.c}
\]

\[
\Theta(V_{\text{eff}}) = V_{\text{eff}} \left( x - \frac{i}{4\pi} \nabla_k \right) - V_{\text{eff}} \left( x + \frac{i}{4\pi} \nabla_k \right). \tag{2.59.d}
\]

The system (2.59.a)–(2.59.d) is to be solved subject to the condition

\[
w(x, k, t = 0) = w_f(x, k). \tag{2.59.e}
\]
The regularity of $w_I(x,k)$ will determine what is meant by a solution. In the next chapter a suitable space on which to study possible solutions is constructed and the regularity properties of any solutions found is described.
Chapter 3

Global Existence and Uniqueness

3.1 Preliminaries

This chapter begins with a restatement of the Wigner-Poisson (WP) system. It should be emphasized that \( w(x, k, t) \) is defined on \( \mathbb{R}^2 \times \mathbb{R}^2 \times [0, \infty) \) and describes the behaviour of an effective one-particle distribution in the presence of many other particles. For brevity the subscript on the potential energy is dropped so that \( V_{\text{eff}} \) will be simply denoted as \( V \). With this change, one arrives at the WP system

\[
\frac{\partial w}{\partial t} + v \cdot \nabla w - \frac{i}{\hbar} \Theta(V) w = 0, \quad x, v \in \mathbb{R}^3, t > 0. \tag{3.1.a}
\]

In the above equation \( \Theta = \mathcal{F}^{-1} \delta V \mathcal{F} \) is the pseudo-differential operator with symbol

\[
\delta V = V \left( x + \frac{\zeta}{2}, t \right) - V \left( x - \frac{\zeta}{2}, t \right), \tag{3.1.b}
\]

\( v = 2\pi\hbar k/m \) and \( V \) is the potential energy\(^1\) given by

\[
V(x, t) = \frac{\beta}{4\pi|x|} + \frac{\alpha}{4\pi} \int_{\mathbb{R}^3} \frac{n(y, t)}{|y - x|} \, dy, \quad \alpha, \beta \in \mathbb{R}, \tag{3.1.c}
\]

\(^1\) In this chapter all integrals are over the space \( \mathbb{R}^3 \) unless otherwise stated.
with \[ n(x, t) = \int_{R^3} w(x, k, t) \, dk. \tag{3.1.d} \]

The system (3.1.a–3.1.d) is to be solved subject to the initial condition\(^2\)

\[ w(x, k, t = 0) = w_f(x, k). \tag{3.1.e} \]

### 3.1.1 WP to SP Transformation

To reduce the WP system to the Schrödinger–Poisson (SP) system a method described by Brezzi and Markowich [10] is utilized. One begins by taking the Fourier transform of equation (3.1.a) which gives an equation for \( \hat{w}(x, \zeta, t) = \mathcal{F}w(x, k, t) \):

\[
\frac{\partial \hat{w}}{\partial t} + \frac{i\hbar}{m} \nabla \zeta \cdot \nabla_x \hat{w} - i \frac{\hbar}{\eta} \left[ V\left(x + \frac{\zeta}{2}, t \right) - V\left(x - \frac{\zeta}{2}, t \right) \right] \hat{w} = 0 \tag{3.2}
\]

where the expressions \( v = 2\pi \hbar k/m \) and \( \mathcal{F}(2\pi ku) = i\nabla \zeta(\mathcal{F}u) \) have been used. This second relationship is a result of our definition of the Fourier transform given by expression (2.3.a). Taking \( \eta = \zeta/\hbar \), changing variables to

\[ r = x + \frac{\hbar \eta}{2} \quad s = x - \frac{\hbar \eta}{2} \]

and defining the dependent variable

\[ z(r, s) = \hat{w}(x(r, s), \eta(r, s)), \tag{3.3} \]

equation (3.2) is transformed to

\[ i\hbar \frac{\partial z}{\partial t} - (H_s - H_r)z = 0. \tag{3.4} \]

In (3.4)

\[ H_x = -\frac{\hbar^2}{2m} \Delta_x + V(x, t) \tag{3.5} \]

\(^2\) The subscript \( f \) denotes initial time \( t = 0 \).
is a single particle quantum mechanical Hamiltonian. Equations (3.4)-(3.5) are to be solved subject to the initial condition

\[ z(r, s, t = 0) = z_l(r, s) \quad (3.6.a) \]

where

\[ z_l(r, s) = \mathcal{T} \mathcal{F} w_l(x, k). \quad (3.6.b) \]

The \( \mathcal{T} \) denotes the coordinate transformation \((x, \eta) \rightarrow (r, s)\).

Suppose that \( w \) is the Wigner transform of some density operator \( \rho \). Up to this point only the fact that \( w \) satisfies a Wigner equation has been used. However, there are solutions to the Wigner equation which cannot be a Wigner transform of any density operator [64]. From this point forward, the assumption will be made that \( w \) is the Wigner transform of some well defined density operator \( \rho \). Hence \( w \) will be replaced by \( \rho_w \) in the work that follows.

In section 2.3 it was found that if \( \rho \) is a density operator, the normalization

\[ \text{Tr } \rho = 1 \quad \Rightarrow \quad \int_{\mathbb{R}^3} \rho_w(x, k, t) \, dk \, dx = 1, \quad t \geq 0. \quad (3.7) \]

Relation (3.3) gives

\[ \rho_w(x, \eta, t) = \int e^{-2i\eta k} \rho_w(x, k, t) \, dk = z(x + \hbar \eta/2, x - \hbar \eta/2, t). \]

For \( \eta = 0 \), one has \( r = x = s \) and

\[ \rho_w(x, 0, t) = \int \rho_w(x, k, t) \, dk = z(x, x, t). \]

Hence, the condition on \( z(r, s, t) \) corresponding to (3.7) is

\[ \int z(r, r, t) \, dr = 1, \quad t \geq 0. \quad (3.8) \]

\(^3\) In this situation there is only one effective particle \((M = 1)\).
Consider the integral operator $Z_t : L^2(\mathbb{R}^3) \to L^2(\mathbb{R}^3)$ defined by

$$
(Z_t f)(s) = \int z_t(r, s)f(r)dr = \int_{\mathbb{R}^3 \times \mathbb{R}^3} e^{-2\pi i(r-s)\cdot k}\rho_{w,t}((r+s)/2, k)f(r)dk dr.
$$

If $\rho_{w,t}$ satisfies the condition to be a Wigner distribution, $z_t(r, s)$ defines a kernel for a positive trace class\(^4\) operator with trace equal to one [51]. Additionally, if $\rho_t$ is a density operator [64], $\rho_t(x, x') = \rho_{w,t}(x', x)$ and from chapter 2, $\rho_{w,t}(x, k)$ is real valued ($\rho_{w,t}(x, k) = \bar{\rho}_{w,t}(x, k)$). This implies that

$$
Z_t(s, r) = \int e^{2\pi i(s-r)\cdot k}\rho_{w,t}((s+r)/2, k)dk = z_t(r, s).
$$

Therefore the integral operator $Z_t$ has the Hilbert-Schmidt property and is self-adjoint [38]. Consequently $z_t$ has a sequence $\{\lambda_j\}_{j \in \mathbb{N}} \in l^2$ of eigenvalues and a complete orthonormal set $\{\psi_j(x) \in L^2(\mathbb{R}^3)\}_{j \in \mathbb{N}}$ of eigenvectors. The Fourier expansion of the kernel $z_t$ then has the form

$$
z_t(r, s) = \sum_{j=1}^{\infty} \lambda_j \bar{\psi}_j(r)\psi_j(s). \quad (3.10)
$$

The series is convergent in $L^2(\mathbb{R}^3 \times \mathbb{R}^3)$.

The representation (3.10) leads one to consider the set of equations

$$
\begin{align*}
i\hbar \frac{\partial \psi_j}{\partial t} &= H\psi_j, \quad x \in \mathbb{R}^3, \ t > 0, \ \forall j \in \mathbb{N} \quad (3.11.a) \\
\psi_j(x, t = 0) &= \varphi_j(x), \quad x \in \mathbb{R}^3, \ \forall j \in \mathbb{N}. \quad (3.11.b)
\end{align*}
$$

By directly substituting the function

$$
z(r, s, t) = \sum_{j=1}^{\infty} \lambda_j \bar{\psi}_j(r, t)\psi_j(s, t) \quad (3.12)
$$

\(^4\) Recall that an operator $T$ is trace class if the eigenvalues of $T$ sum to a finite number, the trace of $T$. An operator that is trace class is necessarily compact [66].
into equation (3.11.a) and using the fact that the Hamiltonian is real valued, one can verify that (3.12) is a solution. From (3.11.b), it is obvious that the function (3.12) satisfies the initial condition (3.10). Thus, the WP system (3.4)-(3.8) has been reduced to the SP system (3.11.a-3.11.b). Recovering the Wigner function \( \rho_w(x, k, t) \) from \( z(r, s, t) \) gives the expression

\[
\rho_w(x, k, t) = \sum_{j=1}^{\infty} \lambda_j \int e^{2\pi i k \cdot \eta} \overline{\psi_j(x + \eta/2, t)} \psi_j(x - \eta/2, t) \, d\eta.
\]

Additionally,

\[
n(x, t) = z(x, x, t) = \sum_{j=1}^{\infty} \lambda_j |\psi_j(x, t)|^2.
\]

A comparison of expression (3.13) with equation (2.27) of chapter 2 indicates that \( \lambda_j \) can be interpreted as the probability of finding the system in the state \( \psi_j(x, t) \).

### 3.1.2 A Change of Variable

Before commencing with the analysis of the SP system, it is useful to rescale the variables so as to eliminate any explicit dependence upon either \( h \) or \( m \). If the SP system was simply a linear equation then this process would be trivial. Since this is a nonlinear, self-consistent system, this rescaling process is described in detail. Our specific interest in is the conversion\(^5\) of

\[
\begin{align*}
\text{(SP)}_h \quad & \begin{cases}
ih \partial_t \tilde{\psi}_j = -\frac{\hbar^2}{2m} \Delta_x \tilde{\psi}_j + \tilde{V} \tilde{\psi}_j \\
\Delta_x \tilde{V} = -\alpha \sum_{j=1}^{\infty} \lambda_j |\tilde{\psi}_j|^2 - \beta \delta(x)
\end{cases} \\
\text{(SP)} \quad & \begin{cases}
i \partial_t \psi_j = -\frac{1}{2} \Delta_x \psi_j + V \psi_j \\
\Delta_x V = -\alpha \sum_{j=1}^{\infty} \lambda_j |\psi_j|^2 - \beta C_{h,m} \delta(x)
\end{cases}
\end{align*}
\]

\(^5\) Partial derivatives will occasionally be denoted by a subscript. For example, \( \partial_t = \frac{\partial}{\partial t} \).
3.1: Preliminaries

where $C_{h,m}$ is some constant that depends on the transformation.

The variables are rescaled via

$$
\tilde{x} = h^{u_1}m^{v_1}x, \quad \tilde{t} = h^{u_2}m^{v_2}t, \quad \tilde{\psi}_j = h^{u_3}m^{v_3}\psi_j, \quad \tilde{V} = h^{u_4}m^{v_4}V, \quad \tilde{\lambda} = h^\sigma m^s \lambda.
$$

The first set of equations follows from

$$
i\hbar \partial_t \tilde{\psi}_j + \frac{\hbar^2}{2m} \Delta_x \tilde{\psi}_j - \tilde{V} \tilde{\psi}_j = h^{u_3+u_4}m^{v_3+v_4} \left( i\hbar^{1-u_2-u_4}m^{-v_2-v_4} \partial_t \psi_j 
+ \frac{1}{2} h^{2-2u_1-u_4}m^{-1-2v_1-v_4} \Delta_x \psi_j - V \psi_j \right)
$$

which gives four relationships: $1 - u_2 - u_4 = 0$, $-v_2 - v_4 = 0$, $2 - 2u_1 - u_4 = 0$ and $-1 - 2v_1 - v_4 = 0$. A second set of equations comes from the equation for the potential:

$$
\Delta_x \tilde{V} = h^{-2u_1+u_4}m^{-2v_1+v_4} \Delta_x V
$$

which implies that $-2u_1 + u_4 - 2u_3 = \sigma$ and $-2v_1 + v_4 - 2v_3 = s$.

Another condition arises by specifying that the transformation of the variables does not affect the overall number of particles. This can be ensured by setting

$$
1 = \int \left| \tilde{\psi}_j \right|^2 d\tilde{x} = h^{2u_3+3u_1}m^{2v_3+3v_1} \int \left| \psi_j \right|^2 dx = h^{2u_3+3u_1}m^{2v_3+3v_1}.
$$

This yields, $2u_3 + 3u_1 = 0$ and $2v_3 + 3v_1 = 0$. Notice that this condition implies that the constant $C_{h,m}$ above depends only upon $\sigma$ and $s$.

There exists a unique solution to the above defined system. In vector notation,

$$
\langle u_1, u_2, u_3, u_4 \rangle = (2,3,-3,-2) + \sigma(-1,-2,3/2,2)
$$

$$
\langle v_1, v_2, v_3, v_4 \rangle = (-1,-1,3/2,1) + s(-1,-2,3/2,2).
$$
Values for $\sigma$ and $s$ are obtained by forcing the total probability of finding a particle to be invariant under the transformation in question. The corresponding condition is

$$1 = \sum_{j=1}^{\infty} \lambda_j = h^\alpha m^s \sum_{j=1}^{\infty} \lambda_j = h^\sigma m^s$$

which will be unity provided $\sigma = s = 0$. This implies that under the rescaling

$$\tilde{x} = \frac{h^2}{m} x, \quad \tilde{t} = \frac{h^3}{m} t, \quad \tilde{\psi}_j = \frac{m^{3/2}}{h^3} \psi_j, \quad \tilde{V} = \frac{m}{h^2} V, \quad \tilde{\lambda} = \lambda,$$

one obtains $C_{h,m} = 1$. Hence the final form of the SP system is recovered:

$$i \partial_t \psi_j = -\frac{1}{2} \Delta_x \psi_j + V \psi_j$$
$$\Delta_x V = -\alpha \sum_{j=1}^{\infty} \lambda_j |\psi_j|^2 - \beta \delta(x).$$

### 3.2 Statement of the Problem

The transformation of the WP into the SP system leads to the consideration of the system

$$i \partial_t \psi_j = -\frac{1}{2} \Delta_x \psi_j + V \psi_j, \quad x \in \mathbb{R}^3, \quad t > 0, \quad \forall j \in \mathbb{N}$$

$$\psi_j(x, t = 0) = \varphi_j(x), \quad x \in \mathbb{R}^3, \quad \forall j \in \mathbb{N}$$

coupled to the potential equation

$$\Delta V = -\alpha \sum_{j=1}^{\infty} \lambda_j |\psi_j|^2 - \beta \delta(x)$$

where $\delta(x)$ is a delta function. This set of equations describes the evolution of a system of quantum states $\{\psi_j(x, t)\}_{j \in \mathbb{N}}$ with $\lambda_j$ the probability of the system being in state $j$. The system interacts under a self-consistent potential $V(x, t)$ which contains a point Coulomb source of strength $\beta$ situated at the origin. Because $\lambda_j$ is
interpreted as the probability of finding the system in state \( j \), one must necessarily have \( 0 \leq \lambda_j \leq 1 \) and \( \sum_j \lambda_j = 1 \).

Factoring out the external Coulomb energy explicitly, the original problem can be viewed as finding a sequence of functions \( \psi_j = \psi_j(x, t), \ x \in \mathbb{R}^3, \ t > 0 \) that satisfy:

\[
\begin{align*}
    i \partial_t \psi_j &= -\frac{1}{2} \Delta \psi_j + V \psi_j + \beta V_0 \psi_j, \quad \forall j \in \mathbb{N}, \\
    V &= \frac{1}{4\pi|x|}, \\
    \Delta V &= -\alpha n(x, t), \\
    n(x, t) &= \sum_{j=1}^{\infty} \lambda_j |\psi_j|^2.
\end{align*}
\]  

(3.15)  

(3.16)

For the remainder of this chapter, \( V \) will refer to only the self-consistent potential energy.

Our purpose is to show that there exists a unique solution to the system of equations (3.15)–(3.16) subject to the initial condition\(^6\)

\[
    \psi_j(x, t = 0) = \varphi_j \in H^1(\mathbb{R}^3), \quad \forall j \in \mathbb{N}. 
\]  

(3.17)

In addition, the normalization conditions,

\[
    \begin{align*}
        (i) \quad 0 &\leq \lambda_j \leq 1 \\
        (ii) \quad \|\varphi_j\|_2 &= 1, \quad \|\lambda_j\|_\text{tv} = 1
    \end{align*}
\]  

(3.18.a)  

(3.18.b)

must hold for all \( j \in \mathbb{N} \).

It will be shown that \( V \) is only a weak solution to (3.16). However, during construction of solutions to (3.16), the right hand side \( n(x, t) \) will always be in some \( L^p(\mathbb{R}^3) \) \((1 \leq p \leq \infty)\). Hence one may use either equation (3.16) or the explicit integral representation of the self-consistent potential energy\(^7\)

\[
    V(x, t) = \frac{\alpha}{4\pi} \int \frac{n(y, t) \ dy}{|y - x|} = \frac{\alpha}{4\pi} \sum_{j=1}^{\infty} \lambda_j \int \frac{|\psi_j(y, t)|^2 \ dy}{|y - x|} 
\]  

(3.19)

\[^6\] A description of the space \( H^1(\mathbb{R}^3) \) can be found in appendix A.

\[^7\] A proof of this statement can be found in the paper by Brezzi and Markowich [10] pp. 53-54.
3.2: Statement of the Problem

(necessarily a real valued quantity).

The sequence of wave functions is denoted by $\Psi = \{\psi_j\}_{j \in \mathbb{N}}$. Moreover, it will be convenient to introduce the following weighted direct sum Hilbert spaces

$$
X := \{\Gamma = \{\gamma_j\}_{j \in \mathbb{N}} : \gamma_j \in L^2(\mathbb{R}^3) \quad \forall j, \|\Gamma\|_X^2 = \sum_j \lambda_j \|\gamma_j\|^2 < \infty\},
$$

$$
Y := \{\Gamma = \{\gamma_j\}_{j \in \mathbb{N}} : \gamma_j \in H^1(\mathbb{R}^3) \quad \forall j, \|\Gamma\|_Y^2 = \sum_j \lambda_j \|\gamma_j\|_{1,2}^2 < \infty\},
$$

$$
Z := \{\Gamma = \{\gamma_j\}_{j \in \mathbb{N}} : \gamma_j \in H^2(\mathbb{R}^3) \quad \forall j, \|\Gamma\|_Z^2 = \sum_j \lambda_j \|\gamma_j\|_{2,2}^2 < \infty\}.
$$

It is understood that differential and multiplication operators acting on sequences of wave functions are defined componentwise. Since it has already been assumed that our region of integration extends over $\mathbb{R}^3$ unless specified otherwise, $L^2(\mathbb{R}^3)$ will be denoted as $L^2$ for the rest of this chapter. Accordingly, $H^1(\mathbb{R}^3)$ and $H^2(\mathbb{R}^3)$ will be abbreviated to $H^1$ and $H^2$ respectively. As an example, condition (3.18.b) yields

$$
\|\Phi\|_X^2 = \sum_{j=1}^{\infty} \lambda_j \|\varphi_j\|^2 = \sum_{j=1}^{\infty} \lambda_j = 1.
$$

Also notice that the definition of $z(r, s, t)$ as

$$
z(r, s, t) = \sum_{j=1}^{\infty} \lambda_j \overline{\psi}_j(r, t)\psi_j(s, t)
$$

implies that

$$
\|z(\cdot, \cdot, t)\|_{L^2(\mathbb{R}^3 \times \mathbb{R}^3)} \leq \sum_{j=1}^{\infty} \lambda_j \|\overline{\psi}_j(\cdot, t)\psi_j(\cdot, t)\|_{L^2(\mathbb{R}^3 \times \mathbb{R}^3)}
$$

$$
= \sum_{j=1}^{\infty} \lambda_j \|\psi_j(\cdot, t)\|_2^2 = \|\Psi\|_X^2.
$$

Through the use of such inequalities, properties of the SP problem (3.15)-(3.18.b) can be transferred to the WP problem (3.4)-(3.8).
3.3 Self-Adjointness on $Y$

Defining a linear operator $A_\beta$ by $D(A_\beta) = Y \subset X$ with $\beta \in \mathbb{R}$ and

$$A_\beta \Psi = -i \left( \frac{\Delta}{2} - \beta V_0 \right) \Psi$$

for $\Psi \in D(A_\beta)$, the initial value problem (3.15)-(3.17) can be rewritten as

$$\frac{d\Psi}{dt} + A_\beta \Psi + iJ(\Psi) = 0$$

(3.20)

$$\Psi(0) = \Phi \in Y,$$  

(3.21)

where $J(\Psi) = V(\Psi)\Psi$ and $V(\Psi)$ is given either by (3.16) or (3.19).

To consider the Hamiltonian $-iA_\beta$, it is useful to introduce the notion of relative boundedness. An operator $A$ is relatively bounded with respect to $T$, or $T$-bounded, if $D(A) \supset D(T)$ and there exists some $C > 0$ such that

$$\|Au\| \leq C(\|u\| + \|Tu\|), \quad u \in D(T).$$

If $A$ is $T$-bounded, then the infimum of all numbers $b \geq 0$ for which there exists some $a > 0$ such that

$$\|Au\| \leq a\|u\| + b\|Tu\|, \quad \forall u \in D(T),$$

is called the $T$-bound of $A$. Using this concept, one has the theorem due to Rellich as cited in Kato [40], p. 287:

**Theorem 3.1 (Kato-Rellich).** Let $T$ be self-adjoint. If $A$ is symmetric and $T$-bounded with $T$-bound smaller than one, then $T + A$ is self-adjoint. In particular, $T + A$ is self-adjoint if $A$ is bounded and symmetric with $D(A) \supset D(T)$.

---

8 For any operator $T$, $D(T)$ denotes the domain of $T$. 

3.3: Self-Adjointness on Y

**Proof.** The proof can be found in Kato [40], p. 288. □

This theorem reveals a method for showing that the operator $-iA_\beta$ is self-adjoint. First show that $-iA_0 = -\Delta/2$ is self-adjoint and then show that for any $\beta \in \mathbb{R}$, the operator $\beta V_0$ is symmetric and relatively bounded with respect to $-\Delta/2$ with a $-\Delta/2$-bound less that one.

### 3.3.1 Self-Adjointness of $-iA_0$ on $X$

The first step in showing the self-adjointness of the perturbed operator $-iA_\beta$ on the space $Y$ is to prove that the unperturbed operator $-iA_0$ is self-adjoint on $X$.

**Lemma 3.2** The operator $-iA_0$ is self-adjoint in $X$.  

**Proof.** Integrating by parts yields

$$
\langle v, -\Delta u/2 \rangle = -\sum_{j=1}^{\infty} \lambda_j \int \bar{v}_j \cdot \Delta u_j/2 \, dx = \sum_{j=1}^{\infty} \lambda_j \int \Delta \bar{u}_j/2 \cdot u_j \, dx = -\sum_{j=1}^{\infty} \lambda_j \int \Delta v_j/2 \cdot \bar{u}_j \, dx = \langle -\Delta v/2, u \rangle
$$

which implies that $-iA_0 = -\Delta/2$ is symmetric. If $-iA_0$ is symmetric then $-iA_0$ is self-adjoint provided for every $\lambda$ with $\text{Im} \lambda \neq 0$, the range of $\lambda I - (-iA_0)$ is dense\(^9\) in $X$.

Define the space

$$
\mathcal{C} := \{ \Gamma = \{ \gamma_j \}_{j \in \mathbb{N}} : \gamma_j \in C^\infty_0(\mathbb{R}^3) \ \forall j, \| \Gamma \|_\mathcal{C} = \sum \lambda_j \| \gamma_j \|_\infty < \infty \}. 
$$

It is enough to show that $-iA_0$ is self-adjoint in $\mathcal{C}$, since $\mathcal{C}$ is dense\(^10\) in $X$. Let $\mathcal{V} = \{ v_j \}_{j \in \mathbb{N}} \in \mathcal{C}$ then using the Fourier transform\(^11\), the solution of $(\lambda I + iA_0)U = \mathcal{V}$ is

$$
U(x) = \frac{1}{(2\pi)^{3/2}} \int \frac{\hat{\mathcal{V}}(\xi)e^{ix\cdot\xi}}{\lambda + |\xi|^2/2} \, d\xi.
$$

\(^9\) See Pazy [54] p. 223.  

\(^10\) A generalization of theorem B.9 of appendix B.  

\(^11\) Here the standard definition of the Fourier transform given in appendix A is used. $\mathcal{F}f = \hat{f} = (2\pi)^{-3/2} \int e^{-ix\cdot\xi} f(x) \, dx.$
### 3.3: Self-Adjointness on $Y$

The $L^\infty$ bound of a function is defined as $\|f\|_\infty := \text{ess sup}_x |f(x)|$. Depicted is the functional form of $f(|\xi|^2) = \frac{(1 + |\xi|^2)}{\lambda + |\xi|^2/2}$ on $0 \leq |\xi|^2 < \infty$. This justifies the statement that for $\text{Im} \lambda \neq 0$, $\|f\|_\infty < \infty$.

That is, $(\lambda + |\xi|^2/2)\hat{U} = \hat{V}$. As a result,

$$
\left\| \frac{1 + |\xi|^2}{\lambda + |\xi|^2/2} \hat{\theta}_j \right\|_2 \leq \left( \sum_{j=1}^\infty \lambda_j \left\| \frac{1 + |\xi|^2}{\lambda + |\xi|^2/2} \hat{\theta}_j \right\|_2^2 \right)^{1/2}
$$

Notice that having $\text{Im} \lambda \neq 0$ ensures that the $\| \cdot \|_\infty$ norm is bounded. Figure 3.1 shows the functional form of the argument of the $\| \cdot \|_\infty$ term for a general $\lambda \in \mathbb{C}$. This inequality implies that $\mathcal{U} = \{u_j\}_{j \in \mathbb{N}} \in D(\mathcal{A}_0) = \mathbb{Z}$. This implies that the range of $(\lambda I + i\mathcal{A}_0)$ contains $\mathbb{C}$. □

Having established that the unperturbed operator is indeed self-adjoint on $X$, consider the full perturbed operator.
3.3: Self-Adjointness on $Y$

3.3.2 Self-Adjointness of $-iA_\beta$ on $X$ 

Since $V_0$ is real valued, the operator of multiplication by $V_0$ is self-adjoint on 

$$D(V_0) = \{ \Psi : \Psi \in X, V_0\Psi \in X \}.$$ 

Theorem 3.1 indicates self-adjointness of the unperturbed Hamiltonian is assured if it can be shown that 

$$\|\beta V_0 u\|_X \leq a\|u\|_X + b - \Delta u/2\|_X, \quad \forall u \in D(-\Delta/2) = Z \subset X, 0 \leq b < 1.$$ 

For any $\epsilon > 0$, $V_0$ can be broken into two disjoint pieces 

$$V_0 = \frac{1}{4\pi|x|} = \frac{1}{4\pi|x|} \chi_{\{x:|x|<\epsilon\}} + \frac{1}{4\pi|x|} \chi_{\{x:|x|\geq \epsilon\}}$$ 

where $\chi$ is the characteristic function on the indicated set. Estimation with the Minkowski and Hölder inequalities\textsuperscript{12} yields 

$$\|V_0\psi_j\|_2 \leq \left\| \frac{1}{4\pi|x|} \chi_{\{x:|x|<\epsilon\}} \right\|_2 \|\psi_j\|_\infty + \left\| \frac{1}{4\pi|x|} \chi_{\{x:|x|\geq \epsilon\}} \right\|_\infty \|\psi_j\|_2$$ 

Therefore,

$$\|V_0\Psi\|_X^2 = \sum_{j=1}^{\infty} \lambda_j \|V_0\psi_j\|_2^2 = \left\| \lambda_j \|V_0\psi_j\|_2^2 \right\|_{l_1}$$

$$= \left\| \lambda_j^{1/2} \|V_0\psi_j\|_2 \right\|_{l_2}^2$$

$$\leq \left\| \lambda_j^{1/2} \left( \frac{\epsilon}{4\pi} \right)^{1/2} \|\psi_j\|_\infty + \frac{1}{4\pi\epsilon} \|\psi_j\|_2 \right\|_{l_2}^2$$

$$\leq \left( \left( \frac{\epsilon}{4\pi} \right)^{1/2} \lambda_j^{1/2} \|\psi_j\|_\infty \right)^2 + \left( \frac{1}{4\pi\epsilon} \lambda_j^{1/2} \|\psi_j\|_2 \right)^2$$

$$= \left( \left( \frac{\epsilon}{4\pi} \right)^{1/2} \left( \sum_{j=1}^{\infty} \lambda_j \|\psi_j\|_\infty^2 \right)^{1/2} + \frac{1}{4\pi\epsilon} \|\Psi\|_X \right)^2$$

\textsuperscript{12} Appendix B section B.1 contains a listing of all of the fundamental inequalities used in the dissertation.
which shows that \( C \subset D(V_0) \). However, for any \( \psi_j \in C_0^\infty(\mathbb{R}^3) \) and \( a > 0 \) there exists some \( b \), independent of \( \psi_j \), such that

\[
\|\psi_j\|_\infty \leq a\|\Delta \psi_j\|_2 + b\|\psi_j\|_2.
\]

Consequently,

\[
\sum_{j=1}^\infty \lambda_j \|\psi_j\|_\infty^2 \leq \sum_{j=1}^\infty \lambda_j (a\|\Delta \psi_j\|_2 + b\|\psi_j\|_2)^2 \\
\leq 2 \sum_{j=1}^\infty \lambda_j \left(a^2\|\Delta \psi_j\|_2^2 + b^2\|\psi_j\|_2^2\right) \\
= 2a^2\|\Delta \Psi\|^2_X + 2b^2\|\Psi\|^2_X
\]

which implies, by using the inequality (3.22), that

\[
\|\beta V_0 \Psi\|^2_X \leq 2\beta^2 \left[ \frac{\epsilon}{4\pi} \left( \sum_{j=1}^\infty \lambda_j \|\psi_j\|_\infty^2 \right) + \left( \frac{1}{4\pi \epsilon} \right)^2 \|\Psi\|^2_X \right] \\
\leq 4\pi^{-1}\beta^2\epsilon \| - \Delta \Psi \|_X^2 + \left( \pi^{-1}\beta^2 \epsilon + \pi^{-2}\epsilon^{-2}/8 \right) \beta^2\|\Psi\|^2_X.
\]

Thus \( \beta V_0 \) is \(-\Delta/2\)-bounded in \( X \) and by choosing an appropriate value for \( \epsilon \), this bound can be made arbitrarily small. By lemma 3.2, \(-iA_0\) is self-adjoint on \( X \).

Therefore, from the above bound and theorem 3.1, it has been proved that

**Lemma 3.3** \(-iA_\beta = -iA_0 + \beta V_0\) is self-adjoint on \( X \). \( \Box \)

Before the self-adjointness of \(-iA_\beta\) is extended to the space \( Y \) an estimate on the growth of the self-consistent potential energy is required.

### 3.3.3 An Independent Estimate

To continue the analysis of our system, a number of Sobolev estimates are required. Presented here are the first of these estimates. Although this particular estimate

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3.3: Self-Adjointness on $Y$

will be used primarily in section 3.5 with the estimation of the self-consistent potential $V$ and its derivatives, it is presented here because of the role that it plays in section 3.3.4.

**Lemma 3.4** For $f \in C_0^\infty(\mathbb{R}^m)$ ($m \geq 3$) the following inequality holds

$$
\int_{\mathbb{R}^m} \frac{|f(x)|^2}{|x|^2} \, dx \leq \frac{4}{(m-2)^2} \int_{\mathbb{R}^m} \sum_{j=1}^{m} \left| \frac{\partial}{\partial x_j} f(x) \right|^2 \, dx.
$$

**Proof.** The following proof is from [66]. Denote the unit sphere in $\mathbb{R}^m$ as $\Omega_m$ and its differential surface element as $d\omega_m$. Converting to spherical coordinates

$$
\int_{\mathbb{R}^m} \frac{|f(x)|^2}{|x|^2} \, dx = \int_{\Omega_m} r^{m-3} \int_{\Omega_m} |f(r,\omega)|^2 \, d\omega_m \, dr
$$

$$
= \lim_{\varepsilon \to 0} \int_{\Omega_m} r^{m-3} \int_{\Omega_m} |f(r,\omega)|^2 \, d\omega_m \, dr. \quad (3.23)
$$

Provided $m \geq 3$, the expression (3.23) can now be integrated by parts to yield

$$
\lim_{\varepsilon \to 0} \left\{ \frac{r^{m-2}}{(m-2)} \int_{\Omega_m} |f(r,\omega)|^2 \, d\omega_m \int_{\Omega_m} f^*(r,\omega) \frac{\partial}{\partial r} f(r,\omega) \, d\omega_m \, dr \right\}.
$$

The first term vanishes since $f \in C_0^\infty(\mathbb{R}^m)$ and the lower limit converges to

$$
\frac{1}{(m-2)} \varepsilon^{m-2} |f(0)|^2 \int_{\Omega_m} d\omega_m \to 0.
$$

Thus, one is left with the expression

$$
\left| -\frac{2}{(m-2)} \int_{\Omega_m} f^*(r,\omega) \frac{\partial}{\partial r} f(r,\omega) \, d\omega_m \, dr \right|
$$

$$
\leq \frac{2}{(m-2)} \int_{\Omega_m} |f(r,\omega)| \left| \frac{\partial}{\partial r} f(r,\omega) \right| \, d\omega_m \, dr
$$

$$
\leq \frac{2}{(m-2)} \int_{\mathbb{R}^m} \frac{1}{|x|} |f(x)| \left\{ \sum_{j=1}^{m} \left| \frac{\partial}{\partial x_j} f(x) \right|^2 \right\}^{1/2} \, dx
$$
where the last expression has been converted back to rectangular coordinates. Applying Hölder’s inequality gives

\[ \int_{\mathbb{R}^m} \frac{|f(x)|^2}{|x|^2} \, dx \leq \frac{2}{(m-2)} \left( \int_{\mathbb{R}^m} \frac{|f(x)|^2}{|x|^2} \, dx \right)^{1/2} \left( \int_{\mathbb{R}^m} \sum_{j=1}^m \left| \frac{\partial}{\partial x_j} f(x) \right|^2 \, dx \right)^{1/2}. \]

Solving for the left hand side completes the proof. □

This estimate will allow the extension of the self-adjointness of the operator \(-iA_\beta\) to the space \(Y\) which is the topic of the next section.

### 3.3.4 Extension to the Space \(Y\)

It can now be shown that the Coulomb Hamiltonian, \(-iA_\beta\), can be treated within the space \(Y\). This technical result extends the argument found in the paper of Chadam and Glassey [14].

**Theorem 3.5** For any \(\beta \in \mathbb{R}\) there exists a \(\mu_\beta\) such that

\[ H_\mu = -iA_\beta + \mu_\beta = -\frac{\Delta}{2} + \frac{\beta}{4\pi|x|} + \mu_\beta \] (3.24)

is a positive self-adjoint operator with domain \(D(-\Delta) = Z\). Hence \(H_\mu^{1/2}\) exists as a positive self-adjoint operator with domain \(D((-\Delta)^{1/2})\). The norm \(\|H_\mu^{1/2}\cdot\|_X\) is equivalent to the \(Y\) norm.

**Proof.** For any fixed \(m > 0\) and \(\beta \leq 0\), the spectrum of the operator

\[ -\frac{\Delta}{2m} + \frac{\beta}{4\pi|x|} \] (3.25)

is the set

\[ \left\{ -\frac{m\beta^2}{8\pi m^2} \right\}_{n=1}^{\infty} \cup [0, \infty) \] (3.26)

and if \(\beta \geq 0\) the spectrum is just the set \([0, \infty)\). A proof of this fact in the case \(X = L^2, Z = H^2\) can be found in any intermediate level quantum mechanics text.
3.3: Self-Adjointness on $Y$

For $\beta < 0$ (an attractive Coulomb potential) one has both a continuous spectrum and a discrete spectrum with an accumulation point at $x = 0$. For $\beta \geq 0$ (a repulsive Coulomb potential) the spectrum contains just a continuous part.

See for example [25, 43]. An illustration of the spectra is shown in figure 3.2. Noting that equation (3.24) has $m = 1$, one only needs to choose $\mu_\beta \geq \beta^2/8\pi$ to ensure the first two statements of the theorem\textsuperscript{14} [40].

To illustrate the norm equivalence begin by choosing $\mu_\beta \geq 1/4 + \beta^2/4\pi > \beta^2/8\pi$ to ensure positivity. If $\beta \leq 0$ then for any $\psi_j \in D(-\Delta) = D(-\Delta/2 - \beta/4\pi|x| + \mu_\beta)$ the self-adjointness of this operator implies that its eigenfunctions $\{f_j\}_{j \in \mathbb{N}}$ form a complete set on $L^2$. By expressing $\psi_j$ as a linear combination of these eigenfunctions, $\psi_j = \sum_n a_n f_n$, one computes $\langle f_j, (-\Delta/2m + \beta/4\pi|x| + \mu_\beta)f \rangle$. This projects out the eigenvalues

$$\sum_{n=1}^{\infty} |a_n|^2 \left( \mu_\beta - \frac{m\beta^2}{8\pi n^2} \right) \langle f_n, f_n \rangle \geq \sum_{n=1}^{\infty} |a_n|^2 \left( \mu_\beta - \frac{m\beta^2}{8\pi} \right) \langle f_n, f_n \rangle \geq \left( \mu_\beta - \frac{m\beta^2}{8\pi} \right) \langle f, f \rangle.$$

Therefore,

$$\langle \psi_j, \left( -\frac{\Delta}{2} + \frac{\beta}{4\pi|x|} + \mu_\beta \right) \psi_j \rangle = \langle \psi_j, \left( -\frac{\Delta}{4} + \frac{\beta}{4\pi|x|} + \mu_\beta \right) \psi_j \rangle + \langle \psi_j, -\frac{\Delta}{4} \psi_j \rangle \geq \langle \psi_j, \left( \mu_\beta - \frac{\beta^2}{4\pi} \right) \psi_j \rangle + \langle \psi_j, -\frac{\Delta}{4} \psi_j \rangle$$

\textsuperscript{14} This estimate assumes that $\beta \leq 0$. For $\beta \geq 0$ one need only assume that $\mu_\beta \geq 0$. 
where the spectrum given by (3.26) with \( m = 2 \) has been used. For \( \beta > 0 \) the same lower bound is attained since in this case

\[
\left\langle \psi_j, \left( -\frac{\Delta}{2} + \frac{\beta}{4\pi|x|} + \mu_\beta \right) \psi_j \right\rangle \geq \left\langle \psi_j, \left( -\frac{\Delta}{2} + \mu_\beta \right) \psi_j \right\rangle \\
\geq \left\langle \psi_j, \left( -\frac{\Delta}{2} + \frac{1}{4} \right) \psi_j \right\rangle \\
\geq \frac{1}{4} \langle \psi_j, (1 - \Delta) \psi_j \rangle.
\]

For an upper bound, apply lemma 3.4 and the Hölder inequality which gives

\[
\left\langle \psi_j, \frac{\beta}{|x|} \psi_j \right\rangle = \beta \left\| \frac{\psi_j}{|x|} \right\|_1
\leq |\beta| \left\| \psi_j \right\|_2 \left\| \frac{\psi_j}{|x|} \right\|_2
\leq 2|\beta| \left\| \psi_j \right\|_2 \left\| \nabla \psi_j \right\|_2
\leq |\beta| \left( \left\| \psi_j \right\|_2^2 + \left\| \nabla \psi_j \right\|_2^2 \right)
= |\beta| \left( \langle \psi_j, \psi_j \rangle + \langle \nabla \psi_j, \nabla \psi_j \rangle \right)
= |\beta| \langle \psi_j, (1 - \Delta) \psi_j \rangle.
\]

Hence,

\[
\left\langle \psi_j, \left( -\frac{\Delta}{2} + \frac{\beta}{4\pi|x|} + \mu_\beta \right) \psi_j \right\rangle \leq \frac{1 + |\beta|/2\pi}{2} \left\langle \psi_j, \left( \frac{2\mu_\beta + |\beta|/2\pi}{1 + |\beta|/2\pi} - \Delta \right) \psi_j \right\rangle \\
\leq \frac{1 + |\beta|/2\pi}{2} \langle \psi_j, (c_\beta - \Delta) \psi_j \rangle
\]

where \( c_\beta = \max\{1, 2\mu_\beta\} \). Thus independent of the sign of \( \beta \),

\[
\frac{1}{4} \langle \psi_j, (1 - \Delta) \psi_j \rangle \leq \left\langle \psi_j, \left( -\frac{\Delta}{2} + \frac{\beta}{4\pi|x|} + \mu_\beta \right) \psi_j \right\rangle \leq \frac{1 + |\beta|/2\pi}{2} \langle \psi_j, (c_\beta - \Delta) \psi_j \rangle.
\]
3.3: Self-Adjointness on $Y$

Taking a weighted sum over $\{\lambda_j\}_{j \in \mathbb{N}}$ and using our choice of $\mu_\beta$, all the operators are positive. Consequently,

$$\frac{1}{4}\|(1 - \Delta)^{1/2}\Psi\|^2_X \leq \left( -\frac{\Delta}{2} + \frac{\beta}{4\pi|x|} + \mu_\beta \right)^{1/2} \Psi \|_X^2 \leq \frac{1 + |\beta|/2\pi}{2\|c_\theta - \Delta\|^{1/2}} \Psi \|_X^2.$$

Since $D(-\Delta)$ is a core\(^{15}\) for all of the above operators, the inequality can be extended to $\psi_j \in D((-\Delta)^{1/2}) [14]$. This completes the proof since the first and last expressions are equivalent to the $Y$ norm by the spectral theorem [40]. □

The subsequent work in this chapter will consider $-iA_\theta$ as the unperturbed Hamiltonian. Therefore, for the sake of brevity, $H_c$ will denote the operator

$$H_c := -iA_\theta = -\frac{\Delta}{2} + \beta V_0.$$

**Corollary 3.6** $-i\tilde{H}_c$ with $D(\tilde{H}_c) = \{\Gamma \in Y|H_c\Gamma \in Y\}$ is the infinitesimal generator of a $C_0$ group of operators

$$\tilde{U}(t) = \begin{cases} 
 e^{-it\tilde{H}_c} & t \geq 0 \\
 e^{+it\tilde{H}_c} & t \leq 0
\end{cases}$$

on the Hilbert space $Y$.

**Proof.** Lemma 3.3 gives the self-adjointness on $X$ and theorem 3.5 shows that $D(H^{1/2}_\mu)$ is isomorphic to $Y$ under norm equivalence. Now consider $\tilde{U}(t)$ which denotes $U(t)$ restricted to $Y$. This is a $C_0$ group on $Y$ with an infinitesimal generator $\tilde{H}_c$ with $D(\tilde{H}_c) = \{\Gamma \in Y|H_c\Gamma \in Y\}$. Furthermore, one has the representation $\tilde{U}(t) = e^{-it\tilde{H}_c}$ for $t \geq 0$ and $\tilde{U}(-t) = e^{+it\tilde{H}_c}$ for $t \leq 0$. □

From this point forward, the tildes on $U(t)$ and $H_c$ are dropped.

\(^{15}\) If an operator $T$ is closed then a subset $\Omega \subset D(T)$ is called a core for $T$ if $\overline{T \upharpoonright \Omega} = T$ (the closure of $T$ restricted to $\Omega$ is all of $T$). See reference [55] p. 256.
3.4 Classes of Solutions

Having defined the unitary group \( \{ e^{-itH_{c}} \}_{t \in \mathbb{R}} \), some classes of solutions to (3.15)–(3.17) can be defined. If \( \Phi \in Y \) then a function\(^{16} \) \( \Psi \in C([0,T);Y) \) satisfying

\[
\Psi(t) = e^{-itH_{c}}\Phi - i \int_{0}^{t} e^{-i(t-s)H_{c}} J(\Psi(s)) \, ds \quad 0 \leq t < T,
\]

is called a mild solution of the initial value problem (3.15)–(3.17) on \([0,T)\). A strong solution of (3.15)–(3.17) on \( Y \) and the time interval \([0,T)\) is a function \( \Psi \in C([0,T);Y) \cap C^{1}([0,T);X) \) such that (3.15)–(3.17) is valid on \([0,T)\). If \( \Psi \in C([0,T);Y) \) it will be called a mild \( Y \)-valued solution. If \( \Psi \in C^{1}([0,T);X) \) it will be called a strong \( X \)-valued solution. A global mild or strong solution of (3.15)–(3.17) is one in which the defining properties hold for \( T = \infty \).

In this chapter it is proved that (3.15)–(3.17) has a unique global mild solution on \( Y \) which can be viewed as a unique global strong solution on \( X \). This is done in a number of stages as indicated in figure 3.3. First it is shown that the nonlinear map \( J : Y \times [0,T) \to Y \) and is locally Lipschitz in \( \Psi \) uniformly on \( t \in [0,T) \). This property is sufficient to prove that there exists a unique mild solution on an interval \([0,t_{\text{max}})\) and that if \( t_{\text{max}} < \infty \) then \( \lim_{t \to t_{\text{max}}} \| \Psi(t) \|_{Y} = \infty \). One then proceeds to show that this unique mild solution on \( Y \) is in fact a strong solution on \( X \) by using the fact that \( J : Y \times [0,t_{\text{max}}) \to Y \) is continuously differentiable from \( Y \times [0,t_{\text{max}}) \) into \( Y \).

The final stage is to extend the solution to an arbitrarily large time by ensuring that the quantity \( \| \Psi(t) \|_{Y} \) remains bounded for all \( t \in [0,T) \). That this is indeed the case is established by analyzing both the probability and energy conservation laws of the system. This shows that our locally defined solution is actually a global solution.

\(^{16} \Psi \in C([0,T);Y) \) implies that \( \| \Psi(\cdot,t) \|_{Y} \) is continuous as a function of time \( t \) on the interval \( 0 \leq t < T \).
3.4: Classes of Solutions

Strategy for Proving Global Existence and Uniqueness of
\[ \frac{d\Psi}{dt} + A_\beta \Psi + iJ(\Psi) = 0 \] where \(-iA_\beta = iH_c = -\left(\frac{\Delta}{2} - \beta V_0\right)\); \(J(\Psi) = V(\Psi)\Psi\)

---

**Figure 3.3:** A strategy for proving global existence and uniqueness.

*Illustrated is a schematic of the following sections and how they connect together to prove global existence and uniqueness for the SP system. The notation is: L-lemma, P-proposition, § denotes section and §§ denotes subsection. The abbreviation s.a. means self-adjoint.*
3.5 Estimation of $V$

The following estimates of the self-consistent potential will hold for any potential that can be expressed in the form given by (3.19) irrespective of the external Coulomb potential. The very versatile Gagliardo–Nirenberg (GN) inequality is presented first.

**Lemma 3.7 (The GN inequality for $\mathbb{R}^3$)**

Let $1 \leq q, r \leq \infty$ and let $j, m \in \mathbb{N} \cup \{0\}$ satisfy $0 \leq j < m$. Then

$$\sum_{|\beta|=j} \|D^\beta f\|_p \leq C_{m,j,q,r,a} \sum_{|\alpha|=m} \|D^\alpha f\|_q \|f\|_q^{1-a}$$

for any $f \in W^{m-r} \cap L^q$ where

$$\frac{1}{p} = \frac{j}{3} + \left(\frac{1}{r} - \frac{m}{3}\right) a + \frac{1-a}{q}$$

for all $a$ in the interval $j/m \leq a < 1$, with the following exception: if $m - j - 3/r$ is a nonnegative integer, then the above inequality is asserted for $j/m < a < 1$.

**Proof.** The book by Tanabe [63] proves this inequality in detail. Theorem 3.4 of this reference considers the specific exceptional case $m - j - 3/r = 0$. □

Because of the proliferation of inequalities used throughout this dissertation every distinct proportionality constant will not be renamed. Rather, for the sake of brevity and clarity $C$ will denote generic, but not necessarily equal, positive constants. When necessary, $C(\cdot, \ldots, \cdot)$ will denote constants depending only on the quantities appearing in the parenthesis.

**Lemma 3.8** If $\Gamma \in Y$ then $V = V(\Gamma) \in L^\infty$ and

$$\|V(\Gamma)\|_\infty \leq C\|\Gamma\|_X\|\Gamma\|_Y.$$

Also, if $\Gamma, \tilde{\Gamma} \in Y$ then

$$\|V(\Gamma) - V(\tilde{\Gamma})\|_\infty \leq C(\|\Gamma\|_X, \|\tilde{\Gamma}\|_X)\|\Gamma - \tilde{\Gamma}\|_Y.$$
Proof. Let $\Gamma \in Y \subset X$. Using (3.19) gives

$$
\|V(\Gamma)\|_\infty \leq C \sum_{j=1}^{\infty} \lambda_j \left\| \int \frac{|\gamma_j(y)|^2}{|y - \cdot|} \, dy \right\|_\infty
\leq C \sum_{j=1}^{\infty} \lambda_j \left\| \gamma_j \|_2 \left( \int \frac{|\gamma_j(y)|^2}{|y - \cdot|^2} \, dy \right)^{1/2} \right\|_\infty
\leq C \sum_{j=1}^{\infty} \lambda_j \|\nabla \gamma_j\|_2
\leq C \left( \sum_{j=1}^{\infty} \lambda_j \|\gamma_j\|_2^2 \right)^{1/2} \left( \sum_{j=1}^{\infty} \lambda_j \|\nabla \gamma_j\|_2^2 \right)^{1/2}
\leq C \|\Gamma\|_X \|\Gamma\|_Y.
$$

The second step proceeded using lemma 3.4 and the third step required the use of the Cauchy–Schwarz inequality. Using a similar argument produces

$$
\|V(\Gamma) - V(\bar{\Gamma})\|_\infty \leq C \sum_{j=1}^{\infty} \lambda_j \left\| \int \frac{|\gamma_j(y)|^2 - |\bar{\gamma}_j(y)|^2}{|y - \cdot|} \, dy \right\|_\infty
\leq C \sum_{j=1}^{\infty} \lambda_j \left\| \int \frac{|\gamma_j(y) - \bar{\gamma}_j(y)| + |\bar{\gamma}_j(y) - \gamma_j(y)|}{|y - \cdot|} \, dy \right\|_\infty
\leq C \sum_{j=1}^{\infty} \lambda_j (\|\gamma_j\|_2 + \|\bar{\gamma}_j\|_2) \|\nabla (\gamma_j - \bar{\gamma}_j)\|_2
\leq C \left( \|\Gamma\|_X + \|\bar{\Gamma}\|_X \right) \left[ \sum_{j=1}^{\infty} \lambda_j \|\nabla (\gamma_j - \bar{\gamma}_j)\|_2^2 \right]^{1/2}
\leq C (\|\Gamma\|_X, \|\bar{\Gamma}\|_X) \|\Gamma - \bar{\Gamma}\|_Y. \quad \Box
$$

Lemma 3.9 If $\Gamma \in Y$ then $\nabla V(\Gamma) \in L^2$ and

$$
\|\nabla V(\Gamma)\|_2^2 \leq C \|\Gamma\|_X^3 \|\Gamma\|_Y.
$$

Moreover, if $\Gamma, \bar{\Gamma} \in Y$ then

$$
\|\nabla V(\Gamma) - \nabla V(\bar{\Gamma})\|_2 \leq C (\|\Gamma\|_X, \|\bar{\Gamma}\|_X) \|\Gamma - \bar{\Gamma}\|_Y.
$$
Proof. Because $\Gamma \in Y \subset X$ it follows that

$$\Delta V = -\alpha \sum_{j=1}^{\infty} \lambda_j |\gamma_j|^2 \in L^1$$

and from lemma 3.8, that $V \in L^\infty$. These remarks validate the following manipulations:

$$\|\nabla V\|^2_2 = \int |\nabla V|^2 \, dx \leq \int |V \Delta V| \, dx$$

$$\leq \|V\|_\infty \int \alpha \sum_{j=1}^{\infty} \lambda_j |\gamma_j|^2 \, dx$$

$$\leq C \|V\|_\infty \sum_{j=1}^{\infty} \lambda_j \int |\gamma_j|^2 \, dx$$

$$= C \|V\|_\infty \|\Gamma\|_X^2$$

$$\leq C \|\Gamma\|^3_\infty \|\Gamma\|_Y$$

where the $\|V\|_\infty$ estimate from lemma 3.8 and Gauss' theorem have been used.

For the second half of the lemma a similar argument gives

$$\|\nabla \tilde{V} - \nabla \tilde{V}\|^2_2 = \int |\nabla \tilde{V} - \nabla \tilde{V}|^2 \, dx$$

$$\leq \int |(V - \tilde{V}) \Delta (V - \tilde{V})| \, dx$$

$$\leq \|V - \tilde{V}\|_\infty \int \alpha \sum_{j=1}^{\infty} \lambda_j \left(|\gamma_j|^2 - |\tilde{\gamma}_j|^2\right) \, dx$$

$$\leq C \|V - \tilde{V}\|_\infty \sum_{j=1}^{\infty} \lambda_j \int \left[|\tilde{\gamma}_j(\gamma_j - \tilde{\gamma}_j)| + |\tilde{\gamma}_j(\gamma_j - \tilde{\gamma}_j)|\right] \, dx$$

$$\leq C \|V - \tilde{V}\|_\infty \sum_{j=1}^{\infty} \lambda_j \left(\|\gamma_j\|_2 + \|\tilde{\gamma}_j\|_2\right) \|\gamma_j - \tilde{\gamma}_j\|_2$$

$$\leq C \|V - \tilde{V}\|_L^\infty \left(\|\Gamma\|_X + \|\Gamma\|_X\right) \left(\sum_{j=1}^{\infty} \lambda_j \|\gamma_j - \tilde{\gamma}_j\|_2^2\right)^{1/2}$$

---

17 One can interchange the order of summation and integration by applying Lebesgue's monotone convergence theorem to $\{\lambda_j |\psi_j|^2\}_{j \in \mathbb{N}}$ which is a sequence of nonnegative measurable functions on $L^2(\mathbb{R}^3)$ [58].
Lemma 3.10 If $\Gamma \in Y$ then $\Delta V(\Gamma) \in L^2$ and

$$\|\Delta V(\Gamma)\|_2 \leq C\|\Gamma\|_Y^2.$$

In addition, if $\Gamma, \tilde{\Gamma} \in Y$ then

$$\|\Delta V(\Gamma) - \Delta V(\tilde{\Gamma})\|_2 \leq C(\|\Gamma\|_Y, \|\tilde{\Gamma}\|_Y)\|\Gamma - \tilde{\Gamma}\|_Y.$$

Proof.

$$\|\Delta V\|_2 = \left\| \sum_{j=1}^{\infty} \lambda_j \gamma_j \right\|_2$$

$$\leq C \sum_{j=1}^{\infty} \lambda_j \|\gamma_j\|_2$$

$$= C \sum_{j=1}^{\infty} \lambda_j \|\gamma_j\|_4^2.$$

The sequence $\Gamma \in Y \subset X$ so that $\gamma_j \in W^{1,2} \cap L^2$. Therefore using the GN inequality (lemma 3.7) with $j = 0$, $p = 4$, $m = 1$, $q = r = 2$, $a = 3/4$ and $f = \gamma_j$ furnishes the estimate

$$\|\gamma_j\|_4 \leq C\|\nabla \gamma_j\|_{2/2}^{3/4}\|\gamma_j\|_2^{1/4}.$$

Continuing with the original estimate and using Hölder's inequality

$$\|\Delta V\|_2 \leq C \sum_{j=1}^{\infty} \lambda_j \|\nabla \gamma_j\|_2^{3/2}\|\gamma_j\|_2^{1/2}$$

$$\leq C \left( \sum_{j=1}^{\infty} \lambda_j \|\nabla \gamma_j\|_2^2 \right)^{3/4} \left( \sum_{j=1}^{\infty} \lambda_j \|\gamma_j\|_2^2 \right)^{1/4}$$

$$\leq C \left( \sum_{j=1}^{\infty} \lambda_j \|\gamma_j\|_2^2 + \sum_{j=1}^{\infty} \lambda_j \|\nabla \gamma_j\|_2^2 \right)$$

$$= C\|\Gamma\|_Y^2.$$
3.5: Estimation of $V$

For the second half of the lemma let $I = \|\Delta V(\Gamma) - \Delta V(\tilde{\Gamma})\|_2^2$. Using Hölder's inequality,

$$I \leq C \sum_{j=1}^{\infty} \lambda_j \|\gamma_j^2 - \tilde{\gamma}_j^2\|_2^2$$

$$\leq \sum_{j=1}^{\infty} \lambda_j \|\gamma_j - \tilde{\gamma}_j\|_2 \|\gamma_j - \tilde{\gamma}_j\|_2$$

$$\leq \sum_{j=1}^{\infty} \lambda_j \left(\|\gamma_j\|_4^2 + \|\tilde{\gamma}_j\|_4^2\right) \|\gamma_j - \tilde{\gamma}_j\|_4^2.$$

Continuing with the GN inequality,

$$I \leq C(\|\Gamma\|_Y, \|\tilde{\Gamma}\|_Y) \sum_{j=1}^{\infty} \lambda_j \|\nabla (\gamma_j - \tilde{\gamma}_j)\|_2^{3/2} \|\gamma_j - \tilde{\gamma}_j\|_2^{1/2}$$

$$\leq C(\|\Gamma\|_Y, \|\tilde{\Gamma}\|_Y) \left(\sum_{j=1}^{\infty} \lambda_j \|\nabla (\gamma_j - \tilde{\gamma}_j)\|_2^2\right)^{3/4} \left(\sum_{j=1}^{\infty} \lambda_j \|\gamma_j - \tilde{\gamma}_j\|_2^2\right)^{1/4}$$

$$\leq C(\|\Gamma\|_Y, \|\tilde{\Gamma}\|_Y) \|\Gamma - \tilde{\Gamma}\|_Y^2. \quad \Box$$

Lemma 3.11 If $\Gamma \in Y$ then $\nabla V(\Gamma) \in L^\infty$ and

$$\|\nabla V(\Gamma)\|_\infty \leq C\|\Gamma\|_Y^2.$$

Furthermore, if $\Gamma, \tilde{\Gamma} \in Y$ then

$$\|\nabla V(\Gamma) - \nabla V(\tilde{\Gamma})\|_\infty \leq C(\|\Gamma\|_Y, \|\tilde{\Gamma}\|_Y) \|\Gamma - \tilde{\Gamma}\|_Y.$$

Proof. One proceeds as in lemma 3.8. Taking $\Gamma \in Y$ and using the representation (3.19) yields

$$\|\nabla V(\Gamma)\|_\infty \leq C \sum_{j=1}^{\infty} \lambda_j \left\| \int \frac{|\gamma_j(y)|^2}{|y - \cdot|^2} \, dy \right\|_\infty$$

$$\leq C \sum_{j=1}^{\infty} \lambda_j \|\nabla \gamma_j\|_2^2$$

$$\leq C\|\Gamma\|_Y^2.$$
The second half proceeds as in lemma 3.11. In detail
\[
\| \nabla V(\Gamma) - \nabla V(\tilde{\Gamma}) \|_\infty \leq C \sum_{j=1}^\infty \lambda_j \left\| \int \frac{\Gamma_j(y) - \tilde{\Gamma}_j(y)}{|y - i|^2} \, dy \right\|_\infty
\]
\[
\leq C \sum_{j=1}^\infty \lambda_j \left\| \int \frac{|\Gamma_j(y) - \tilde{\Gamma}_j(y)| + |\Gamma_j(y) - \tilde{\Gamma}_j(y)|}{|y - i|^2} \, dy \right\|_\infty
\]
\[
\leq C \sum_{j=1}^\infty \lambda_j (\| \nabla \Gamma_j \|_2 + \| \nabla \tilde{\Gamma}_j \|_2) \| \nabla (\Gamma_j - \tilde{\Gamma}_j) \|_2
\]
\[
\leq C \left( \| \nabla \Gamma \|_X + \| \nabla \tilde{\Gamma} \|_X \right) \left( \sum_{j=1}^\infty \lambda_j \| \nabla (\Gamma_j - \tilde{\Gamma}_j) \|_2^2 \right)^{1/2}
\]
\[
\leq C (\| \Gamma \|_Y, \| \tilde{\Gamma} \|_Y) \| \Gamma - \tilde{\Gamma} \|_Y. \quad \square
\]

3.6 Local Existence of a Unique Strong Solution

Verifying that the map \( J \) has the required property to ensure the local existence of a unique mild solution in the space \( Y \cap X \) is established with the following proposition.

**Proposition 3.12** For every \( T > 0 \) the map \( J : Y \times [0, T] \to Y \) defined by
\[
J(\Psi)_j = V(\Psi) \psi_j
\]
is locally Lipschitz on \( Y \). That is, there exists a constant \( C = C(\| \Psi \|_Y, \| \tilde{\Psi} \|_Y) \) depending on \( \| \Psi \|_Y \) and \( \| \tilde{\Psi} \|_Y \) such that
\[
\| J(\Psi) - J(\tilde{\Psi}) \|_Y \leq C(\| \Psi \|_Y, \| \tilde{\Psi} \|_Y) \| \Psi - \tilde{\Psi} \|_Y. \quad (3.28)
\]

**Proof.** Let \( \Psi, \tilde{\Psi} \in Y \) and denote \( V = V(\Psi), \tilde{V} = V(\tilde{\Psi}) \). First consider
\[
\| J(\Psi) - J(\tilde{\Psi}) \|_2^2 = \sum_{j=1}^\infty \lambda_j \| V \psi_j - \tilde{V} \tilde{\psi}_j \|_{1,2}^2
\]
\[
\leq C_1 \sum_{j=1}^\infty \lambda_j \| V \psi_j - \tilde{V} \tilde{\psi}_j \|_2^2 + C_2 \sum_{j=1}^\infty \lambda_j \| \nabla (V \psi_j - \tilde{V} \tilde{\psi}_j) \|_2^2. \quad (3.29)
\]
Expression (3.29) consists of two pieces. Estimation of the first piece is accomplished as follows:

\[ \sum_{j=1}^{\infty} \lambda_j \| V \psi_j - \tilde{V} \tilde{\psi}_j \|_2^2 = \sum_{j=1}^{\infty} \lambda_j \| V (\psi_j - \tilde{\psi}_j) + (V - \tilde{V}) \tilde{\psi}_j \|_2^2 \leq 2 \sum_{j=1}^{\infty} \lambda_j \left[ \| V (\psi_j - \tilde{\psi}_j) \|_2^2 + \| (V - \tilde{V}) \tilde{\psi}_j \|_2^2 \right]. \]

From lemma 3.8,

\[ \sum_{j=1}^{\infty} \lambda_j \| V (\psi_j - \tilde{\psi}_j) \|_2^2 \leq \| V \|_\infty^2 \sum_{j=1}^{\infty} \lambda_j \| \psi_j - \tilde{\psi}_j \|_2^2 \leq C \| \psi \|_X \| \psi \|_2 \| \psi - \tilde{\psi} \|_X^2 \leq C (\| \psi \|_Y) \| \psi - \tilde{\psi} \|_Y^2. \]

Again using lemma 3.8 and the fact that our initial wave function lies in \( Y \),

\[ \sum_{j=1}^{\infty} \lambda_j \| (V - \tilde{V}) \tilde{\psi}_j \|_2^2 \leq \| V - \tilde{V} \|_\infty^2 \sum_{j=1}^{\infty} \lambda_j \| \tilde{\psi}_j \|_2^2 \leq C (\| \psi \|_X, \| \tilde{\psi} \|_X) \| \psi - \tilde{\psi} \|_Y \| \tilde{\psi} \|_X^2 \leq C (\| \psi \|_X, \| \tilde{\psi} \|_X) \| \psi - \tilde{\psi} \|_Y^2. \]

Collecting these two results gives

\[ \sum_{j=1}^{\infty} \lambda_j \| V \psi_j - \tilde{V} \tilde{\psi}_j \|_2^2 \leq C (\| \psi \|_Y, \| \tilde{\psi} \|_X) \| \psi - \tilde{\psi} \|_Y^2 \] \hspace{1cm} (3.30)

which completes the estimate of the first piece of equation (3.29).

To estimate the second term in expression (3.29), one can split the term into two separate pieces and then apply the gradient operator. This gives a total of four terms which will be labelled \( T_1 \) to \( T_4 \). That is,

\[ \| \nabla (V \psi_j - \tilde{V} \tilde{\psi}_j) \|_2^2 = \| \nabla [V (\psi_j - \tilde{\psi}_j) + (V - \tilde{V}) \tilde{\psi}_j] \|_2^2 \leq C \left\{ \| \nabla [V (\psi_j - \tilde{\psi}_j)] \|_2^2 + \| \nabla [(V - \tilde{V}) \tilde{\psi}_j] \|_2^2 \right\} \]
3.6: Local Existence of a Unique Strong Solution

\[
\begin{align*}
\leq C \left\{ \| (\psi_j - \tilde{\psi}_j) \nabla V \|_2^2 + \| V \nabla (\psi_j - \tilde{\psi}_j) \|_2^2 \\
+ \| \tilde{\psi}_j \nabla (V - \tilde{V}) \|_2^2 + \| (V - \tilde{V}) \nabla \tilde{\psi}_j \|_2^2 \right\}
\end{align*}
\]

\[= C(T_1 + T_2 + T_3 + T_4).\]

These terms are dealt with sequentially. For \( T_1 \)

\[T_1 = \| (\psi_j - \tilde{\psi}_j) \nabla V \|_2^2 \leq \| \nabla V \|_\infty^2 \| \psi_j - \tilde{\psi}_j \|_2^2 \]
\[\leq C \| \Psi \|_X^2 \| \psi_j - \tilde{\psi}_j \|_2^2 \]
\[\leq C(\| \Psi \|_Y) \| \psi_j - \tilde{\psi}_j \|_{1,2}^2.\]

Furthermore,

\[T_2 = \| V \nabla (\psi_j - \tilde{\psi}_j) \|_2^2 \leq \| V \|_\infty^2 \| \nabla (\psi_j - \tilde{\psi}_j) \|_2^2 \]
\[\leq C \| \Psi \|_X^2 \| \Psi \|_Y^2 \| \psi_j - \tilde{\psi}_j \|_{1,2} \]
\[= C(\| \Psi \|_X, \| \Psi \|_Y) \| \psi_j - \tilde{\psi}_j \|_{1,2}.\]

and

\[T_4 = \| (V - \tilde{V}) \nabla \tilde{\psi}_j \|_2^2 \leq \| V - \tilde{V} \|_\infty^2 \| \nabla \tilde{\psi}_j \|_2^2 \]
\[\leq C(\| \Psi \|_X, \| \tilde{\Psi} \|_X) \| \Psi - \tilde{\Psi} \|_Y^2 \| \tilde{\psi}_j \|_{1,2}^2.\]

The \( T_3 \) term requires the GN inequality and both lemmas 3.9 and 3.10. Specifically,

\[T_3 = \| \tilde{\psi}_j \nabla (V - \tilde{V}) \|_2^2 \]
\[\leq \| \nabla (V - \tilde{V}) \|_2^2 \| \tilde{\psi}_j \|_2^2 \]
\[\leq C \| \Delta (V - \tilde{V}) \|_2^{3/2} \| \nabla (V - \tilde{V}) \|_2^{1/2} \| \nabla \tilde{\psi}_j \|_2^{3/2} \| \tilde{\psi}_j \|_2^{1/2} \]
\[\leq C(\| \Psi \|_Y, \| \tilde{\Psi} \|_Y) \| \Psi - \tilde{\Psi} \|_Y^2 \| \tilde{\psi}_j \|_2^{3/2} \| \tilde{\psi}_j \|_2^{1/2}.\]

Collecting all of the four estimates together gives the result

\[\sum_{j=1}^{\infty} \lambda_j \| \nabla (V \psi_j - \tilde{V} \tilde{\psi}_j) \|_2^2 \leq C_1(\| \Psi \|_Y) \| \Psi - \tilde{\Psi} \|_Y^2 + C_2(\| \Psi \|_X, \| \tilde{\Psi} \|_Y) \| \Psi - \tilde{\Psi} \|_Y^2\]
Combining the estimates (3.30) and (3.31) with equation (3.29) gives the property

\[ \| J(\Psi) - J(\bar{\Psi}) \|_Y^2 \leq C(\| \Psi \|_Y, \| \bar{\Psi} \|_Y) \| \Psi - \bar{\Psi} \|_Y^2. \]  

(3.31)

completing the proof of the proposition. □

Proposition 3.12 illustrates that the map \( J : Y \times [0, T] \to Y \) is locally Lipschitz in \( \Psi \) uniformly in \( t \) on bounded intervals. In other words, for all \( t' \geq 0 \) and constant \( C \geq 0 \) there exists a constant \( L(t', C) \) such that

\[ \| J(\Psi(t)) - J(\bar{\Psi}(t)) \|_Y \leq L(t', C)\| \Psi(t) - \bar{\Psi}(t) \|_Y \]

provided \( t \in [0, t'] \), \( \Psi, \bar{\Psi} \in Y \), \( \| \Psi \|_Y \leq C \) and \( \| \bar{\Psi} \|_Y \leq C \).

The main result of this section can now be stated. Its development parallels the work of Pazy [54].

**Theorem 3.13** For every \( \Phi \in Z \) there exists a unique mild solution \( \Psi \) on \( Y \) of the initial value problem (3.15)-(3.17), defined for \( t \in [0, t_{\max}) \) such that

\[ \Psi \in C([0, t_{\max}); Y) \cap C^1([0, t_{\max}); X) \]

with the property that either \( t_{\max} = \infty \) or \( t_{\max} < \infty \) and \( \lim_{t \to t_{\max}} \| \Psi \|_Y = \infty \).

**Proof.** For a given \( t_0 \geq 0 \) and \( \Phi = \Psi(t_0) \in Y \) let

\[ t_1 = t_0 + \min \left\{ 1, \frac{1}{2L} \right\} \]

where \( L = L(t_0 + 1, 2\| \Phi \|) \) is the bound of expression (3.28) in proposition 3.12 for the interval \( 0 \leq t \leq t_0 + 1 \). Consider the ball

\[ B_{\Phi} = \left\{ \Psi \in C([t_0, t_1]; Y) \; : \; \| \Psi \|_{L^\infty([t_0, t_1]; Y)} \leq 2\| \Phi \|_Y \right\} \]
3.6: Local Existence of a Unique Strong Solution

The map $F$ takes values in $B_\Phi$ back into $B_\Phi$. It is shown below that $F^n$ is a strict contraction on $B_\Phi$ and as a result $F$ has a fixed point.

Figure 3.4: The mapping $F : B_\Phi \to B_\Phi$.

Equipped with the distance

$$\|u - v\| = \|u(t) - v(t)\|_{L^\infty([t_0, t_1]; Y)} = \max_{t \in [t_0, t_1]} \|u(t) - v(t)\|_Y$$

so that it forms a closed subset of the Banach space $C([t_0, t_1]; Y)$ and is therefore complete. Unless specified otherwise, all subsequent norms in this proof will be this norm on $C([t_0, t_1]; Y)$. For $\Psi$ in the ball $B_\Phi$, define a mapping $F$ by

$$(F\Psi)(t) = e^{-it(t-t_0)H_\epsilon} \Phi - i \int_{t_0}^t e^{-i(t-s)H_\epsilon} J(\Psi(s)) \, ds, \quad t_0 \leq t \leq t_1$$

and illustrated in figure 3.4. This $F$ maps the space $B_\Phi$ into itself since

$$\|(F\Psi)(t)\|_Y \leq \left\|e^{-it(t-t_0)H_\epsilon} \Phi\right\|_Y + \int_{t_0}^t \left\|e^{-i(t-s)H_\epsilon} J(\Psi(s))\right\|_Y \, ds$$

$$\leq \|\Phi\|_Y + \int_{t_0}^t \left\|J(\Psi(s))\right\|_Y \, ds$$

$$\leq \|\Phi\|_Y + \int_{t_0}^t L\|\Psi(s)\|_Y \, ds$$

$$\leq \|\Phi\|_Y + L(t - t_0)\|\Psi\|_Y$$

$$\leq [1 + 2L(t - t_0)] \|\Phi\|_Y$$
3.6: Local Existence of a Unique Strong Solution

\[ \leq [1 + 2L(t_1 - t_0)] \| \Phi \|_Y \]
\[ \leq 2\| \Phi \|_Y \]

using the choice for \( t_1 \). Throughout \( B_\Phi \) the Lipschitz constant holds uniformly which allows one to construct a contraction mapping. Indeed,

\[
\| (F^\Psi)(t) - (F^\tilde{\Psi})(t) \|_Y \leq \int_{t_0}^{t} \| e^{-i(t-s)H_c} \left[ J(\Psi(s)) - J(\tilde{\Psi}(s)) \right] \|_Y ds \\
\leq L \int_{t_0}^{t} \| \Psi(s) - \tilde{\Psi}(s) \|_Y ds \\
\leq L(t - t_0) \| \Psi - \tilde{\Psi} \|
\]

and given that

\[
\| (F^n\Psi)(t) - (F^n\tilde{\Psi})(t) \|_Y \leq \frac{L^n(t - t_0)^n}{n!} \| \Psi - \tilde{\Psi} \| \quad (3.32)
\]

one has

\[
\| (F^{n+1}\Psi)(t) - (F^{n+1}\tilde{\Psi})(t) \|_Y \leq \int_{t_0}^{t} \| e^{-i(t-s)H_c} \left[ J((F^n\Psi)(s)) - J((F^n\tilde{\Psi})(s)) \right] \|_Y ds \\
\leq \int_{t_0}^{t} L \| (F^n\Psi)(s) - (F^n\tilde{\Psi})(s) \|_Y ds \\
\leq \frac{L^{n+1} \| \Psi - \tilde{\Psi} \|}{n!} \int_{t_0}^{t} (s - t_0)^n ds \\
\leq \frac{L^{n+1}(t - t_0)^{n+1}}{(n+1)!} \| \Psi - \tilde{\Psi} \|.
\]

Therefore, by induction on \( n \), relation (3.32) holds for all \( n \). Provided that \( n \) is large enough

\[
\frac{L^n(t - t_0)^n}{n!} < \frac{L^n(t_1 - t_0)^n}{n!} < 1.
\]

Therefore \( F^n \) is a strict contraction on \( B_\Phi \) and as such\(^\text{18}\), there exists a unique fixed point \( \Psi \in B_\Phi \subset C([t_0, t_1]; Y) \) such that

\[
\Psi(t) = (F\Psi)(t) = e^{-itH_c}\Phi - i \int_{t_0}^{t} e^{-i(t-s)H_c} J(\Psi(s)) ds, \quad 0 \leq t_0 \leq t \leq t_1,
\]

which is a mild solution to (3.20)–(3.21) or equivalently (3.15)–(3.17) on the interval \([t_0, t_1]\).

By the above construction, if \(\gamma\) is a mild solution on the interval \([0, \tau]\) then it can be extended to the interval \([0, \tau + \delta]\) with \(\delta > 0\) by defining \(\tilde{\gamma}(t)\) to be the solution of

\[
\tilde{\gamma}(t) = e^{-i(t-\tau)H_e} \gamma(\tau) - i \int_{\tau}^{t} e^{-i(t-s)H_e} J(\tilde{\gamma}(s)) \, ds, \quad \tau \leq t \leq \tau + \delta
\]

and then setting \(\gamma(t) = \tilde{\gamma}(t)\) for the interval \([\tau, \tau + \delta]\). Recall of course that this \(\delta\) depends only upon \(\|\gamma(t)\|_Y\).

Let \([0, t_{\max}]\) be the maximal interval of existence of (3.20)–(3.21) and consider a sequence \(\{t_n\}_{n \in \mathbb{N}}\) such that \(\lim_{n \to \infty} t_n = t_{\max}\) and \(\|\Psi(t_n)\|_Y \leq C\) for all \(n\). The boundedness of \(\Psi\) ensures that for all \(n\) there exists some \(\delta > 0\) such that a solution on \([0, t_n]\) can be extended to the interval \([0, t_n + \delta]\). Hence for \(n\) sufficiently large, \(\Psi\) can be extended beyond \(t_{\max}\), contradicting its definition. As a result, if \(t_{\max} < \infty\) then \(\lim_{t \to t_{\max}} \|\Psi(t)\|_Y = \infty\).

At this point it has been proved that there exists a unique local mild solution to (3.15)–(3.17) on an interval \([0, t_{\max}]\) and if \(t_{\max} < \infty\) then \(\lim_{t \to t_{\max}} \|\Psi(t)\|_Y = \infty\). To show that this unique mild \(Y\)-valued solution is in fact a strong \(X\)-valued solution of (3.15)–(3.17) one must verify that \(\Psi(t)\) is continuously differentiable on \([0, t_{\max}]\) with respect to the \(X\) topology [54].

Specify \(t_0 = 0\) and for all \(0 \leq t \leq t_{\max}\), consider

\[
(F\Psi)(t) = e^{-itH_e} \Phi + i \int_{0}^{t} e^{-i(t-s)H_e} J(\Psi(s)) \, ds. \tag{3.33}
\]

Since \(\Psi \in C([0, t_{\max}); Y), J(\Psi) \in C([0, t_{\max}); X)\) and therefore,

\[
(T\Psi)(t) = i \int_{0}^{t} e^{-i(t-h-s)H_e} J(\Psi(s)) \, ds \in C^1([0, t_{\max}); X).
\]

That is, \((F\Psi)(t)\) has been reduced to

\[
(F\Psi)(t) = \Psi(t) = U(t)\Phi + (T\Psi)(t) \tag{3.34}
\]
where \((T\Psi)(t) \in C^1([0,t_{\text{max}}); X)\) and \(U(t)\) is the group associated with \(H_c\). Consider equation (3.34) with \(\Phi \in D(H_c)\) as an operator on \(X\) so that \(\Phi \in D(H_c) = Z\). By the semigroup property\(^{19}\) \(U(t)\Phi \in C^1([0,t_{\text{max}}); X)\).

Showing that \(\Psi \in C^1([0,t_{\text{max}}); X)\) could have also been accomplished by using the Lipschitz continuity of \(J(\Psi)\). However in this case, one requires the observation that since \(Y\) is a reflexive Banach space, the fact that \(J\) is Lipschitz continuous with respect to \(t\) is enough to ensure that \(J\) is differentiable with respect to \(t\) a.e.\(^{20}\) and \(J' \in L^1([0,t_{\text{max}}); Y)\). The reader is referred to appendix C theorem C.2 for the proof of this significant detail.

### 3.7 Global Existence

To prove that this local solution is a global solution it is sufficient, by theorem 3.13, to prove that for every \(T > 0\), such that \(\Psi\) is a solution of (3.20)-(3.21) on \([0,T)\), then \(\|\Psi(\cdot,t)\|_Y \leq C(T)\) for every \(0 \leq t < T\) and some constant \(C(T)\). That this is the case for our system will be apparent once some conservation laws have been established.

To establish conservation laws using the original differential equation (3.15) would require that \(\Psi \in Z\) rather than the space \(Y\). One way to circumvent this problem is to take the Galerkin viewpoint [14]. In this viewpoint, one obtains a differential equation in a subspace of \(Y\) that is used in place of the original equation (3.15). Estimates are obtained using the ideas of the previous work and the final result is achieved by passing to the limit.

Let \(P_N\) be the spectral projection for the Hamiltonian \(H_c\) whose range is the closed interval \([-N,N]\). Multiplication of the local unique mild solution (3.33) by

---

\(^{19}\) See Pazy [54] p. 102, theorem 4.1.3 for details of the proof.

\(^{20}\) The term *almost everywhere* (typically denoted as a.e.) is commonly used to designate the phrase: "except for a set whose measure is zero".
3.7: Global Existence

$P_N$ and using the fact that $P_N^2 = P_N$ [55] yields

$$P_N \Psi(t) = P_N e^{-iH_c t} \Phi - i \int_0^t P_N e^{-i(t-s)H_c} P_N J(\Psi(s)) \, ds.$$  

Since $P_N H_c$ is a bounded operator, strong differentiation is allowed [14]. Taking the derivative with respect to $t$ gives the differential equation

$$\frac{d \tilde{\Psi}}{dt} = iH_c \tilde{\Psi} + iP_N J(\Psi), \quad \Psi = P_N \Psi.$$  \hspace{1cm} (3.35)

This will be used instead of the original set of equations given by (3.15). Expanding the vector $\Psi$ in terms of its components and multiplying by $i$ results in the alternative expression

$$i \partial_t \tilde{\psi}_j = -\frac{1}{2} \Delta \tilde{\psi}_j + P_N V \psi_j + \beta V_0 \tilde{\psi}_j, \quad \forall j \in \mathbb{N}. \hspace{1cm} (3.36)$$

In addition, the quantity $\tilde{V}$ is defined by the expression

$$\Delta \tilde{V} = -\alpha n = -\alpha \sum_{j=1}^{\infty} \lambda_j |\tilde{\psi}_j|^2.$$  \hspace{1cm} (3.37)

This bears a closer resemblance to the expressions (3.15)—(3.16).

As a first application in the use of equations (3.36)—(3.37) it is shown that if the initial function $\Phi$ is restricted to the space $Z \subset Y$ then $\|\Psi(\cdot, t)\|_Z$ is exponentially bounded.

**Proposition 3.14** If $\Phi \in Z$ and $\Psi(x, t)$ is the unique mild $Y$-valued solution of theorem 3.13 then there exists constants $C_1 = C_1(\|\Phi\|_Z)$ and $C_2 = C_2(\|\Phi\|_Y)$ such that

$$\|\Psi(\cdot, t)\|_Z \leq C_1 e^{C_2 t}.$$  

**Proof.** One begins by computing

$$\frac{d}{dt} \left( \|\partial_t \tilde{\Psi}(\cdot, t)\|_X^2 \right) = \sum_{j=1}^{\infty} \lambda_j \int \left( \frac{\partial \tilde{\psi}_j}{\partial t} \frac{\partial^2 \tilde{\psi}_j}{\partial t^2} + \frac{\partial \tilde{\psi}_j}{\partial t} \frac{\partial^2 \tilde{\psi}_j}{\partial t^2} \right) dx$$
where equation (3.36) has been used followed by an integration by parts and an application of both the Hölder and Cauchy–Schwarz inequalities. Lemma 3.4 gives the estimate

\[ \| \partial_t \tilde{V}(\cdot, t) \|_{\infty} \leq C \| \partial_t \tilde{V}(\cdot, t) \|_X \| \tilde{V}(\cdot, t) \|_Y \] (3.38)

and in a similar fashion,

\[ \| \partial_t (V - \tilde{V}) \|_{\infty} \leq C (\| \partial_t \tilde{V}(\cdot, t) \|_X + \| \partial_t \tilde{V}(\cdot, t) \|_X \| \tilde{V}(\cdot, t) - \tilde{V}(\cdot, t) \|_Y). \]

Using estimate (3.38) one finds that

\[ \frac{d}{dt} \left( \| \partial_t \tilde{V}(\cdot, t) \|_X^2 \right) \leq C \| \partial_t \tilde{V}(\cdot, t) \|_X^2 \]

with \( C = C(\| \tilde{V} \|_Y) \) and by a standard application of Gronwall's theorem\(^{22}\),

\[ \| \partial_t \tilde{V}(\cdot, t) \|_X^2 \leq \| \partial_t \tilde{V}(\cdot, 0) \|_X^2 e^{Ct}. \]

\(^{21}\) Differentiation of equation (3.36) with respect to \( t \) is justified by a regularity theorem of Segal [59] (theorem 3, p. 353).

\(^{22}\) See theorem C.1 in appendix C.
Letting $N \to \infty$ one obtains

$$\|\partial_t \psi(\cdot, t)\|_{L^2}^2 \leq C_1 e^{C_2 t} \tag{3.39}$$

with $C_1 = C_1(\|\Phi\|_Z)$ and $C_2 = C_2(\|\Phi\|_Y)$. By rewriting equation (3.36) in the form

$$\frac{1}{2} \Delta \tilde{\psi}_j = -i \partial_t \tilde{\psi}_j + P_N V \tilde{\psi}_j + \beta V_0 \tilde{\psi}_j,$$

summing over the $\lambda_j$ and then taking the $L^2$ norm of both sides one has

$$\|\Delta \tilde{\psi}(\cdot, t)\|_{L^2}^2 = \sum_{j=1}^{\infty} \lambda_j \|\Delta \tilde{\psi}_j\|_{L^2}^2 \leq C_1 \sum_{j=1}^{\infty} \lambda_j \|\partial_t \tilde{\psi}_j\|_{L^2}^2 + C_2 \sum_{j=1}^{\infty} \lambda_j \|V \psi_j\|_{H^2}^2 + C_3 \sum_{j=1}^{\infty} \lambda_j \|V_0 \tilde{\psi}_j\|_{L^2}^2.$$

The first term is estimated with equation (3.39). For the second term, item (i) of theorem 3.23 gives $\|V(\cdot, t)\|_{L^\infty} \leq C$ so that

$$\sum_{j=1}^{\infty} \lambda_j \|V \psi_j\|_{H^2}^2 \leq \|V(\cdot, t)\|_{L^\infty} \|\Psi(\cdot, t)\|_{H^2}^2 \leq C \|\Phi\|_{H^2}^2 \leq C$$

uniformly in $N$ by the conservation of probability. The final term can be bounded above using lemma 3.4

$$\sum_{j=1}^{\infty} \lambda_j \|V_0 \tilde{\psi}_j\|_{L^2}^2 \leq C \sum_{j=1}^{\infty} \lambda_j \|\nabla \tilde{\psi}_j\|_{L^2}^2 \leq C \|\nabla \tilde{\psi}(\cdot, t)\|_{L^2}^2 \leq C$$

again, uniformly in $N$. Using these estimates, as well as the fact that the $H^2$ norm is equivalent to the graph norm of the Laplacian operator [1], implies that

$$\|\Psi(\cdot, t)\|_{L^2}^2 \leq C \left(\|\Psi(\cdot, t)\|_{H^2}^2 + \|\Delta \Psi(\cdot, t)\|_{L^2}^2\right)$$

$$\leq C_1 e^{C_2 t}$$

where $C_1 = C_1(\|\Phi\|_Z)$ and $C_2 = C_2(\|\Phi\|_Y)$ which completes the proof. □
3.7.1 Conservation of Probability

**Proposition 3.15 (Conservation of Probability)**

*If \( \Phi \in Z \) and \( \Psi(x,t) \) is the unique mild \( Y \)-valued solution of theorem 3.13 on the interval \([0, t_{\text{max}})\) which is a strong \( X \)-valued solution then

\[
\|\Psi(\cdot,t)\|_X = \|\Phi\|_X = 1
\]

for all \( t \in [0, t_{\text{max}}) \).

**Proof.** Applying \( \bar{\psi}_j \) to (3.36) and subtracting the result of applying \( \bar{\psi}_j \) to the complex conjugate of (3.36) one obtains

\[
i(\bar{\psi}_j \partial_t \bar{\psi}_j + \bar{\psi}_j \partial_t \psi_j) = \frac{1}{2}(\bar{\psi}_j \Delta \bar{\psi}_j - \bar{\psi}_j \Delta \psi_j).
\]

Using the vector identity

\[
\nabla \cdot (v \nabla u) = \nabla v \cdot \nabla u + v \Delta u
\] (3.40)

gives

\[
i \frac{\partial}{\partial t} \left( |\bar{\psi}_j(x,t)|^2 \right) = \frac{1}{2} \nabla \cdot \left( \bar{\psi}_j \nabla \bar{\psi}_j - \bar{\psi}_j \nabla \psi_j \right).
\]

Finally, by integrating over all space and using Gauss' divergence theorem yields

\[
\frac{\partial}{\partial t} \left( \|\bar{\psi}_j(\cdot,t)\|_2^2 \right) = \int \partial_t \left( |\bar{\psi}_j(x,t)|^2 \right) dx = 0.
\]

This implies that

\[
\|\bar{\psi}_j(\cdot,t)\|_2^2 = \|\phi_j\|_2^2
\]

which upon multiplication by \( \lambda_j \), summing on \( j \) and using the normalization given by (3.18.b) gives

\[
\|\bar{\Psi}(\cdot,t)\|_X^2 = \|\Phi\|_X^2.
\]

Letting \( N \to \infty \) proves the proposition. \( \square \)
3.7: Global Existence

3.7.2 Conservation of Energy

Proposition 3.16 (Conservation of Energy)

If $\Phi \in Z$ and $\Psi(x,t)$ is the unique mild $Y$-valued solution of theorem 3.13 on the interval $[0, t_{\text{max}}]$ which is a strong $X$-valued solution then

$$\frac{1}{2} \| \nabla \Psi(\cdot,t) \|^2_X + E_{\alpha,\beta}(t) = \frac{1}{2} \| \nabla \Phi \|^2_X + E_{\alpha,\beta}(0)$$

(3.41)

for all $t_0, t_1 \in [0, t_{\text{max}})$ where

$$E_{\alpha,\beta}(t) = \frac{1}{2} \int V_n \, dx + \beta \int V_0n \, dx.$$  

(3.42)

Proof. Since $\tilde{\Psi}$ is a solution of (3.35), there exists a time interval $[0, t_{\text{max}})$ such that $\tilde{\Psi} \in C([0, t_{\text{max}}); Y) \cap C^1([0, t_{\text{max}}); X)$. Take $\delta > 0$ and consider

$$\frac{1}{\delta} \int \left[ |\nabla \tilde{\Psi}(t + \delta)|^2 - |\nabla \tilde{\Psi}(t)|^2 \right] \, dx$$

$$= \sum_{j=1}^{\infty} \lambda_j \left[ \frac{1}{\delta} \int \tilde{\Psi}_j(t) \Delta \tilde{\Psi}_j(t) \, dx - \frac{1}{\delta} \int \tilde{\Psi}_j(t + \delta) \Delta \tilde{\Psi}_j(t + \delta) \, dx \right]$$

$$= - \sum_{j=1}^{\infty} \lambda_j \int \frac{1}{\delta} [\tilde{\Psi}_j(t + \delta) - \tilde{\Psi}_j(t)] \Delta \tilde{\Psi}_j(t) \, dx$$

$$- \sum_{j=1}^{\infty} \lambda_j \int \frac{1}{\delta} [\tilde{\Psi}_j(t) - \tilde{\Psi}_j(t + \delta)] \Delta \tilde{\Psi}_j(t + \delta) \, dx$$

obtained by using the identity (3.40) and Gauss' theorem. Letting $\delta \to 0$ and using the fact that $\tilde{\Psi} \in C^1([0, t_{\text{max}}); X)$ shows that $\partial_t \left( \| \nabla \tilde{\Psi}(\cdot,t) \|^2_X \right)$ exists and

$$\frac{d}{dt} \left( \| \nabla \tilde{\Psi}(\cdot,t) \|^2_X \right) = -2 \text{Re} \sum_{j=1}^{\infty} \lambda_j \int (\Delta \tilde{\Psi}_j) \partial_t \tilde{\Psi}_j \, dx.$$  

The integrand can be simplified by a method similar to proposition 3.15. Applying $\partial_t \tilde{\Psi}_j$ to (3.36) gives

$$i|\partial_t \tilde{\Psi}_j|^2 + \frac{1}{2} (\partial_t \tilde{\Psi}_j) \Delta \tilde{\Psi}_j = (\tilde{V} + \beta V_0) (\partial_t \tilde{\Psi}_j) \tilde{\Psi}_j + (P_N V_j - \tilde{V} \tilde{\Psi}_j) \partial_t \tilde{\Psi}_j.$$
Adding this to its complex conjugate yields

\[
\text{Re}(\Delta \bar{\psi}_j) \partial_t \tilde{\psi}_j = (\bar{V} + \beta V_0) \partial_t (|\bar{\psi}_j|^2) + \frac{1}{2} \text{Re}(V \psi_j - \bar{V} \tilde{\psi}_j) \partial_t \bar{\psi}_j
\]  

(3.43)

where the fact that \( \bar{V} + \beta V_0 \) is real valued and that \( P_N V \psi_j \partial_t \bar{\psi}_j = V \psi_j \partial_t \bar{\psi}_j = V \psi_j \partial_t \bar{\psi}_j \) have been used. Summing expression (3.43) over the probabilities \( \lambda_j \) one obtains the expression

\[
\sum_{j=1}^{\infty} \lambda_j \left[ (\Delta \bar{\psi}_j) \partial_t \tilde{\psi}_j + (\Delta \tilde{\psi}_j) \partial_t \bar{\psi}_j \right] = 2(\bar{V} + \beta V_0) \partial_t \bar{n} + \text{Re} \sum_{j=1}^{\infty} \lambda_j (V \psi_j - \bar{V} \tilde{\psi}_j) \partial_t \bar{\psi}_j.
\]

(3.44)

From equation (3.37)

\[
\Delta \bar{V} = -\alpha \sum_{j=1}^{\infty} \lambda_j |\bar{\psi}_j|^2 = -\alpha \bar{n}
\]

one obtains

\[
\bar{V} \partial_t (\Delta \bar{V}) = \nabla \cdot (\bar{V} \partial_t (\nabla \bar{V})) - \nabla \bar{V} \cdot \partial_t (\nabla \bar{V}) = -\alpha \bar{V} \partial_t \bar{n}
\]

and

\[
\partial_t (\bar{V} \Delta \bar{V}) = \nabla \cdot \partial_t (\bar{V} \nabla \bar{V}) - \partial_t (\nabla \bar{V} \cdot \nabla \bar{V}) = -\alpha \partial_t (\bar{V} \bar{n}).
\]

It now follows that

\[
-\alpha \bar{V} \partial_t \bar{n} = \nabla \cdot [\bar{V} \partial_t (\nabla \bar{V})] - \frac{1}{2} \partial_t (\nabla \bar{V} \cdot \nabla \bar{V})
\]

\[
= \nabla \cdot [\bar{V} \partial_t (\nabla \bar{V})] - \frac{1}{2} \nabla \cdot \partial_t (\bar{V} \nabla \bar{V}) - \frac{\alpha}{2} \partial_t (\bar{V} \bar{n})
\]

or, by integrating over \( \mathbb{R}^3 \) and using Gauss' divergence theorem,

\[
\int \bar{V} \partial_t \bar{n} \, dx = \frac{1}{2} \int \partial_t (\bar{V} \bar{n}) \, dx.
\]

(3.45)

Additionally \( \partial_t V_0 = 0 \) so that

\[
\int V_0 \partial_t \bar{n} \, dx = \frac{d}{dt} \int V_0 \bar{n} \, dx.
\]

(3.46)
Hence, an application of relations (3.45) and (3.46) to equation (3.44) gives

\[
\frac{d}{dt} \left( \| \nabla \tilde{\psi}(\cdot, t) \|_{X}^2 \right) = - \frac{d}{dt} \int \tilde{V} \tilde{n} \, dx - 2\beta \frac{d}{dt} \int V_0 \tilde{n} \, dx
\]

\[
- \operatorname{Re} \sum_{j=1}^{\infty} \lambda_j (V \psi_j - \tilde{V} \tilde{\psi}_j) \partial_t \tilde{\psi}_j \, dx.
\]

Integrating over the interval \((0, t)\) and then applying the definition of \(E_{\alpha, \beta}\) given by equation (3.42), reveals

\[
\frac{1}{2} \| \nabla \tilde{\psi}(\cdot, t) \|_{X}^2 + \tilde{E}_{\alpha, \beta}(t) = \frac{1}{2} \| \nabla \Phi \|_{X}^2 + E_{\alpha, \beta}(0)
\]

\[
- \frac{1}{2} \operatorname{Re} \sum_{j=1}^{\infty} \lambda_j \int_0^t \int (V \psi_j - \tilde{V} \tilde{\psi}_j) \partial_t \tilde{\psi}_j \, dx \, ds \tag{3.47}
\]

with

\[
\tilde{E}_{\alpha, \beta}(t) = \frac{1}{2} \int \tilde{V} \tilde{n} \, dx + \beta \int V_0 \tilde{n} \, dx.
\]

The final step is to take the limit as \(N \to \infty\). The estimates that follow are essentially the same as those used to exhibit the Lipschitz property of the map \(J\) in proposition 3.12. The gradient term can be estimated with theorem 3.5 as

\[
\| \nabla (\tilde{\psi}(\cdot, t) - \psi(\cdot, t)) \|_{X}^2 \leq C \| (H_c + \mu_\beta)^{1/2} (\tilde{\psi}(\cdot, t) - \psi(\cdot, t)) \|_{X}^2
\]

\[
= C \| (P_N - I)(H_c + \mu_\beta)^{1/2} \psi(\cdot, t) \|_{X}^2. \tag{3.48}
\]

This last expression goes to zero by the spectral theorem and the fact that for each \(t \in [0, t_{\text{max}})\), \(\psi(t) \in Y = D((H_c + \mu_\beta)^{1/2})\). The external Coulomb energy is also estimated with theorem 3.5:

\[
\int (V_0 \tilde{n} - V_0 n) \, dx \leq \sum_{j=1}^{\infty} \lambda_j \left\| V_0 \left( |\tilde{\psi}_j|^2 - \tilde{\psi}_j \tilde{\psi}_j + \tilde{\psi}_j \tilde{\psi}_j - |\psi_j|^2 \right) \right\|_1
\]

\[
\leq C \sum_{j=1}^{\infty} \lambda_j \left( \| \tilde{\psi}_j \|_2 \left\| \frac{\tilde{\psi}_j - \psi_j}{|\cdot|} \right\|_2 + \left\| \frac{\tilde{\psi}_j}{|\cdot|} \right\|_2 \left\| \tilde{\psi}_j - \psi_j \right\|_2 \right)
\]

\[
\leq C \sum_{j=1}^{\infty} \lambda_j \left( \| \tilde{\psi}_j \|_2 \| \nabla (\tilde{\psi}_j - \psi_j) \|_2 + \| \nabla \psi_j \|_2 \| \tilde{\psi}_j - \psi_j \|_2 \right)
\]
The Minkowski and H"older inequalities, lemma 3.4 and theorem 3.5 have been applied in that order. This last expression also goes to zero as $N \to \infty$ using the previous argument. For the self-consistent energy term one uses the Minkowski, H"older and Cauchy-Schwarz inequalities to break the estimate into three separate pieces defined $T_1$, $T_2$ and $T_3$ below:

\[
\int (\tilde{V} n - V n) \, dx \leq \sum_{j=1}^{\infty} \lambda_j \left\| \tilde{V} |\tilde{\psi}_j|^2 - V |\tilde{\psi}_j|^2 + V |\psi_j|^2 - V |\psi_j|^2 \right\|_1
\]

\[
\leq \sum_{j=1}^{\infty} \lambda_j \left\| (\tilde{V} - V) |\tilde{\psi}_j|^2 \right\|_1 + \sum_{j=1}^{\infty} \lambda_j \left\| V \left( |\psi_j|^2 - |\tilde{\psi}_j|^2 \right) \right\|_1
\]

\[
\leq \| \tilde{V} - V \|_\infty \| \tilde{\Psi} \|_X^2 + \| V \|_\infty \sum_{j=1}^{\infty} \lambda_j \left\| |\psi_j|^2 - |\tilde{\psi}_j|^2 \tilde{\psi}_j + \tilde{\psi}_j \psi_j - |\psi_j|^2 \right\|_1
\]

\[
\leq \| \tilde{V} - V \|_\infty \| \tilde{\Psi} \|_X^2 + \| V \|_\infty \sum_{j=1}^{\infty} \lambda_j \| \tilde{\psi}_j (\psi_j - \tilde{\psi}_j) \|_1 + \| V \|_\infty \sum_{j=1}^{\infty} \lambda_j \| \tilde{\psi}_j (\psi_j - \tilde{\psi}_j) \|_1
\]

\[
\leq \| \tilde{V} - V \|_\infty \| \tilde{\Psi} \|_X^2 + \| V \|_\infty \| \tilde{\Psi} \|_X^2 \| |\psi - \tilde{\psi}|^2 \|_X + \| V \|_\infty \| \tilde{\Psi} \|_X \| \tilde{\Psi} - \tilde{\psi}\|_X^2
\]

\[
:= T_1 + T_2 + T_3.
\]

One now proceeds as in proposition 3.12. From lemma 3.8,

\[
T_2 = \| V \|_\infty \| \tilde{\Psi} \|_X \| \tilde{\Psi} - \tilde{\psi}\|_X^2
\]

\[
\leq C \| \tilde{\Psi} \|_X \| \tilde{\psi}\|_X \| \tilde{\psi} - \tilde{\psi}\|_X^2
\]

\[
= C \| \tilde{\Psi} \|_X \| \tilde{\psi}\|_X \| (P_N - I) \tilde{\psi}\|_X^2,
\]

\[
T_3 = \| V \|_\infty \| \tilde{\Psi} \|_X \| \tilde{\psi}\|_X^2
\]

\[
\leq C \| \tilde{\Psi} \|_X \| \tilde{\psi}\|_X \| \tilde{\psi} - \tilde{\psi}\|_X^2
\]

\[
= C \| \tilde{\Psi} \|_X \| \tilde{\psi}\|_X \| P_N \tilde{\psi}\|_X^2 \| (P_N - I) \tilde{\psi}\|_X^2
\]

and

\[
T_1 = \| \tilde{V} - V \|_\infty \| \tilde{\Psi} \|_X^2
\]

\[
\leq C (\| \tilde{\Psi} \|_X + \| \tilde{\psi}\|_X) \| \tilde{\psi}\|_X \| \tilde{\psi} - \tilde{\psi}\|_X
\]

\[
= C (\| \tilde{\Psi} \|_X + \| P_N \tilde{\psi}\|_X) \| P_N \tilde{\psi}\|_X^2 \| (P_N - 1)(H_c + \mu_\beta)^{1/2} \tilde{\psi}\|_X.
\]
These all go to zero as $N \to \infty$ by the spectral theorem. Finally, the integrand (with respect to the $s$ variable) of expression (3.47) can be written as

$$i \sum_{j=1}^{\infty} \lambda_j \left[ \langle V \psi_j - \tilde{V} \tilde{\psi}_j, (H_c + \mu) \tilde{\psi}_j \rangle + \langle V \psi_j - \tilde{V} \tilde{\psi}_j, P_N V \psi_j \rangle - \mu \langle V \psi_j - \tilde{V} \tilde{\psi}_j, \tilde{\psi}_j \rangle \right]$$

$$:= T_4 + T_5 + T_6.$$

The $T_4$ term is written as

$$\sum_{j=1}^{\infty} \lambda_j \langle (H_c + \mu)^{1/2} (V \psi_j - \tilde{V} \tilde{\psi}_j), (H_c + \mu)^{1/2} \tilde{\psi}_j \rangle$$

$$\leq C \sum_{j=1}^{\infty} \lambda_j \|V \psi_j - \tilde{V} \tilde{\psi}_j\|_{1,2} \|\tilde{\psi}_j\|_{1,2}$$

$$\leq C \|V \Psi - \tilde{V} \tilde{\Psi}\|_Y \|\Psi\|_Y$$

$$\leq C (\|\Psi\|_Y, \|\tilde{\Psi}\|_Y) \|\Psi - \tilde{\Psi}\|_Y$$

by using the Lipschitz bound of proposition 3.12. For the $T_5$ term,

$$\sum_{j=1}^{\infty} \lambda_j \langle V \psi_j - \tilde{V} \tilde{\psi}_j, P_N V \psi_j \rangle \leq \sum_{j=1}^{\infty} \lambda_j \|V \psi_j - \tilde{V} \tilde{\psi}_j\|_2 \|V \psi_j\|_2$$

$$= \sum_{j=1}^{\infty} \lambda_j \|V \psi_j - V \tilde{\psi}_j + V \tilde{\psi}_j - \tilde{V} \tilde{\psi}_j\|_2 \|V \psi_j\|_2$$

$$\leq \|V\|_\infty^2 \|\Psi - \tilde{\Psi}\|_X \|\Psi\|_X + \|V\|_\infty \|V - \tilde{V}\|_\infty \|\Psi\|_X \|\tilde{\Psi}\|_X$$

$$\leq C_1 (\|\Psi\|_Y) \|\Psi - \tilde{\Psi}\|_X + C_2 (\|\Psi\|_Y, \|\tilde{\Psi}\|_X) \|\Psi - \tilde{\Psi}\|_Y$$

using the Minkowski, Hölder inequalities as well as lemma 3.8. The $T_6$ term is estimated in a similar manner:

$$\sum_{j=1}^{\infty} \lambda_j \langle V \psi_j - \tilde{V} \tilde{\psi}_j, \psi_j \rangle \leq \sum_{j=1}^{\infty} \lambda_j \|V \psi_j - \tilde{V} \tilde{\psi}_j\|_2 \|\psi_j\|_2$$

$$= \sum_{j=1}^{\infty} \lambda_j \|V \psi_j - V \tilde{\psi}_j + V \tilde{\psi}_j - \tilde{V} \tilde{\psi}_j\|_2 \|\psi_j\|_2$$

$$\leq \|V\|_\infty \|\Psi - \tilde{\Psi}\|_X \|\Psi\|_X + \|V - \tilde{V}\|_\infty \|\tilde{\Psi}\|_X \|\tilde{\Psi}\|_X$$

$$\leq C_1 (\|\Psi\|_Y) \|\Psi - \tilde{\Psi}\|_X + C_2 (\|\Psi\|_Y, \|\tilde{\Psi}\|_X) \|\Psi - \tilde{\Psi}\|_Y.$$
The above estimates show that integrand is bounded above uniformly in $N$ by a constant that depends only on $\|\Psi\|_Y$ and since $\Psi(t) \in C([0, t_{\text{max}}]; Y)$, this upper bound in integrable on $[0, t_{\text{max}}]$. Therefore by the dominated convergence theorem the integral with respect to $s$ tends to zero as $N \to \infty$ and the difference between the desired conservation law and expression (3.47) tends to zero. □

3.7.3 A Crucial Estimate

The conservation laws derived in the last section are now used to obtain the key bounds on the growth of the vector $\Psi(x, t)$.

**Lemma 3.17** If $\Phi \in \mathbb{Z}$ and $\Psi(x, t)$ is the unique mild $Y$-valued solution of theorem 3.13 on the interval $[0, t_{\text{max}})$ then $\|\Psi(\cdot, t)\|_Y \leq C$ for all $t \in [0, t_{\text{max}})$ where $C$ depends only on $\Phi$.

**Proof.** An upper bound for the energy term $E_{\alpha, \beta}(t)$ of equation (3.42) is exhibited first. For the self-consistent term,

$$\left| \int V_n \, dx \right| \leq \|V(\cdot, t)\|_\infty \|n\|_1$$

$$\leq C\|\Psi(\cdot, t)\|_Y^2 \|\Psi(\cdot, t)\|_Y$$

$$= C\|\Phi\|_X \|\Psi(\cdot, t)\|_Y$$

applying lemma 3.8 and proposition 3.15. For the Coulomb term,

$$\left| \int V_0 n \, dx \right| \leq \sum_{j=1}^{\infty} \lambda_j \int \frac{|\psi_j(x, t)|^2}{|x|} \, dx$$

$$\leq C \sum_{j=1}^{\infty} \lambda_j \|\psi_j\|_2 \left\| \frac{\psi_j}{|x|} \right\|_2$$

$$\leq C\|\Phi\|_X \|\Psi(\cdot, t)\|_Y$$

by using the Hölder inequality, lemma 3.4, proposition 3.15 and the Cauchy–Schwarz inequality. Combining these two results, one obtains the estimate

$$|E_{\alpha, \beta}(t)| \leq C\|\Psi(\cdot, t)\|_Y$$

(3.50)
where $C$ is a constant that depends only upon $\|\Phi\|_X$.

Equation (3.41) and the energy bound (3.50) give

$$
\|\nabla \psi(\cdot,t)\|_X^2 = \|\psi\|_X^2 + 2E_{\alpha,\beta}(0) - 2E_{\alpha,\beta}(t) \\
\leq C_1 + C_2\|\psi(\cdot,t)\|_Y.
$$

(3.51)

Hence, from the definition of the $Y$ norm, one determines that

$$
\|\psi(\cdot,t)\|_Y^2 = \|\psi(\cdot,t)\|_X^2 + \|\nabla \psi(\cdot,t)\|_X^2 \\
\leq 1 + C_1 + C_2\|\psi(\cdot,t)\|_Y \\
\leq C_3 + \frac{1}{2}\|\psi(\cdot,t)\|_Y^2.
$$

This last bound will be satisfied provided $C_3 \geq C_2^2/2 + C_1 + 1$. Solving for $\|\psi(\cdot,t)\|_Y$ yields the result. □

Having shown that $\|\psi(\cdot,t)\|_Y$ remains bounded, theorem 3.13 now implies that the local solution is actually global. This gives the following corollary:

**Corollary 3.18** For every $\Phi \in Z$ there exists a unique global mild $Y$-valued solution which is a strong $X$-valued solution of the initial value problem (3.15)-(3.17) such that

$$
\psi \in C([0,\infty); Y) \cap C^1([0,\infty); X).
$$

**Proof.** This is a direct consequence of applying lemma 3.17 to theorem 3.13. □

In addition, global bounds can now be obtained on the growth of the potential.

**Corollary 3.19** If $\Phi \in Z$ and $\psi(x,t)$ is the unique mild $Y$-valued solution of theorem 3.13 then

$$
\|V(\cdot,t)\|_\infty \leq C, \|\nabla V(\cdot,t)\|_2 \leq C, \|\Delta V(\cdot,t)\|_2 \leq C, \|\nabla V(\cdot,t)\|_\infty \leq C
$$

for all $t$ where $C$ depends only on $\Phi$. 

3.8: Regularity Properties

**Proof.** This follows by simply applying the previous lemma to lemmata 3.8–3.11. □

Emphasis should be made that the existence of the unique global mild solution $\Psi \in Y$ does not depend on either $\alpha$ or $\beta$. By considering the problem on all of $\mathbb{R}^3$ as in [13], instead of a bounded domain $\Omega$, global existence for all four cases of $\alpha$ and $\beta$ listed in table 2.1 is obtained. In addition, this eliminates a technical regularization procedure as one passes to an arbitrarily large domain. Finally, by treating the external Coulomb potential term as part of the *unperturbed* equation, it can be handled with standard semigroup theory. This eliminates many of the complications that arise if the Coulomb potential is treated as a perturbation.

This chapter concludes with some results that summarize the properties of the solution to (3.15)–(3.17).

**3.8 Regularity Properties**

**Theorem 3.20** The SP system (3.15)–(3.17) has a unique global strong $X$-valued solution $(\Psi, V)$ with the properties

(i) $\Psi \in C([0, \infty); Y) \cap C^1([0, \infty); X) \cap L^\infty([0, \infty); Y)$

(ii) $V \in C([0, \infty); L^\infty) \cap L^\infty([0, \infty); L^\infty)$

(iii) $\nabla V \in C([0, \infty); L^2) \cap L^\infty([0, \infty); L^2)$

(iv) $n, \Delta V \in C([0, \infty); L^2) \cap L^\infty([0, \infty); L^2) \cap C^1([0, \infty); L^1)$.

**Proof.** Item (i) follows immediately from lemma 3.17 and corollary 3.18. Items (ii) and (iii) are restatements of lemmas 3.8 and 3.9 respectively where one uses the fact that $\Psi \in C([0, \infty); Y)$. The proof of (iv) is as follows. The first part, $n, \Delta V \in C([0, \infty); L^2) \cap L^\infty([0, \infty); L^2)$, is a direct consequence of lemma 3.10, item (i) and the definition of $\Delta V$ in equation (3.16). To show the second part,
3.8: Regularity Properties

\( n, \Delta V \in C^1([0, \infty); L^1) \), one considers

\[
\| \partial_t \Delta V(t) - \partial_t \Delta V(s) \|_1 = \left\| \sum_{j=1}^{\infty} \lambda_j 2 \text{Re} \left[ \overline{\psi_j(t)} \partial_t \psi_j(t) - \overline{\psi_j(s)} \partial_t \psi_j(s) \right] \right\|_1
\leq C \sum_{j=1}^{\infty} \lambda_j \| \overline{\psi_j(t)} \|_2 \| \partial_t \psi_j(t) - \partial_t \psi_j(s) \|_2
\leq C \| \overline{\psi} \|_X \left( \sum_{j=1}^{\infty} \lambda_j \| \partial_t \psi_j(t) - \partial_t \psi_j(s) \|_2^2 \right)^{1/2}
\leq C \| \partial_t \overline{\psi}(t) - \partial_t \overline{\psi}(s) \|_X.
\]

Since \( \overline{\psi} \in C^1([0, \infty); X) \) the proof is complete. □

Before leaving this section, a few more regularity results are proved. For the most part, these last results are extensions of the original relationships established in theorem 3.20. To facilitate this extension, an additional independent estimate is required. The first lemma is a generalization of the Hardy and Littlewood inequality [34] which is stated without proof.

**Lemma 3.21** Let \( 0 < \mu < m \) and suppose that \( f \in L^p(\mathbb{R}^m) \), \( g \in L^r(\mathbb{R}^m) \) with \( p^{-1} + r^{-1} + \mu m^{-1} = 2 \) and \( 1 < p, r < \infty \). Then

\[
\int_{\mathbb{R}^m} \int_{\mathbb{R}^m} \frac{|f(x)||g(y)|}{|x - y|^{\mu}} \, dy \, dx \leq C_{p, r, \mu, m} \| f \|_p \| g \|_r.
\]

**Proof.** The reader is directed to p. 31 of [56]. □

Using this estimate a closely related inequality is proved that will sharpen our estimates for the self-consistent potential. Our proof originates with Bers, John and Schechter [5].
Lemma 3.22 Let $0 < \lambda < m$ and suppose that $f \in L^p(\mathbb{R}^m)$ with $p > 1$ and $q = p^{-1} + \lambda m^{-1} - 1 > 0$. Then

$$\left\| \int_{\mathbb{R}^m} \frac{f(y)}{|y-x|^{\lambda}} dy \right\|_q \leq C_p, \lambda, m \|f\|_p.$$ 

Proof. By duality, the stated inequality will be true if it can be shown that for all functions $f, g$ with compact support

$$\left| \langle g, |x|^{-\lambda} \ast f \rangle \right| \leq C \|f\|_p \|g\|_r, \quad \frac{1}{q} + \frac{1}{r} = 1.$$ 

However from Lemma 3.21

$$\left| \langle g, |x|^{-\lambda} \ast f \rangle \right| \leq C \int_{\mathbb{R}^m} \int_{\mathbb{R}^m} \frac{|f(x)||g(y)|}{|y-x|^{\lambda}} dy \, dx \leq C \|f\|_p \|g\|_r$$

with $p^{-1} + r^{-1} + \lambda m^{-1} = 2$. Replacing $r^{-1}$ with $1 - q^{-1}$, $p > 1$, $r > 1$ gives the desired result. □

The final regularity theorem of the SP system can now be stated.

Theorem 3.23 The SP system (3.15)--(3.17) described in theorem 3.20 has the following additional properties

(i) $V \in L^\infty([0, \infty); L^p) \cap C([0, \infty); L^p)$ for $3 < p \leq \infty$

(ii) $\nabla V \in L^\infty([0, \infty); L^q) \cap C([0, \infty); L^q)$ for $3/2 < q \leq \infty$

(iii) $\nabla, \Delta V \in L^\infty([0, \infty); L^r) \cap C([0, \infty); L^r)$ for $1 \leq r \leq 3$.

Proof. First note that for any $f \in L^q \cap L^r$

$$\left\| |f(t)|^2 - |f(s)|^2 \right\|_p = \left\| \overline{f(t)}[f(t) - f(s)] + f(s)[\overline{f(t)} - \overline{f(s)}] \right\|_p$$

$$\leq (\|f(t)\|_q + \|f(s)\|_q) \|f(t) - f(s)\|_r$$
where \( p^{-1} = q^{-1} + r^{-1} \) by Hölder's inequality. Hence,

\[
\| \Delta V(\cdot, t) - \Delta V(\cdot, s) \|_p \leq C \sum_{j=1}^{\infty} \lambda_j \left\| \psi_j(t) \right\|^2 - \left\| \psi_j(s) \right\|^2 \|_p \\
\leq C \sum_{j=1}^{\infty} \lambda_j \left( \| \psi_j(t) \|_q + \| \psi_j(s) \|_q \right) \| \psi_j(t) - \psi_j(s) \|_r \\
\leq C \left[ \left( \sum_{j=1}^{\infty} \lambda_j \| \psi_j(t) \|_q^2 \right)^{1/2} + \left( \sum_{j=1}^{\infty} \lambda_j \| \psi_j(s) \|_q^2 \right)^{1/2} \right] \\
\times \left( \sum_{j=1}^{\infty} \lambda_j \| \psi_j(t) - \psi_j(s) \|_r^2 \right)^{1/2}.
\] (3.52)

Substituting \( q = r = 2, p = 1 \) into the relation (3.52) gives

\[
\| \Delta V(\cdot, t) - \Delta V(\cdot, s) \|_1 \leq C \| \Psi(t) - \Psi(s) \|_X
\] (3.53)

and since \( \Psi \in C^1([0, \infty); X) \), one has \( \Delta V \in C([0, \infty); L^1) \). Substituting \( q = r = 6, p = 3 \) yields

\[
\| \Delta V(\cdot, t) - \Delta V(\cdot, s) \|_3 \leq C \| \Psi(t) - \Psi(s) \|_Y
\] (3.54)

by using the inequality \( \| f \|_6 \leq C \| \nabla f \|_2 \). This can be obtained from the GN inequality if one chooses \( r = 2, j = 0, m = 1, p = 6 \) and \( a = 1 \). Since \( \Psi \in C([0, \infty); Y) \), expression (3.54) implies that \( \Delta V \in C([0, \infty); L^3) \). Applying the Riesz–Thorin interpolation theorem to (3.53) and (3.54) allows one to conclude that

\[ n, \Delta V \in C([0, \infty); L^r) \text{ for } 1 \leq r \leq 3 \]

which proves the second half of item (iii).

To show that \( n, \Delta V \in L^\infty([0, \infty); L^r) \) for \( 1 \leq r \leq 3 \), (the first half of item (iii)), consider the inequality

\[
\| \Delta V \|_r \leq C \sum_{j=1}^{\infty} \lambda_j \| \psi_j \|_{2r}^2.
\]

\[ ^{23} \text{It is also possible to use item (iv) of theorem 3.20.} \]
Choosing $r = 1$ gives
\[ \|\Delta V\|_1 \leq C\|\Psi(\cdot, t)\|_X^2 \leq C \]
while $r = 3$ implies
\[ \|\Delta V\|_3 \leq C \sum_{j=1}^{\infty} \lambda_j \|\psi_j\|_6^2 \leq C \sum_{j=1}^{\infty} \lambda_j \|\nabla \psi_j\|_2^2 \leq C\|\Psi(\cdot, t)\|_Y \leq C \]
by using $\|f\|_6 \leq C\|\nabla f\|_2$. $\Psi \in Y$ ensures that these quantities remain bounded.

Items (i) and (ii) follow directly from item (iii) by using the representation
\[ V(x, t) = \frac{1}{4\pi} \int \frac{\Delta V(y, t)}{|y - x|} \, dy \]
which also implies that
\[ \nabla V(x, t) = \frac{1}{4\pi} \int \frac{\Delta V(y, t)}{|y - x|^2} \, dy. \]
Using lemma 3.22 one has the estimate
\[ \|\nabla V(\cdot, t) - \nabla V(\cdot, s)\|_q \leq C\|\Delta V(\cdot, t) - \Delta V(\cdot, s)\|_p \quad (3.55) \]
valid for $p > 1$ and $q^{-1} = p^{-1} - 1/3 > 0$ and
\[ \|V(\cdot, t) - V(\cdot, s)\|_q \leq C\|\Delta V(\cdot, t) - \Delta V(\cdot, s)\|_p \quad (3.56) \]
valid for $p > 1$ and $q^{-1} = p^{-1} - 2/3 > 0$. Item (ii) follows by applying the range $1 < p < 3$ from item (iii) to equation (3.55). The case $q = \infty$ follows from lemma 3.11. Item (i) results by an application of the range $1 < p < 3/2$ from item (iii) to equation (3.56). The case $q = \infty$ is realized by applying item (ii) of theorem 3.20. This completes the proof of the last of the three items. □

It is worth noting that no attempt was made to show that the statements of theorems 3.20 and 3.23 are optimal. The only criteria has been to exhibit a sufficiently broad set of properties so that much of the analysis in the subsequent
Table 3.1: SP regularity for $\beta = 0$ and $\beta \neq 0$.

The regularity results for $\beta = 0$ (no external potential) are compared with those for $\beta \neq 0$. Ranges in round brackets are extended estimates that follow from the case $\beta \neq 0$. All other $\beta = 0$ results can be replaced by the $\beta \neq 0$ ranges.

By transforming from the SP system into the WP system, the regularity properties of the SP system are inherited by the WP system. This procedure begins by recalling the transformation from the SP system to the WP system.
3.9 Global Existence of the WP System

To lift the results to the WP system, first recall the definition of $z(r, s)$ given in equation (3.12) and repeated here for convenience

$$z(r, s, t) = \sum_{j=1}^{\infty} \lambda_j \overline{\psi_j}(r, t)\psi_j(s, t).$$

This equation is invariant under the change of variable introduced in section 3.1.2. Properties of $z$ can be lifted from the properties of $\Psi$ by noting that

$$\|z(\cdot, \cdot, t)\|_{L^2(\mathbb{R}_s^3 \times \mathbb{R}_t^2)} = \left\| \sum_{j=1}^{\infty} \lambda_j \overline{\psi_j}(\cdot, t)\psi_j(\cdot, t) \right\|_{L^2(\mathbb{R}_s^3 \times \mathbb{R}_t^2)}$$

$$\leq \sum_{j=1}^{\infty} \lambda_j \left( \int \int |\overline{\psi_j}(r, t)|^2 |\psi_j(s, t)|^2 \, dr \, ds \right)^{1/2}$$

$$= \sum_{j=1}^{\infty} \lambda_j \|\psi_j(\cdot, t)\|_2^2$$

$$= \|\overline{\Psi}(\cdot, t)\|_{\mathcal{H}}^2. \quad (3.57)$$

Continuing in a similar fashion, theorem 3.20 leads to the following proposition:

**Proposition 3.24** Let $\Psi$ be given as in theorem 3.20. Then

(i) $z \in C([0, \infty); H^1(\mathbb{R}_s^3 \times \mathbb{R}_t^2)) \cap L^\infty([0, \infty); H^1(\mathbb{R}_s^3 \times \mathbb{R}_t^2))$

(ii) $\frac{\partial z}{\partial t} \in C([0, \infty); L^2(\mathbb{R}_s^3 \times \mathbb{R}_t^2))$.

**Proof.** Item (i) of theorem 3.20 gives $\Psi \in C([0, \infty); H^1(\mathbb{R}_s^2 \times \mathbb{R}_t^2)) \cap C^1([0, \infty); X)$. An application of inequalities associated with (3.57) gives the continuity results. The $L^\infty$ bound on $z$ follows from estimating

$$\|z\|_{H^1(\mathbb{R}_s^3 \times \mathbb{R}_t^2)} \leq \|z\|_{L^2(\mathbb{R}_s^3 \times \mathbb{R}_t^2)} + C \left( \|\nabla_x z\|_{L^2(\mathbb{R}_s^3 \times \mathbb{R}_t^2)} + \|\nabla_s z\|_{L^2(\mathbb{R}_s^3 \times \mathbb{R}_t^2)} \right)$$

$$\leq \|\overline{\Psi}(\cdot, t)\|_{\mathcal{H}}^2 + C \sum_{j=1}^{\infty} \lambda_j \|\nabla \psi_j(\cdot, t)\|_2 \|\psi_j(\cdot, t)\|_2$$
3.9: Global Existence of the WP System

\[ \leq \|\Psi(\cdot, t)\|_{L^2}^2 + C \left( \sum_{j=1}^{\infty} \lambda_j \|\nabla \psi_j(\cdot, t)\|_2^2 \right)^{1/2} \left( \sum_{j=1}^{\infty} \lambda_j \|\psi_j(\cdot, t)\|_2^2 \right)^{1/2} \]

\[ \leq \|\Psi(\cdot, t)\|_{L^2}^2 + C(\|\Psi(\cdot, t)\|_{L^2}^2 + \|\Psi(\cdot, t)\|_{L^2}^2) \leq C \]

using the Cauchy–Schwarz and Hölder inequalities, as well as proposition 3.15 and lemma 3.17. □

The properties of the Wigner function can now be lifted from those of \( z \) using the fact that \( \rho_w \) and \( z \) are connected through the relationship \( \rho_w(x, k, t) = \mathcal{F}^{-1}\mathcal{T}^{-1}z(r, s, t) \). The \( \mathcal{T}^{-1} \) denotes the coordinate transformation \( (r, s) \rightarrow (x, \eta) \).

In terms of the \( \psi_j \), one has equation (3.13) which is repeated here for convenience:

\[ \rho_w(x, k, t) = \sum_{j=1}^{\infty} \lambda_j \int e^{2\pi ik \cdot \eta} \overline{\psi_j(x + \eta/2, t)} \psi_j(x - \eta/2, t) \, d\eta. \tag{3.58} \]

This relationship allows one to state the main existence and uniqueness theorem for the WP system.

**Theorem 3.25** If \( \rho_{w, l} \in L^2(\mathbb{R}_x^2 \times \mathbb{R}_x^3) \) is chosen to be a valid Wigner distribution then the WP system (3.1.a)-(3.1.e) has a unique global mild solution \( (\rho_w, n, V_{\text{eff}}) \) with the properties

(i) \( \rho_w \in C([0, \infty); L^2(\mathbb{R}_x^2 \times \mathbb{R}_x^3)) \)

(ii) \( \frac{\partial \rho_w}{\partial t} \in C([0, \infty); L^2(\mathbb{R}_x^2 \times \mathbb{R}_x^3)) \)

(iii) \( \Theta(V_{\text{eff}})\rho_w \in C([0, \infty); L^2(\mathbb{R}_x^2 \times \mathbb{R}_x^3)) \)

(iv) \( n \in L^\infty([0, \infty); L^r) \cap C([0, \infty); L^r) \) for \( 1 \leq r \leq 3 \)

(v) \( n \in C^1([0, \infty); L^1). \)

In addition, \( V_{\text{eff}} = V + \beta V_0 \) and \( V \) satisfies the properties of theorem 3.23.
Proof. These items depend on the isometry properties of the Fourier transform on the space $L^2$ and the fact that the Jacobian of the coordinate transformation $(r, s) \rightarrow (x, k)$ is one. For item (i), this implies that

$$
\|\rho_w(\cdot, \cdot, t) - \rho_w(\cdot, \cdot, s)\|_{L^2(R^3_x \times R^3_r)} = \|z(\cdot, \cdot, t) - z(\cdot, \cdot, s)\|_{L^2(R^3_x \times R^3_r)}
$$

and for item (ii)

$$
\|\partial_t \rho_w(\cdot, \cdot, t) - \partial_t \rho_w(\cdot, \cdot, s)\|_{L^2(R^3_x \times R^3_r)} = \|\partial_z(\cdot, \cdot, t) - \partial_z(\cdot, \cdot, s)\|_{L^2(R^3_x \times R^3_r)}.
$$

Proposition 3.24 completes the proof for these items.

For item (iii) the potential energy is referred to as $V_{\text{eff}}$ rather than just $V$ to emphasize the fact that this potential energy includes the Coulomb potential. As an auxiliary estimate,

$$
\|V_{\text{eff}}(\cdot, t)z(\cdot, \cdot, t)\|_{L^2(R^3_x \times R^3_r)}^2 = \int \int \left[ \sum_{j=1}^{\infty} \lambda_j \left( \frac{\beta}{4\pi |r|} + V(r, t) \right) \overline{\psi}_j(r, t) \psi_j(s, t) \right]^2 \, dr \, ds
$$

$$
= \int \sum_{j=1}^{\infty} \lambda_j \left( \frac{\beta}{4\pi |r|} + V(r, t) \right) \overline{\psi}_j(r, t) \left| \overline{\psi}_j(r, t) \right|^2 \, dr
$$

$$
\times \int \sum_{j=1}^{\infty} \lambda_j |\psi_j(s, t)|^2 \, ds
$$

$$
\leq \left( C\|\overline{\psi}(\cdot, t)\|_{L^2}^2 + \|V(\cdot, t)\|_{L^\infty}^2 \|\psi(\cdot, t)\|_{L^2}^2 \right) \|\overline{\psi}(\cdot, t)\|^2_{L^2}
$$

Under the Fourier transform one also has

$$
\|\Theta(V_{\text{eff}})\rho_w\|_{L^2(R^3_x \times R^3_r)} = \|[V_{\text{eff}}(\cdot, t) - V_{\text{eff}}(\cdot, t)]z(\cdot, \cdot, t)\|_{L^2(R^3_x \times R^3_r)}.
$$

These two estimates give item (iii). Items (iv), (v) and the comment on $V$ are direct restatements of theorems 3.20 and 3.23. □

One can use interpolation to find an $L^\infty$ bound for $\rho_w$ by noting that
The isometry properties of the Fourier transform on $L^2$ also imply that

$$
\| \rho_w(x,\cdot, t) \|_{L^2(R^3)} = \| \Phi \|_X \tag{3.60}
$$

from equation (3.57). This proves the following theorem:

**Theorem 3.26** If $\rho_{w,f} \in L^2(R^3 \times R^3)$ is chosen to be a valid Wigner distribution then the WP system (3.1.a)-(3.1.e) has the property

$$
\rho_w \in L^\infty([0,\infty); L^p(R^3 \times R^3)) \text{ for } 2 \leq p \leq \infty.
$$

**Proof.** Apply the Riesz–Thorin theorem to equations (3.59) and (3.60). □

The $k \cdot \nabla_x \rho_w$ term in the quantum Liouville equation, if treated by itself, gives rise to a Laplacian operator in $r$ and $s$. Therefore one requires a solution that is at least locally in $H^2$ to estimate this term. However, if the initial value $\Phi$ of the SP system is restricted to the space $Z \subset Y$, then $\rho_{w,f} \in H^2(R^3 \times R^3)$. Thus proposition 3.14 produces the following additional regularity property for the WP system:

**Proposition 3.27** If $\rho_w(x,k,t)$ is the unique mild solution of theorem 3.25 and one further specifies that $\rho_{w,f} \in H^2(R^3 \times R^3)$ then there exists constants $C_1, C_2$ that depend only upon $\rho_{w,f}$ such that

$$
\| k \cdot \nabla_x \rho_w \|_{L^2(R^3 \times R^3)} \leq C_1 e^{C_2 t}.
$$
Proof. From the isometry properties of the Fourier transform on the space $L^2$

$$
\|k \cdot \nabla_x \rho \|_{L^2(\mathbb{R}_x^2 \times \mathbb{R}_z)} = \|\Delta_r Z(\cdot, \cdot, t) - \Delta_z Z(\cdot, \cdot, t)\|_{L^2(\mathbb{R}_r^2 \times \mathbb{R}_z^2)}
$$

$$
\leq 2 \int \int \left| \sum_{j=1}^{\infty} \lambda_j \left( \Delta_r \overline{\psi_j(r)} \right) \psi_j(s) \right|^2 \, dr \, ds
$$

$$
\leq 2 \int \sum_{j=1}^{\infty} \lambda_j |\Delta_r \psi_j(r)|^2 \, dr \int \sum_{j=1}^{\infty} \lambda_j |\psi_j(s)|^2 \, ds
$$

$$
\leq \|\Psi(\cdot, t)\|_Z \|\overline{\Psi}(\cdot, t)\|_X.
$$

Proposition 3.14 shows that the $Z$ norm of $\Psi$ is exponentially bounded with constants $C_1$ and $C_2$ that depend solely on the initial wave function $\Phi$. □

The next chapter studies how the WP system evolves in time and determine in which situations the solution decays or approaches a steady state.
Chapter 4
Asymptotic Behaviour

4.1 An Auxiliary System

The success of the previous chapter can be attributed to the convention of treating the external Coulomb field as part of the unperturbed Coulomb Hamiltonian $H_c$. However, when dealing with the asymptotic behaviour of the Schrödinger operator, it is advantageous to utilize the well-known estimates of the free propagator $e^{-itH_0} = e^{-itA/2}$ [39, 56]. For this purpose, it is necessary to separate out the Coulomb field explicitly. To this end, an auxiliary sequence of functions $\Psi = \{\psi_j\} = \{\psi_j(x, t)\}$, $x \in \mathbb{R}^3$, $t \in [0, \infty)$ is defined which satisfies

$$i\partial_t \psi_j = -\frac{1}{2} \Delta \psi_j + V \psi_j + \beta V_\epsilon \psi_j, \quad \forall j \in \mathbb{N}, \quad V_\epsilon = \frac{1}{4\pi(|x| + \epsilon)} \quad (4.1)$$

with $\epsilon > 0$. One requires the $\epsilon$ to ensure that for any $\Gamma \in Y$ one has $V_\epsilon \Gamma \in Y$. In the limit as $\epsilon \to 0$, equation (4.1) reduces to the original equation given by (3.15). Furthermore, $V$ and $n$ are given by expression (3.16) which we repeat for convenience:

$$\Delta V = -\alpha n(x, t), \quad n(x, t) = \sum_{j=1}^{\infty} \lambda_j |\psi_j|^2. \quad (4.2)$$

The function $\Psi$ is also subjected to the initial condition

$$\Psi(0) = \Phi \in Z \quad (4.3)$$
4.1: An Auxiliary System

where $\Phi$ is independent of $\epsilon$.

There exists a unique solution to the system (4.1)–(4.3). The proof is analogous to the method used in chapter 3.

**Proposition 4.1** For every $\Phi \in Z$ there exists a unique strong solution $\Psi_\epsilon$ on $Y$ of the initial value problem (4.1)–(4.3), defined for all $t \in [0, \infty)$ such that

$$\Psi_\epsilon \in C([0, \infty); Y) \cap L^\infty_{loc}([0, \infty); Z), \quad \partial_t \Psi_\epsilon \in C([0, \infty); X) \cap L^\infty_{loc}([0, \infty); X),$$

$$\|\Psi(\cdot, t)\|_X = \|\Phi\|_X, \quad \|\Psi(\cdot, t)\|_Y \leq C.$$  

Moreover,

$$\|V(\cdot, t)\|_\infty \leq C, \quad \|\nabla V(\cdot, t)\|_2 \leq C, \quad \|\Delta V(\cdot, t)\|_2 \leq C, \quad \|\nabla V(\cdot, t)\|_\infty \leq C,$$

where the constant $C$ is independent of $\epsilon$ and depends only on $\Phi$.

**Proof.** Since $\Phi \in Z \subset Y$, theorem 3.13 ensures the existence of a unique mild $Y$-valued solution which can be viewed as a strong $X$-valued solution. This is a direct consequence of the fact that $J(\Psi_\epsilon) = V(\Psi_\epsilon)\Psi_\epsilon + \beta V_\epsilon \Psi_\epsilon$ is locally Lipschitz on $Y$. The statements $\Psi_\epsilon \in L^\infty_{loc}([0, \infty); Z)$ and $\partial_t \Psi_\epsilon \in L^\infty_{loc}([0, \infty); X)$ result from proposition 3.14. The statement $\|\Psi_\epsilon\|_X = \|\Phi\|_X$ follows from the conservation of probability of the system (4.1)–(4.3). In a similar fashion, the estimate $\|\Psi_\epsilon\|_Y \leq C$ is produced as in chapter 3, i.e. through the conservation of energy of (4.1)–(4.3) and lemma 3.17. These two bounds are then used to estimate the potential $V$ by using lemmata 3.8–3.11 of chapter 3. \(\square\)

Having exhibited the existence of a unique solution for the auxiliary system, the free propagator $e^{-itH_0}$ is considered in greater detail below. As an aid to the subsequent calculations, we turn to computing explicit formulas for $e^{-itH_0}$ which, for $t > 0$, are denoted by $G(t)$. This operator is responsible for propagating the
solution forward in time by an amount \( t \). Denoting the Fourier transform and its inverse by \( \mathcal{F} \) and \( \mathcal{F}^{-1} \) respectively, one obtains

\[
H_0 = \mathcal{F}^{-1} \frac{|\xi|^2}{2} \mathcal{F}, \quad f(H_0) = \mathcal{F}^{-1} f \left( \frac{|\xi|^2}{2} \right) \mathcal{F}
\]

where \( f \) is any bounded measurable function [56]. As a result, \( G(t) \) can be expressed as the Fourier multiplier

\[
G(t) = \mathcal{F}^{-1} \left( e^{-i\xi^2/2} \right) \mathcal{F}.
\]

### 4.2 Properties of the Free Propagator

The free Hamiltonian is a special case of the Coulomb Hamiltonian that was considered in chapter 3. Hence, the group of operators \( \{ e^{itH_0} \}_{t \in \mathbb{R}} \) can be characterized with the following lemma:

**Lemma 4.2** \(-iH_0\) is the infinitesimal generator of a \( C_0 \) group of unitary operators \( G(t) = e^{-itH_0} \) on the Hilbert space \( Y \). Furthermore, \( G(t) \) satisfies the relationships \( G^{-1}(t) = G(-t) \), \( ||G(t)|| = 1 \) and \( ||G(-t)|| = 1 \).

**Proof.** Corollary 3.6 with \( \beta = 0 \) proves that \(-iH_0\) is self-adjoint on \( Y \). The proof follows by applying Stone's theorem [54]. \( \square \)

The free Hamiltonian generates the semigroup \( G(t) \). Therefore, one can express the derivatives of \( G(t) \) in terms of \( H_0 \). To this end we present the corollary:

**Corollary 4.3** If \( H_0 \) is the Hamiltonian corresponding to the free propagator \( G(t) \) in lemma 4.2 then for all \( \Phi \in Y \)

\[
\frac{d}{dt} G(t)\Phi = -iG(t)H_0\Phi
\]
Proof. From lemma 4.2, $-iH_0$ and $iH_0$ generate the one dimensional semigroups $G(t)$ and $G(-t)$ on $Y$ respectively. Since $-iH_0$ is the infinitesimal generator of $G(t)$, the semigroup property yields for all $\Phi \in Y$

$$G(t) (-iH_0 \Phi) = G(t) \lim_{\delta \to 0^+} \frac{1}{\delta} (G(\delta) \Phi - \Phi)$$

$$= \lim_{\delta \to 0^+} \frac{1}{\delta} (G(t + \delta) - G(t)) \Phi$$

$$= \frac{d}{dt} G(t) \Phi$$

which is expression (4.5.a). Expressions (4.5.b)-(4.5.d) are exhibited in a similar fashion. □

Having defined the group of operators $G(t)$, the next step in determining the asymptotic behaviour of the solution requires an explicit representation for this group. These remarks follow those of Reed & Simon [56]. As in the previous chapters of the dissertation, integrations are typically taken over $\mathbb{R}^3$ so this information will usually be suppressed. Formally, one expects from equation (4.4)\(^1\)

$$G(t)\varphi = e^{-itH_0}\varphi$$

$$= [\mathcal{F}^{-1} \left( e^{-i|\xi|^2/2} \right)] \mathcal{F}\varphi$$

$$= [\mathcal{F}^{-1} \left( \mathcal{F}\mathcal{F}^{-1}e^{-i|\xi|^2/2} \right)] \mathcal{F}\varphi$$

$$= (2\pi)^{-3/2} \mathcal{F}^{-1} \mathcal{F} \left[ \left( \mathcal{F}^{-1} e^{-i|\xi|^2/2} \right) \ast \varphi \right]$$

$$= (2\pi)^{-3/2} \left[ \mathcal{F}^{-1} \left( e^{-i|\xi|^2/2} \right) \right] \ast \varphi.$$
4.2: Properties of the Free Propagator

However, what is meant by the inverse Fourier transform of \( e^{-it|\xi|^2/2} \) requires clarification since \( e^{-it|\xi|^2/2} \notin L^2 \) and \( \mathcal{F}^{-1}\left(e^{-it|\xi|^2/2}\right) \notin L^1 \). Let \( \lambda \in \mathbb{C} \) with \( \text{Re} \lambda > 0 \) so that \( e^{-\lambda|\xi|^2/2} \in L^2 \cap L^\infty \). With this restriction on \( \lambda \),

\[
\mathcal{F}^{-1}\left(e^{-\lambda|\xi|^2/2}\right) = \frac{1}{(2\pi)^{3/2}} \int e^{ix \cdot \xi} e^{-\lambda|\xi|^2/2} d\xi
\]

\[
= \frac{1}{(2\pi)^{3/2}} \int e^{-|\xi|^2/2\lambda} e^{-i|\xi|^2/2\lambda} d\xi
\]

\[
= \frac{1}{(\pi\lambda)^{3/2}} e^{-|\xi|^2/2\lambda} \int e^{-u^2} du
\]

\[
= \lambda^{-3/2} e^{-|\xi|^2/2\lambda}.
\]

The branch of the square root is chosen so that \( \text{Re} \left(\lambda^{1/2}\right) \) is positive for \( \text{Re} \lambda \) positive, (here the complex plane is being cut along the negative real half axis). Therefore,

\[
(e^{-\lambda H_0}\varphi)(x) = (2\pi\lambda)^{-3/2} e^{-|x|^2/2\lambda} \ast \varphi
\]

\[
= \frac{1}{(2\pi\lambda)^{3/2}} \int e^{-|x-y|^2/2\lambda} \varphi(y) dy.
\]

Suppose \( \varphi \in L^1 \cap L^2 \) so that, in the sense of \( L^2 \), one has

\[
\lim_{\epsilon \downarrow 0} \left\| e^{-i(t-\epsilon)H_0} \varphi - e^{-itH_0} \varphi \right\|_2 = 0.
\]

Therefore, there exists a subsequence that converges pointwise a.e. [58]. Hence, for \( \lambda = \epsilon + it \) with \( t \in \mathbb{R} \) and \( \epsilon > 0 \in \mathbb{R} \),

\[
(e^{-itH_0}\varphi)(x) = \lim_{\epsilon \downarrow 0} (e^{-i(t-\epsilon)H_0}\varphi)(x)
\]

\[
= \lim_{\epsilon \downarrow 0} \frac{1}{(2\pi i(t-\epsilon))^{3/2}} \int e^{-|x-y|^2/2i(t-\epsilon)} \varphi(y) dy
\]

as in figure 4.1. This furnishes a representation of the free propagator as

\[
(G(t)\varphi)(x) = (e^{-itH_0}\varphi)(x)
\]

\[
= \frac{1}{(2\pi it)^{3/2}} \int e^{i|y|^2/2t} \varphi(y) dy
\]

(4.6)
by the dominated convergence theorem. For a general \( \varphi \in L^2 \), \( G(t)\varphi \) is interpreted as the limit in \( L^2 \) as \( R \to \infty \) of the integral restricted to \( |y| \leq R \). That is\(^2\)

\[
(G(t)\varphi)(x) = \lim_{R \to \infty} \frac{1}{(2\pi it)^{3/2}} \int_{|y| \leq R} e^{i|x-y|^2/2t}\varphi(y) \, dy.
\]

The form of the propagator (4.6) allows the extraction the time dependence of the various norms. The first of these results follows:

**Lemma 4.4** If \( 2 \leq q \leq \infty \) then for any \( t \neq 0 \), \( G(t) \) as defined in lemma 4.2, is a bounded operator from \( L^p \) to \( L^q \) where \( p^{-1} + q^{-1} = 1 \). Furthermore, one has the estimate

\[
\|G(t)\varphi\|_q \leq (2\pi |t|)^{3/2} \|\varphi\|_p
\]

for all \( \varphi \in L^p \).

**Proof.** The unitarity of \( G(t) \) on \( L^2 \) implies \( \|G(t)\varphi\|_2 = \|\varphi\|_2 \). From the representation of equation (4.6) it follows that \( G(t) \) is bounded from \( L^1 \) to \( L^\infty \) with

\(^2\) l.i.m. is an abbreviation for limes in medio, i.e. limit in the mean.
norm bounded by \((2\pi|t|)^{-3/2}\). By the Riesz–Thorin interpolation theorem, \(G(t)\) is bounded from \(L^p\) to \(L^q\) with norm bounded by \((2\pi|t|)^{3/q-3/2}\). \(\square\)

4.3 Time Evolution of Operators

If \(\mathcal{A}\) is some quantum mechanical operator at time zero, then the time evolution of this operator is defined by forming the product [25]

\[ \mathcal{A}(t) := G(-t)\mathcal{A}G(t). \tag{4.7} \]

Expression (4.7) can be justified, at least formally, by finding the time dependence of the expectation value of \(\mathcal{A}\). Explicitly,

\[ \langle \mathcal{A} \rangle_t = \langle \psi(t), \mathcal{A}\psi(t) \rangle = \langle G(t)\psi(0), \mathcal{A}G(t)\psi(0) \rangle \\
= \langle \psi(0), G^*(t)\mathcal{A}G(t)\psi(0) \rangle \\
= \langle \psi(0), G(-t)\mathcal{A}G(t)\psi(0) \rangle. \]

Using equations (4.5.a)-(4.5.d) produces

\[ \frac{d}{dt}\mathcal{A}(t) = \frac{d}{dt}[G(-t)\mathcal{A}G(t)] \\
= i\mathcal{H}_0G(-t)\mathcal{A}G(t) - G(-t)\mathcal{A}i\mathcal{H}_0G(t) \\
= i\mathcal{H}_0\mathcal{A}(t) - i\mathcal{A}(t)\mathcal{H}_0 \\
= i[H_0, \mathcal{A}(t)] \tag{4.8} \]

which is Heisenberg’s equation that describes the time evolution of the operator \(\mathcal{A}(t)\) when \(\mathcal{A}\) has no explicit time dependence.

Let \(x_m(t)\) denote the time evolved version of the position operator \(x_m\) where \(m = 1, 2, 3\). This can be expressed as

\[ x_m(t) = G(-t)x_mG(t); \quad m = 1, 2, 3 \tag{4.9} \]
where \( x_m \) is the position operator for the \( m \)th coordinate at time zero. By \( x(t) \) we mean the time dependent vector \( (x_1(t), x_2(t), x_3(t)) \) whereas \( x \) denotes the time independent vector \( (x_1, x_2, x_3) \). As well, we will use the multi-index notation found in appendix A: \( \alpha = (\alpha_1, \alpha_2, \alpha_3) \in (\mathbb{N} \cup \{0\})^3 \) and \( D^\alpha = \partial_1^{\alpha_1}\partial_2^{\alpha_2}\partial_3^{\alpha_3} \), where \( \partial_m = \partial/\partial x_m \) (\( m = 1, 2, 3 \)). The following lemma gives a representation of \( x(t) \).

**Lemma 4.5** Let \( G(t), G(-t) \) be the unitary groups generated by the free Schrödinger equation

\[
\frac{i\partial \psi}{\partial t} = -\frac{1}{2}\Delta \psi.
\]

If \( \varphi \in H^1 \) is such that \( x\varphi \in (L^2)^3 \) then, for all \( t \in \mathbb{R} \), \( \varphi \) satisfies the following equation in \( (L^2)^3 \)

\[
x(t)\varphi = G(-t)xG(t)\varphi = (x - it\nabla)\varphi = e^{-it|x|^2/2t}(-it)\nabla \left(e^{it|x|^2/2t}\right)\varphi.
\]

In particular, \( x(t)\varphi \) remains in \( (L^2)^3 \) for all \( t \).

**Proof.** A formal proof that does not consider any domains is presented. In the scaled coordinates, \( H_0 = p^2/2 \) where the momentum operator \( p = -i\nabla_x \). In addition, the fundamental commutator \( [p, x] = -i \). However, \( p \) commutes with any function of \( p \), \( [p^2, p] = 0 \) and the only nontrivial calculation is \( [p^2, x] = p[p, x] + [p, x]p = -2ip \).

Applying Heisenberg's equation (4.8) yields

\[
\frac{d}{dt} p(t) = i[H_0, p(t)] = i[p^2, p]/2 = 0
\]

while

\[
\frac{d}{dt} x(t) = i[H_0, x(t)] = i[p^2, x]/2 = p.
\]

Therefore, \( p(t) = -i\nabla_x \) and \( x(t) = x - it\nabla_x \). The last equality in the lemma results by simply differentiating and using the fact that \( \partial_m(|x|^2) = 2x_m \). \( \square \)

Lemma 4.5 shows that the position and momentum operators recover the classical equations of motion for a particle without any external forces acting on it.
4.4 An Approximate Conservation Law

In this section an approximate conservation law is developed which is related to an approximate invariance of the system (4.1)-(4.3). Ginibre and Velo [27] state that this invariance is the nonrelativistic analogue of conformal invariance. The term pseudoconformal conservation law is used in [27] to describe this approximate conservation law.

4.4.1 Preliminary Lemmata

For the results that follow, a restriction on the admissible initial values of the $X$-valued solution to the SP system is required. A possible restriction is indicated by lemma 4.5. Define the Hilbert space [36] as

\[ X := \left\{ f \in H^1(\mathbb{R}^3) : \| f \|_X^2 = \sum_{|\alpha| \leq 1} \left( \| D^\alpha f \|_2^2 + \| x_\alpha f \|_2^2 \right) < \infty \right\}. \]

The lemma and corollary that follow give estimates on the $L^p$ norms of functions that lie in $X$.

**Lemma 4.6** If $f \in X$ and $G(-t)$ is the unitary operator given in lemma 4.4 then $f \in L^p$ for $2 \leq p < 6$ and

\[ \| f \|_p \leq C_p \| G(-t)f \|_2^2 \| xG(-t)f \|_2^{1-a}, \quad t > 0, \]

where $1 - a = 3(1/2 - 1/p)$.

**Proof.** The proof is similar to that given in Ginibre and Velo [27]. An alternative proof can be found in [37]. Lemma 4.4 implies that for $p \geq 2$,

\[ \| f \|_p = \| G(t)G(-t)f \|_p \leq C_p t^{a-1} \| G(-t)f \|_p^2. \quad (4.10) \]
4.4: An Approximate Conservation Law

The subtlety of the proof lies in finding a sharp estimate for the $\|G(-t)f\|_{p/(p-1)}$ term. From Hölder's inequality, for any $\epsilon > 0$ and $p < 6$,

$$\|G(-t)f\|_{\frac{p}{p-1}} \leq \left\| (x^2 + \epsilon^2)^{1/2} G(-t)f \right\|_2 \left\| (x^2 + \epsilon^2)^{-1/2} \right\|_1$$

(4.11)

since, by the definition of $\alpha$, $1 - \frac{1}{p} = \frac{1}{2} + \frac{(1 - \alpha)}{3}$. To ensure that the right hand side of this inequality remains bounded one has to make the restriction $p < 6$. This will be made clear in a moment. Provided the restriction on $p$ is enforced, each term of (4.11) is subsequently estimated:

$$\left\| (x^2 + \epsilon^2)^{1/2} G(-t)f \right\|_2 = \left\| (x^2 + \epsilon^2)|G(-t)f|^2 \right\|_1^{1/2}$$

$$\leq \left( \|xG(-t)f\|_2^2 + \epsilon^2 \|G(-t)f\|_2^2 \right)^{1/2}$$

(4.12)

through the use of the Minkowski and Hölder inequalities and

$$\left\| (x^2 + \epsilon^2)^{-1/2} \right\|_{\frac{3}{1-\alpha}} = \left[ \int (x^2 + \epsilon^2)^{-3/(2-2\alpha)} dx \right]^{(1-\alpha)/3}$$

$$= \left[ \int (y^2 + \epsilon^2)^{-3/(2-2\alpha)} \epsilon^2 dy \right]^{(1-\alpha)/3}$$

$$= \epsilon^{-\alpha} \left\| (x^2 + 1)^{-1/2} \right\|_{\frac{3}{1-\alpha}}$$

(4.13)

through a change of variable. Combining relations (4.11), (4.12) and (4.13) gives

$$\|G(-t)f\|_{\frac{p}{p-1}} \leq \left( \|xG(-t)f\|_2^2 + \epsilon^2 \|G(-t)f\|_2^2 \right)^{1/2} \epsilon^{-\alpha} \left\| (x^2 + 1)^{-1/2} \right\|_{\frac{3}{1-\alpha}}.$$  

(4.14)

The upper limit on $p$ follows by considering $\left\| (x^2 + 1)^{-1/2} \right\|_r^r$ for some $r \geq 1$. Integrating explicitly$^3$ yields

$$\left\| (x^2 + 1)^{-1/2} \right\|_r^r = 4\pi \int_0^\infty \frac{x^2 dx}{(x^2 + 1)^{r/2}} = 2\pi \frac{\Gamma(3/2)\Gamma((r - 3)/2)}{\Gamma(r/2)} < \infty$$

$^3$ This expression is a special case of formula 8.384.1 of [31]. $\Gamma(x)$ in this expression is the gamma function.
provided \( r > 3 \). The condition \( r = 3/(1 - a) > 3 \) translates into \( p < 6 \) and justifies the interval \( 2 \leq p < 6 \). Specifying \( \epsilon = \|xG(-t)f\|_2/\|G(-t)f\|_2 \) reduces expression (4.14) to

\[
\|G(-t)f\|_p \leq \sqrt{2} \|xG(-t)f\|_2^{1-a}\|G(-t)f\|_2^a \left( x^2 + 1 \right)^{-1/2} \|1\|_{p/2-1}.
\]  

(4.15)

Applying the estimate (4.15) to (4.10) completes the result. □

A corollary to lemma 4.6 follows immediately.

**Corollary 4.7** If \( f \) satisfies the conditions of lemma 4.6 then

\[
\|f\|_p \leq C_p \|f\|_2^{\frac{p}{2}} \|(x + it\nabla)f\|_2^{1-a} t^{a-1}.
\]

*Proof.* Applying the case \( q = p = 2 \) of lemma 4.4 gives \( \|G(-t)f\|_2 = \|f\|_2 \). Replacing \( t \) with \(-t\) in the representation of lemma 4.5 and again using lemma 4.4 implies

\[
\|G(t)xG(-t)f\|_2 = \|(x + it\nabla)f\|_2 = \|xG(-t)f\|_2.
\]

The result follows from lemma 4.6. □

The space \( \mathcal{X} \) defines the direct sum Hilbert space

\[
\Xi := \left\{ \Gamma = \{\gamma_j\}_{j \in \mathbb{N}} : \gamma_j \in \mathcal{X}(\mathbb{R}^3) \forall j, \|\Gamma\|_\mathcal{X}^2 = \sum \lambda_j \|\gamma_j\|_\mathcal{X}^2 < \infty \right\}.
\]

The space \( \Xi \) is naturally associated with the three conservation laws (probability, energy and pseudoconformal) since it is the largest space where all three conservation laws make sense. It is necessary to ensure that solutions which are restricted to this space do not leave it at some later time. This fact is established by the following lemma.

---

4 If \( \|G(-t)f\|_2 = \|f\|_2 = 0 \) then \( f = 0 \) a.e. which would satisfy the lemma vacuously.
Figure 4.2: Behaviour of an explicit \( \{ \theta_n(x) \} \) sequence.

The sequence \( \{ \theta_n(x) \} \) defines a set of functions whose derivatives of up to second order are continuous. Also, in the limit as \( n \to \infty \), the \( \theta_n(x) \) converge to the characteristic function on \( \mathbb{R}^3 \). The nature of the construction ensures \( \| x^n \nabla \theta_n \|_\infty \leq \| \nabla \theta_1 \|_\infty \) for all \( n \).

**Lemma 4.8** If \( \Phi \in \Xi \subseteq Y \) and \( \Psi \) is the unique global strong \( X \)-valued solution of proposition 4.1 then \( \forall t \geq 0, \Psi(t) \in \Xi \) and for \( m = 1, 2, 3 \)

\[
\| x_m \Psi(t) \|_X \leq \| x_m \Phi \|_X + Ct
\]

where \( C \) depends on \( \| \Phi \|_\Xi \).

**Proof.** Consider a set of functions \( \{ \theta_n(x) \}_{n \in \mathbb{N}} \) generated by the following procedure. Take a real valued, time independent function \( \theta_1(x) \in C^2(\mathbb{R}^3) \) such that \( 0 \leq \theta_1 \leq 1, \theta_1(x) = 1 \) if \( |x| \leq 1/2 \) and \( \theta_1(x) = 0 \) if \( |x| \geq 1 \). For \( n \geq 1 \) define \( \theta_n(x) := \theta_1(x/n) \).

An explicit example of such a sequence of functions is detailed in figure 4.2. Because the support of \( \theta_n(x) = \{ x : |x| \leq n \} \), for any \( f \in L^2 \) and finite \( n, \| x_m \theta_n f \|_2 \leq n \| f \|_2 \).

The crucial property is the uniform boundedness of the gradient, i.e. for any \( n \in \mathbb{N} \)

\[
\| x_m \nabla \theta_n \|_\infty = \left\| \frac{x_m}{n} \nabla \theta_1 \right\|_\infty \leq \| \nabla \theta_1 \|_\infty.
\]
Take $\psi_j \in \mathcal{X}$ so that equation (4.1) with $\psi_j = \psi_{\epsilon j}$ can be written as

$$i \partial_t (x_m \theta_n \psi_j) = -\frac{1}{2} x_m \theta_n \Delta \psi_j + (V + \beta V_\epsilon) x_m \theta_n \psi_j.$$  \hspace{1cm} (4.17)

Multiplication by $x_m \theta_n \psi_j$ and rearranging terms gives

$$i \partial_t (x_m \theta_n \psi_j) x_m \theta_n \psi_j = \frac{1}{2} \Delta (x_m \theta_n \psi_j) x_m \theta_n \psi_j + (V + \beta V_\epsilon) x_m^2 \theta_n^2 |\psi_j|^2$$

$$+ \frac{1}{2} x_m \theta_n \psi_j [\Delta (x_m \theta_n \psi_j) - x_m \theta_n \Delta \psi_j].$$  \hspace{1cm} (4.18)

Taking the imaginary part of the relation (4.18) and using the fact that for any complex number $z$, $\text{Im}(iz) = \text{Re} z$, produces

$$2 \text{Re} \left[ \partial_t (x_m \theta_n \psi_j) x_m \theta_n \psi_j \right] = -\text{Im} \left[ \Delta (x_m \theta_n \psi_j) x_m \theta_n \psi_j \right]$$

$$+ \text{Im} \left\{ x_m \theta_n \psi_j [\Delta (x_m \theta_n \psi_j) - x_m \theta_n \Delta \psi_j] \right\}$$

$$= -\text{Im} \left[ \Delta (x_m \theta_n \psi_j) x_m \theta_n \psi_j \right]$$

$$+ 2 \text{Im} \left[ x_m \theta_n \psi_j (x_m \nabla \theta_n \cdot \nabla \psi_j + \theta_n \partial_m \psi_j) \right].$$

These steps proceeded by consistently removing any real valued terms in the argument of the operation that takes the imaginary part. Integrating over $\mathbb{R}^3$ and invoking Gauss' theorem furnishes the estimate

$$\frac{d}{dt} \left( \|x_m \theta_n \psi_j\|_2^2 \right) = 2 \text{Im} \int x_m \theta_n \psi_j (x_m \nabla \theta_n \cdot \nabla \psi_j + \theta_n \partial_m \psi_j) \, dx$$

$$\leq C \left\| x_m \theta_n \psi_j (x_m \nabla \theta_n \cdot \nabla \psi_j + \theta_n \partial_m \psi_j) \right\|_1$$

$$\leq C \|x_m \theta_n \psi_j\|_2 (\|x_m \nabla \theta_n\|_\infty \|\nabla \psi_j\|_2 + \|\theta_n\|_\infty \|\partial_m \psi_j\|_2)$$

$$\leq C \|x_m \theta_n \psi_j\|_2 \|\nabla \psi_j\|_2.$$ \hspace{1cm} (4.19)

Property (4.16) and both the Hölder and Minkowski inequalities have been utilized. Let $f_n(t) = \|x_m \theta_n \psi_j\|_2 \geq 0$ so that (4.19) implies

$$f_n \frac{d}{dt} f_n \leq C \|\nabla \psi_j\|_2 f_n.$$
and therefore
\[ f_n(t) \leq f_n(0) + C \int_0^t \| \nabla \psi_j(s) \|_2 \, ds. \]

Sending \( n \to \infty \), the monotone convergence theorem and lemma 3.17 give
\[
\| x_m \psi_j(t) \|_2 \leq \| x_m \varphi_j \|_2 + C \int_0^t \| \nabla \psi_j(s) \|_2 \, ds
\leq \| x_m \varphi_j \|_2 + C t.
\]

Squaring both sides, summing over the \( \lambda_j \) and then applying the Cauchy–Schwarz inequality yields
\[
\| x_m \Psi_\varepsilon(t) \|_X^2 = \sum_{j=1}^\infty \lambda_j \| x_m \psi_j(t) \|_2^2
\leq \sum_{j=1}^\infty \lambda_j \left( \| x_m \varphi_j \|_2^2 + 2 C t \| x_m \varphi_j \|_2 + C^2 t^2 \right)
\leq \| x_m \Phi \|_X^2 + 2 C t \left( \sum_{j=1}^\infty \lambda_j \right)^{1/2} \left( \sum_{j=1}^\infty \lambda_j \| x_m \varphi_j \|_2^2 \right)^{1/2} + C^2 t^2
\leq (\| x_m \Phi \|_X + C t)^2. \quad \Box \tag{4.20}
\]

A version of the pseudoconformal conservation law valid for any \( \varepsilon > 0 \) can now be proved by using this lemma.

**Proposition 4.9** If \( \Phi \in \Xi \) and \( \Psi_\varepsilon \) is the unique strong \( X \)-valued solution of proposition 4.1 on the interval \([0,T), (\Psi_\varepsilon \in C([0,T); X) \cap C^1([0,T); X) \) with \( T > 0 \) then \( xG(-t)\Psi_\varepsilon(t) \in X^3 \) and for all \( t_0, t_1 \in [0,T), \)
\[
\left\{ \| xG(-t)\Psi_\varepsilon(t) \|_X^2 + 2 t^2 E_{a,\beta}(t) \right\} \bigg|_{t_0}^{t_1} = \int_{t_0}^{t_1} 2 t \left[ E_{a,\beta}(s) + \epsilon \beta \int \frac{n_\varepsilon(x,s)}{|x| + \epsilon} \, dx \right] \, ds. \tag{4.21}
\]

\( E_{a,\beta}(t) \) is the energy of the system and is given by
\[
E_{a,\beta}(t) = \frac{1}{2} \int V(\Psi_\varepsilon)n_\varepsilon \, dx + \beta \int V_\varepsilon n_\varepsilon \, dx.
\]
4.4: An Approximate Conservation Law

Proof. The proof follows that of reference [18] and by analogy one lets

\[ J = V(\Psi) + \beta V_c. \]

For simplicity in this proof we will take, \( n = n_c, \ \Psi = \psi_c \) and correspondingly \( \psi_j = \psi_{j,c} \). Since \((|x| + e)^{-1}\) has replaced \(|x|^{-1}\), the expression \( J\psi \in Y \). One proceeds as in reference [18] by computing

\[
\frac{\partial}{\partial t} \left( xG(-t)\psi_j(t) \right) = xG(-t)\partial_t \psi_j + x \frac{d}{dt} G(-t)\psi_j(t)
\]

\[
= xG(-t)\partial_t \psi_j + x \frac{d}{dt} G H_0 \psi_j(t)
\]

\[
= -i xG(-t) (i\partial_t - H_0) \psi_j(t)
\]

\[
= -i xG(-t) J\psi_j(t)
\]

\[
= -i G(-t) \left( x + it\nabla \right) J\psi_j(t), \tag{4.22}
\]

using in sequence, equation (4.5.c) of corollary 4.2, the original equation (4.1) and corollary 4.3. The conservation law comes about by considering the inner product of expression (4.22) with \( xG(\tau)\psi_j(t) \). Therefore we first need to verify that under the assumptions of the proposition, both \( xG(-t)\psi_j(t) \) and expression (4.22) remain in \( (L^2)^3 \). Since \( \Phi \in \Xi, \) lemma 4.8 gives \( \Psi(x,t) \in \Xi \). The definition of \( \Xi \) implies that \( |x|\Psi(x,t) \in X \). From proposition 4.1, \( ||V(\Psi(-, t))||_\infty < \infty \) and hence \( |x|J\psi_j \in L^2 \).

The application of lemma 4.5 shows that \( xG(-t)\psi_j \in (L^2)^3 \) and \( xG(-t)J\psi_j \in (L^2)^3 \). Therefore, equation (4.22) can be used to construct the inner product

\[
\frac{1}{2} \frac{d}{dt} \left( \|xG(-t)\psi_j(t)\|^2 \right) = \text{Re} \left( xG(-t)\psi_j(t), \frac{\partial}{\partial t} \left( xG(-t)\psi_j(t) \right) \right)
\]

\[
= \text{Re} \left( G(-t) \left( x + it\nabla \right) \psi_j(t), -i G(-t) \left( x + it\nabla \right) J\psi_j(t) \right)
\]

\[
= \text{Im} \left( \left( x + it\nabla \right) \psi_j(t), \left( x + it\nabla \right) J\psi_j(t) \right)
\]

\[
= \text{Im} \left( x\psi_j(t), xJ\psi_j(t) \right) + t^2 \text{Im} \left( i\nabla \psi_j(t), i\nabla (J\psi_j(t)) \right)
\]

\[
+ t \text{Im} \left[ (x\psi_j(t), i\nabla (J\psi_j(t))) + (i\nabla \psi_j(t), xJ\psi_j(t)) \right]
\]
4.4: An Approximate Conservation Law

\[ = \text{Im} \langle x\psi_j(t), xJ\psi_j(t) \rangle + t^2 \text{Im} \langle \nabla\psi_j(t), \nabla(J\psi_j(t)) \rangle \\
+ t \text{Re} \left[ (x\psi_j(t), \nabla(J\psi_j(t))) - \langle \nabla\psi_j(t), xJ\psi_j(t) \rangle \right] \\
= a_j + b_j t + c_j t^2, \quad (4.23) \]

where

\[ a_j = \text{Im} \langle x\psi_j(t), xJ\psi_j(t) \rangle, \]
\[ b_j = \text{Re} \left[ (x\psi_j(t), \nabla(J\psi_j(t))) - \langle \nabla\psi_j(t), xJ\psi_j(t) \rangle \right], \]
\[ c_j = \text{Im} \langle \nabla\psi_j(t), \nabla(J\psi_j(t)) \rangle. \]

The above steps rely on the various properties of the inner product, the fact that \( G(-t) \) is unitary on \( L^2 \) and the expression \( \text{Re}(iz) = -\text{Im} \, z \) which is valid for any complex number \( z \).

Simplifying the coefficients of the quadratic polynomial (4.23) on an individual basis, they are considered in order of complexity. Since

\[ \langle x\psi_j, xJ\psi_j \rangle = \int x^2 J |\psi_j|^2 \, dx \]

is real valued, \( a_j = 0 \). For \( c_j \) one integrates by parts twice and uses equation (4.1) to find

\[ \text{Im} \langle \nabla\psi_j, \nabla(J\psi_j) \rangle = -\text{Im} \langle \Delta \psi_j, J\psi_j \rangle \\
= \text{Im} \langle J\psi_j, \Delta \psi_j \rangle \\
= 2 \text{Im} \langle J\psi_j, J\psi_j - i\partial_t \psi_j \rangle \\
= -2 \text{Re} \langle J\psi_j, \partial_t \psi_j \rangle \\
= -\langle J\psi_j, \partial_t \psi_j \rangle - \overline{\langle J\psi_j, \partial_t \psi_j \rangle} \\
= -\left\langle J, \left( \overline{\psi_j} \partial_t \psi_j + \partial_t \overline{\psi_j} \psi_j \right) \right\rangle \\
= -\left\langle J, \frac{\partial}{\partial t} |\psi_j|^2 \right\rangle. \quad (4.24) \]
A further simplification is possible by utilizing equation (3.45) which is restated here for convenience
\[
\int V \partial_t n \, dx = \frac{1}{2} \int \partial_t (V n) \, dx. \quad (4.25)
\]
Computing the weighted sum by using equation (4.25) and recalling \( n = \sum \lambda_j |\psi_j|^2 \) yields
\[
\sum_{j=1}^{\infty} \lambda_j c_j = - \sum_{j=1}^{\infty} \lambda_j \left\langle J, \frac{\partial}{\partial t} \left(|\psi_j|^2\right) \right\rangle
= - \sum_{j=1}^{\infty} \lambda_j \int V \frac{\partial}{\partial t} \left(|\psi_j|^2\right) \, dx - \beta \sum_{j=1}^{\infty} \lambda_j \int V_c \frac{\partial}{\partial t} \left(|\psi_j|^2\right) \, dx
= - \int V \partial_t n \, dx - \beta \int V_c \partial_t n \, dx
= - \frac{d}{dt} \left[ \frac{1}{2} \int V n \, dx + \beta \int V_c n \, dx \right]
= - \frac{d}{dt} E_{a,b}(t). \quad (4.26)
\]
The time independence of \( V_c \) allows the time derivative to be pulled out of the second term. This leaves only the \( b_j \) to evaluate. Integrating by parts once again and using the fact that \( \nabla \cdot x = 3 \) in \( \mathbb{R}^3 \) gives
\[
b_j = \text{Re} \left\langle x \psi_j, \nabla (J \psi_j) \right\rangle - \text{Re} \left\langle \nabla \psi_j, x J \psi_j \right\rangle
= \text{Re} \left\langle x \psi_j, \psi_j \nabla J + J \nabla \psi_j \right\rangle + \text{Re} \left\langle \psi_j, (\nabla \cdot x) J \psi_j + (x \cdot \nabla J) \psi_j + (x \cdot \nabla \psi_j) J \right\rangle
= 3 \text{Re} \left\langle J, |\psi_j|^2 \right\rangle + 2 \text{Re} \left\langle \psi_j, (x \cdot \nabla J) \psi_j \right\rangle + 2 \text{Re} \left\langle \psi_j, (x \cdot \nabla J) \psi_j \right\rangle
= 3 \left\langle J, |\psi_j|^2 \right\rangle + \left\langle \psi_j, (x \cdot \nabla J) \psi_j \right\rangle + \left\langle (x \cdot \nabla J) \psi_j, \psi_j \right\rangle
+ \left\langle \psi_j, (x \cdot \nabla \psi_j) J \right\rangle + \left\langle ((x \cdot \nabla \psi_j) J, \psi_j \right\rangle. \quad (4.27)
\]
A closer look at the second term in the right hand side of relation (4.27) reveals
\[
\left\langle \psi_j, (x \cdot \nabla J) \psi_j \right\rangle = \left\langle x J \psi_j, \nabla \psi_j \right\rangle
= - \left\langle (\nabla \cdot x) J \psi_j, \psi_j \right\rangle - \left\langle (x \cdot \nabla J) \psi_j, \psi_j \right\rangle - \left\langle (x \cdot \nabla \psi_j) J, \psi_j \right\rangle
= -3 \left\langle J \psi_j, \psi_j \right\rangle - \left\langle (x \cdot \nabla J) \psi_j, \psi_j \right\rangle - \left\langle (x \cdot \nabla \psi_j) J, \psi_j \right\rangle. \quad (4.28)
\]
4.4: An Approximate Conservation Law

Therefore equation (4.27) reduces to the expression

\[ b_j = \langle \psi_j, (x \cdot \nabla J)\psi_j \rangle = \langle \psi_j, (x \cdot \nabla V)\psi_j \rangle + \langle \psi_j, (x \cdot \nabla V_e)\psi_j \rangle. \] (4.29)

where the definition of \( J \) allows the \( J \) to be broken into into two separate pieces. Using relation (3.19) for the self-consistent potential produces

\[ \langle \psi_j, (x \cdot \nabla V)\psi_j \rangle = \int (x \cdot \nabla V) |\psi_j|^2 \, dx \]

\[ = \int_{\mathbb{R}^2} x \cdot \left( \frac{1}{4\pi} \int_{\mathbb{R}^2} \frac{(x-y)}{|x-y|^3} \Delta V(y) \, dy \right) |\psi_j|^2 \, dx. \]

Summing over the \( \lambda_j \) and using equation (4.2) yields

\[-\alpha \sum_{j=1}^{\infty} \lambda_j \langle \psi_j, (x \cdot \nabla V)\psi_j \rangle = \frac{1}{4\pi} \int_{\mathbb{R}^2} \int_{\mathbb{R}^2} (x-y+y) \cdot \frac{(x-y)}{|x-y|^3} \Delta V(y) \Delta V(x) \, dy \, dx \]

\[ = \int_{\mathbb{R}^2} \left( \frac{1}{4\pi} \int_{\mathbb{R}^2} \frac{\Delta V(y)}{|x-y|^3} \, dy \right) \Delta V(x) \, dx \]

\[ + \frac{1}{4\pi} \int_{\mathbb{R}^2} \int_{\mathbb{R}^2} y \cdot \frac{(x-y)}{|x-y|^3} \Delta V(y) \Delta V(x) \, dy \, dx \]

\[ = -\int V \Delta V \, dx + \alpha \sum_{j=1}^{\infty} \lambda_j \langle \psi_j, (x \cdot \nabla V)\psi_j \rangle. \]

The last step takes advantage of the antisymmetry of \( x - y \) under the exchange of \( x \) and \( y \). Solving for the left hand side shows

\[ \sum_{j=1}^{\infty} \lambda_j \langle \psi_j, (x \cdot \nabla V)\psi_j \rangle = \frac{1}{2\alpha} \int V \Delta V \, dx = -\frac{1}{2} \int Vn \, dx. \] (4.30)

The second term of relation (4.29) stems from the external potential. It can be handled directly as

\[ \langle \psi_j, (x \cdot \nabla V_e)\psi_j \rangle = \beta \int \left[ x \cdot \nabla \left( \frac{1}{|x|+\epsilon} \right) \right] |\psi_j|^2 \, dx \]

\[ = -\beta \int \left[ x \cdot \frac{|x|}{(|x|+\epsilon)^2} \right] |\psi_j|^2 \, dx \]

\[ = -\beta \int \frac{|x||\psi_j|^2}{(|x|+\epsilon)^2} \, dx. \] (4.31)
Summing equation (4.29) over the $\lambda_j$ and utilizing equations (4.30) and (4.31) yields
\[
\sum_{j=1}^{\infty} \lambda_j b_j = -\frac{1}{2} \int Vn \, dx - \beta \int \frac{|x|^n}{(|x|+\epsilon)^2} \, dx
\]
\[
= -\frac{1}{2} \int Vn \, dx - \beta \int V_n n \, dx + \epsilon \beta \int \frac{n}{(|x|+\epsilon)^2} \, dx
\]
\[
= -E_{\alpha,\beta}^\epsilon + \epsilon \beta \int \frac{n}{(|x|+\epsilon)^2} \, dx. \quad (4.32)
\]
Equations (4.23), (4.26) and (4.32) now combine to determine that for all $\epsilon > 0$,
\[
\frac{1}{2} \frac{d}{dt} \left( \|xG(-t)\Psi\|^2_X \right) = \frac{1}{2} \frac{d}{dt} \left( \sum_{j=1}^{\infty} \lambda_j \|xG(-t)\psi_j\|^2_X \right)
\]
\[
= \sum_{j=1}^{\infty} \lambda_j \left( a_j + b_j t + c_j t^2 \right)
\]
\[
= \left( -t^2 \frac{d}{dt} - t \right) E_{\alpha,\beta}^\epsilon(t) + \epsilon \beta t \int \frac{n(t)}{|x|+\epsilon} \, dx. \quad (4.33)
\]
The differential operator on the right hand side of this formula can be expressed as
\[
-t^2 \frac{d}{dt} E_{\alpha,\beta}^\epsilon(t) - t E_{\alpha,\beta}^\epsilon(t) = \frac{d}{dt} \left( -t^2 E_{\alpha,\beta}^\epsilon(t) \right) + t E_{\alpha,\beta}^\epsilon(t).
\]
Therefore, by integrating relationship (4.33) over the time interval $[t_0, t_1]$, gives
\[
\left\{ \|xG(-t)\Psi(t)\|^2_X + 2t^2 E_{\alpha,\beta}^\epsilon(t) \right\} \bigg|_{t_0}^{t_1} = \int_{t_0}^{t_1} 2s \left[ E_{\alpha,\beta}^\epsilon(s) + \epsilon \beta \int \frac{n(x,s)}{|x|+\epsilon} \, dx \right] \, ds
\]
which completes the proof of the proposition. \( \square \)

Passing to the limit as $\epsilon \to 0^+$ requires a weak compactness argument in concert with the structure of the SP system (4.1)-(4.3). The next section begins with a review of the notation and fundamental results concerning weakly convergent sequences of functions.

### 4.4.2 The Notion of Weak Convergence

Denote by $\Omega$ an open, bounded, smooth subset of $\mathbb{R}^n (m \geq 2)$. Assume $1 \leq p < \infty$, $q = p/(p-1)$. A sequence $\{f_j\}_{j \in \mathbb{N}} \subset L^p(\Omega)$ converges weakly to $f \in L^p(\Omega)$, written
\[
f_j \overset{w}{\to} f \text{ in } L^p(\Omega),
\]
provided
\[ \int_{\Omega} f_j g \, dx \to \int_{\Omega} f g \, dx \] (4.34)
as \( j \to \infty \) for each \( g \in L^q(\Omega) \). This is to be contrasted with strong convergence. A sequence \( \{f_j\}_{j \in \mathbb{N}} \subset L^p(\Omega) \) converges strongly to \( f \in L^p(\Omega) \), written
\[ f_j \xrightarrow{s} f \text{ in } L^p(\Omega), \]
provided \( f_j \to f \) in \( L^p(\Omega) \) as \( j \to \infty \). The use of a topological word without a modifier always refers to the strong topology. This convention has already been observed in the preceding chapters. To review the properties of weakly convergent sequences of functions a few theorems are presented without proof. Details can be found in [22].

**Theorem 4.10 (Boundedness of Weakly Convergent Sequences).** Assume \( f_j \xrightarrow{w} f \) in \( L^p(\Omega) \). Then

(i) \( \{f_j\}_{j \in \mathbb{N}} \) is bounded in \( L^p(\Omega) \)

(ii) \( \|f\|_p \leq \liminf_{j \to \infty} \|f_j\|_p \).

Statement (i) yields the following refinement (the details of which can be found in [13]).

**Corollary 4.11** If \( f_j \xrightarrow{w} f \) in \( L^p(\Omega) \) and \( g_j \) is bounded in \( L^q(\Omega) \) with \( g_j \xrightarrow{s} g \) in \( L^q(\Omega) \) with \( p^{-1} + q^{-1} = 1 \) then
\[ f_j g_j \xrightarrow{w} fg \text{ in } L^1(\Omega). \]

There is also a refinement of statement (ii) in the case of the Hilbert space \( L^2(\Omega) \) [33].

**Corollary 4.12** If \( f_j \xrightarrow{w} f \) in \( L^2(\Omega) \) and \( \lim_{j \to \infty} \|f_j\|_2 = \|f\|_2 \) then \( f_j \xrightarrow{s} f \) in \( L^2(\Omega) \).
This shows that a weakly convergent sequence on which the norm behaves itself is automatically strongly convergent.

**Theorem 4.13 (Weak Compactness).** Assume $1 < p < \infty$ and that the sequence \( \{f_j\}_{j \in \mathbb{N}} \) is bounded in \( L^p(\Omega) \). Then there exists a subsequence \( \{f_{j_n}\}_{n \in \mathbb{N}} \subset \{f_j\}_{j \in \mathbb{N}} \) and a function \( f \in L^p(\Omega) \) with \( f_{j_n} \overset{u}{\rightharpoonup} f \) in \( L^p(\Omega) \).

In the case \( p = \infty \) the notation is slightly different. A sequence \( \{f_j\}_{j \in \mathbb{N}} \subset L^\infty(\Omega) \) is said to converge weakly star to \( f \in L^\infty(\Omega) \), denoted as \( f_j \rightharpoonup f \) provided expression (4.34) holds for all \( g \in L^1(\Omega) \).

One of the major difficulties with weak convergence is that in general, nonlinear functions are not weakly continuous. It may be that the sequence \( \{f_j\}_{j \in \mathbb{N}} \) converges weakly to \( f \) by virtue of perhaps unbounded, very high frequency and quite irregular oscillations. To illustrate this point for the function \( y(x) = x^2 \) consider a simple example from reference [22]. Select two real numbers \( a < b \) and consider the sequence with terms on \( \Omega = (0, 1) \)

\[
f_j(x) = \begin{cases} 
a & \text{if } \frac{n}{j} \leq x \leq \frac{n+1/2}{j}, \ n = 0, \ldots, j - 1 \\
b & \text{otherwise}
\end{cases}
\]

which is illustrated in figure 4.3. Then \( f_j \rightharpoonup f = (a + b)/2 \) whereas \( f_j^2 \rightharpoonup g = (a^2 + b^2)/2 \neq f^2 \).

In the following section the uniform estimates with respect to time \( t \), given by proposition 4.1, overcome this difficulty and let \( \epsilon \to 0^+ \) in the pseudoconformal conservation law (4.21) given in section 4.4.1.

### 4.4.3 Taking the Limit \( \epsilon \to 0^+ \)

The goal of this section is the establishment of the following theorem:
Theorem 4.14 If $\Phi \in \Xi \cap Z$ and $\Psi$ is the unique strong $X$-valued solution of the system (3.15), (4.2), on the interval $[0, \infty)$ then $x\Psi(t) \in X^3$, $xG(-t)\Psi(t) \in X^3$ and

$$\left\{ \|xG(-t)\Psi(t)\|^2_X + 2t^2E_{\alpha,\beta}(t) \right\}_{t_0}^{t_1} = \int_{t_0}^{t_1} 2sE_{\alpha,\beta}(s)\,ds \quad (4.35)$$

a.e. $t_0, t_1 \in [0, \infty)$, where $E_{\alpha,\beta}(t)$ is given by (3.42).

Proof. The first two points are verified with a few quick observations. Replacing $V_\varepsilon$ with $V_0$ in lemma 4.8 and observing lemma 4.8 only requires $V_\varepsilon$ be real valued gives the conclusion that $x\Psi(x,t) \in X^3$ which is the first point. Moreover, $x\psi_j(x,t) \in (L^2)^3$ and $\psi_j(x,t) \in H^1$, lemma 4.5 implies $xG(-t)\psi_j(x,t) \in (L^2)^3$. Therefore $xG(-t)\Psi(x,t) \in X^3$ which is the second point.

This leaves the justification of the conservation law (4.35). Consider a sequence $\{\Psi_\varepsilon\}_{\varepsilon > 0}$ of solutions to (4.1)-(4.2) obtained in proposition 4.1 for the time interval $(0,T)$. From proposition 4.1, $\Psi_\varepsilon \in C([0,\infty);Y) \cap L^\infty_{\text{loc}}([0,\infty);Z)$ with $\partial_t\Psi_\varepsilon \in C([0,\infty);X) \cap L^\infty_{\text{loc}}([0,\infty);X)$ which implies that $T$ is arbitrary. Proposition 4.9 yields the conservation law (4.21) for each $\Psi_\varepsilon$ on this common interval.
Having established the interval of solution, the justification of letting \( \epsilon \to 0 \) in proposition 4.9 can proceed.

**Step 1: Extraction of weakly convergent subsequences.**

The fact that \( \Psi_\epsilon \in C([0, \infty); Y) \cap L^\infty_{\text{loc}}([0, \infty); Z) \) and \( \partial_t \Psi_\epsilon \in C([0, \infty); X) \) as well as the properties of \( V(\Psi_\epsilon) \) (versions of lemma 3.8 and lemma 3.11) yield some additional estimates. A simple application of the Minkowski and Hölder inequalities gives

\[
\| V(\Psi_\epsilon) \psi_{j,\epsilon} \|_{1,2}^2 \leq \| V(\Psi_\epsilon) \psi_{j,\epsilon} \|_2^2 + \| V(\Psi_\epsilon) \nabla \psi_{j,\epsilon} \|_2^2 + \| \psi_{j,\epsilon} \nabla V(\Psi_\epsilon) \|_2^2 \\
\leq \| V(\Psi_\epsilon) \|_2^2 \left( \| \psi_{j,\epsilon} \|_2^2 + \| \nabla \psi_{j,\epsilon} \|_2^2 \right) + \| \nabla V(\Psi_\epsilon) \|_\infty \| \psi_{j,\epsilon} \|_2^2 \\
\leq C \| \phi \|_X^2 \| \Psi_\epsilon \|_Y^2 \| \psi_{j,\epsilon} \|_{1,2}^2 + C_2 \| \Psi_\epsilon \|_Y \| \psi_{j,\epsilon} \|_2^2 \\
\leq C(\| \Psi_\epsilon \|_Y) \| \psi_{j,\epsilon} \|_{1,2}^2. \tag{4.36}
\]

Furthermore, lemma 3.4 implies

\[
\left\| \frac{\psi_{j,\epsilon}}{|x| + \epsilon} \right\|_2 \leq 2 \| \nabla \psi_{j,\epsilon} \|_2 \\
\leq C \| \psi_{j,\epsilon} \|_{1,2}. \tag{4.37}
\]

The bound for \( V(\Psi_\epsilon) \) requires the Sobolev estimate \( \| f \|_3 \leq C \| \nabla f \|_{1/2} \| f \|_{1/2} \) valid for any \( f \in W^{1,2} \). This estimate together with lemma 3.22 infer that

\[
\| V(\Psi_\epsilon) \|_6 = \left\| \frac{\alpha}{4\pi} \int \frac{n_\epsilon(y,t)}{|y - x|} \, dy \right\|_6 \leq C \| n_\epsilon \|_{6/5} \\
\leq C \sum_{j=1}^{\infty} \lambda_j \| \psi_{j,\epsilon} \|_{6/5} \\
\leq C \sum_{j=1}^{\infty} \lambda_j \| \psi_{j,\epsilon} \|_3 \| \psi_{j,\epsilon} \|_2 \\
\leq C \sum_{j=1}^{\infty} \lambda_j \| \nabla \psi_{j,\epsilon} \|_{1/2} \| \psi_{j,\epsilon} \|_2^{3/2}. \tag{4.38}
\]
4.4: An Approximate Conservation Law

Using the Cauchy–Schwarz inequality on expression (4.38) conveys the estimate

\[
\|V(\psi_\varepsilon)\|_6 \leq C \left( \sum_{j=1}^{\infty} \lambda_j \|\nabla \psi_{j,\varepsilon}\|_2^2 \right)^{1/4} \left( \sum_{j=1}^{\infty} \lambda_j \|\psi_{j,\varepsilon}\|_2^2 \right)^{3/4}
\]

\[
\leq C \|\psi_\varepsilon\|_{V}^{1/2} \|\Phi\|_{X}^{3/2}.
\]

(4.39)

Using the weak compactness property (theorem 4.13) as in [18] implies that for each \(j\) there exists a subsequence \(\{\psi_{j,k}\}_{k=1}^{\infty} \subset \{\psi_{j,\varepsilon}\}_{\varepsilon>0}\) such that as \(k \to \infty (\varepsilon \to 0^+)\)

\[
\psi_{j,\varepsilon} \rightharpoonup \tilde{\psi}_j \text{ in } L^2((0,T);H^1),
\]

\[
\partial_t \psi_{j,\varepsilon} \rightharpoonup \partial_t \tilde{\psi}_j \text{ in } L^2((0,T);L^2),
\]

\[
V(\psi_\varepsilon)\psi_{j,\varepsilon} \rightharpoonup v_{1,j} \text{ in } L^2((0,T);H^1),
\]

\[
V(\psi_\varepsilon) \rightharpoonup v_2 \text{ in } L^2((0,T);L^5),
\]

\[
\frac{\psi_{j,\varepsilon}}{|x| + \varepsilon} \rightharpoonup v_{3,j} \text{ in } L^2((0,T);L^2).
\]

Step 2: Relationships amongst the weak limits.

Having demonstrated the existence of a weakly convergent set of sequences, it is now possible to establish some relationships amongst the weak limits. Let \(\Omega = (0,T) \times \mathbb{R}^3\) and \(\zeta \in C_0^\infty(\Omega)\). It has already been established that \(\psi_{j,\varepsilon} \rightharpoonup \tilde{\psi}_j\) in \(L^2((0,T);H^1)\). This implies that\(^5\)

\[
\zeta \psi_{j,\varepsilon} \rightharpoonup \zeta \tilde{\psi}_j \text{ in } L^2((0,T);L^2).
\]

(4.40)

Hölder’s inequality gives \(\|\zeta \psi_{j,\varepsilon} - \zeta \tilde{\psi}_j\|_{6/5} \leq \|\zeta\|_3 \|\psi_{j,\varepsilon} - \tilde{\psi}_j\|_2\). This fact together with property (4.40) allows the observation that

\[
\zeta \psi_{j,\varepsilon} \rightharpoonup \zeta \tilde{\psi}_j \text{ in } L^2((0,T);L^{6/5}).
\]

\(^5\) This conclusion is attained in [18] with an application of Aubin’s compactness theorem which is theorem 5.1 in chapter 1 of reference [45].
So $V(\Psi_{\epsilon_k}) \xrightarrow{w} v_2$ in $L^2(0,T;L^6)$ and since $\|\zeta \psi_{j,\epsilon_k}\|_{6/5} \leq \|\zeta\|_3 \|\psi_{j,\epsilon_k}\|_2 < \infty$, $\zeta \psi_{j,\epsilon_k}$ is bounded in $L^2((0,T);L^{6/5})$ with $\zeta \psi_{j,\epsilon_k} \xrightarrow{s} \zeta \tilde{\psi}_j$ in $L^2((0,T);L^{6/5})$. Applying corollary 4.11 gives

$$V(\Psi_{\epsilon_k}) \zeta \psi_{j,\epsilon_k} \xrightarrow{w} v_2 \zeta \tilde{\psi}_j \text{ in } L^2((0,T);L^1)$$

and so

$$\int_0^T \int_{\mathbb{R}^3} V(\Psi_{\epsilon_k}) \zeta \psi_{j,\epsilon_k} g \, dx \, dt \xrightarrow{k \to \infty} \int_0^T \int_{\mathbb{R}^3} v_2 \zeta \tilde{\psi}_j g \, dx \, dt$$

as $k \to \infty$ for all $g \in L^\infty(\Omega)$ and any $\zeta \in C_0^\infty(\Omega)$. Considering the product $f = \zeta g$ as an arbitrary function $f \in L^\infty(\Omega)$ gives $v_{1,j} = v_2 \tilde{\psi}_j$.

Showing that $v_{3,j} = \tilde{\psi}_j/|x|$ requires a similar argument. First notice that $1/(|x| + \epsilon_k) \xrightarrow{\epsilon \to 0^+} 1/|x|$ in $L^2((0,T);L^2)$. Since $\zeta \psi_{j,\epsilon_k}$ is bounded in $L^2((0,T);L^2)$ with $\zeta \psi_{j,\epsilon_k} \xrightarrow{s} \zeta \tilde{\psi}_j$ in $L^2((0,T);L^2)$ one can again apply corollary 4.11 to yield

$$\frac{1}{|x| + \epsilon_k} \zeta \psi_{j,\epsilon_k} \xrightarrow{s} \frac{1}{|x|} \zeta \tilde{\psi}_j \text{ in } L^2((0,T);L^1).$$

Therefore following the above argument $v_{3,j} = \tilde{\psi}_j/|x|$.

Step 3: Using uniqueness to show $\Psi_\epsilon \to \tilde{\Psi} = \Psi$.

Consider the Schrödinger equation (4.1) in the weak limit as $\epsilon \to 0^+$. In this limit, $\partial_t \psi_{j,\epsilon_k} \xrightarrow{w} \partial_t \tilde{\psi}_j$ in $L^2(0,T;L^2)$ and $\psi_{j,\epsilon_k} \xrightarrow{w} \tilde{\psi}_j$ in $L^2(0,T;H^1)$ so that $\Delta \psi_{j,\epsilon_k} \xrightarrow{w} \Delta \tilde{\psi}_j$ in $L^2(0,T;H^{-1})$. Also, $\psi_{j,\epsilon_k}/(|x| + \epsilon_k) \xrightarrow{w} v_{3,j} = \tilde{\psi}_j/|x|$ in $L^2(0,T);L^2)$ and $V(\Psi_{\epsilon_k}) \psi_{j,\epsilon_k} \xrightarrow{w} v_{1,j} = v_2 \tilde{\psi}_j$ in $L^2(0,T);H^1)$. This last condition implies $V(\Psi_{\epsilon_k}) \psi_{j,\epsilon_k} \xrightarrow{w} v_2 \tilde{\psi}_j$ in $L^2(0,T);L^2)$. Therefore in the weak limit as $\epsilon \to 0^+$ the Schrödinger equation (4.1) can be written, in the sense of distributions, as

$$i \partial_t \tilde{\psi}_j = -\frac{1}{2} \Delta \tilde{\psi}_j + v_2 \tilde{\psi}_j + \beta \frac{1}{|x|} \tilde{\psi}_j \quad \forall j \in \mathbb{N}$$

(4.41)

with the initial condition $\tilde{\Psi}(0) = \Phi$ (\tilde{\Psi} denotes the sequence \{\tilde{\psi}_1, \tilde{\psi}_2, \ldots\}). From equation (4.41) and the statement of proposition 4.1,

$$\|\tilde{\Psi}(\cdot,t)\|_X = \|\Phi\|_X = \|\Psi_\epsilon(\cdot,t)\|_X$$
and therefore
\[ \| \Psi_\epsilon \|_{L^2((0,T);X)} = \| \tilde{\Psi} \|_{L^2((0,T);X)}. \]

Corollary 4.12 allows the conclusion that as \( \epsilon \to 0^+ \),
\[ \Psi_\epsilon \overset{\epsilon}{\longrightarrow} \tilde{\Psi} \text{ in } L^2((0,T);X). \] (4.42)

This property can be lifted to \( V \) by estimating \( \| V(\Psi_\epsilon) - V(\tilde{\Psi}) \|_6 \) as in the first step. Commencing with the estimate given by lemma 3.22 and using the Minkowski, Hölder and Cauchy–Schwarz inequality justifies the bound
\[ \| V(\Psi_\epsilon) - V(\tilde{\Psi}) \|_6 \leq C \| \Delta V(\Psi_\epsilon) - \Delta V(\tilde{\Psi}) \|_{6/5} \]
\[ \leq C \sum_{j=1}^{\infty} \lambda_j \| |\psi_{j,e}|^2 - |\tilde{\psi}_j|^2 \|_{6/5} \]
\[ \leq C \sum_{j=1}^{\infty} \lambda_j \| \psi_{j,e} (\overline{\psi_{j,e}} - \overline{\tilde{\psi}_j}) + (\psi_{j,e} - \tilde{\psi}_j) \tilde{\psi}_j \|_{6/5} \]
\[ \leq C \sum_{j=1}^{\infty} \lambda_j (\| \psi_{j,e} \|_3 + \| \tilde{\psi}_j \|_3) \| \psi_{j,e} - \tilde{\psi}_j \|_2 \]
\[ \leq C (\| \Psi_\epsilon \|_V, \| \tilde{\Psi} \|_V) \| \Psi_\epsilon - \tilde{\Psi} \|_X. \]

Therefore in view of (4.42)
\[ V(\Psi_\epsilon) \overset{\epsilon}{\longrightarrow} V(\tilde{\Psi}) \text{ in } L^2((0,T);L^6). \] (4.43)

Consequently, \( v_2 = V(\tilde{\Psi}) \) and equation (4.41) becomes the original Schrödinger equation (3.15) without the regularization. Since the solution in corollary 3.18 is unique we must have \( \tilde{\Psi} = \tilde{\Psi} \).

**Step 4:** Allowing \( \epsilon \to 0^+ \) in the conservation law.

Applying the same estimates used to derive expressions (4.38), (4.39) as well as (4.43) gives the estimate.
4.4: An Approximate Conservation Law

\[ \left| \int [V(\Psi_e(x,t))n_e(x,t) - V(\nu(x,t))n(x,t)] \, dx \right| \]
\[ \leq \|V(\Psi(t))\|_6 \|n_e(t) - n(t)\|_{6/5} + \|V(\Psi_e(t)) - V(\nu(t))\|_6 \|n(t)\|_{6/5} \]
\[ \leq C(\|\Psi(t)\|_\infty, \|\nu(t)\|_\infty) \|\Psi_e(t) - \nu(t)\|_X. \]

In view of (4.42) this allows the conclusion

\[ \int V(\Psi_e(x,t))n_e(x,t) \, dx \overset{\epsilon \to 0^+}{\longrightarrow} \int V(\nu(x,t))n(x,t) \, dx \quad \text{a.e. } t \in (0,T). \quad (4.44) \]

Estimating in a similar fashion,

\[ \left| \int \frac{n_e(x,t) - n(x,t)}{|x| + \epsilon} \, dx \right| \leq \sum_{j=1}^{\infty} \lambda_j \left[ \int \frac{\|\psi_{j,\epsilon}(x,t)\|^2 - \|\psi_j(x,t)\|^2}{|x|} \, dx \right] \]
\[ \leq \sum_{j=1}^{\infty} \lambda_j \left( \left\| \psi_{j,\epsilon}(t) \right\|_1 \left\| \psi_j(t) \right\|_1 \right) \left\| \psi_{j,\epsilon}(t) - \psi_j(t) \right\|_2 \]
\[ \leq C(\|\Psi_e(t)\|_\infty, \|\nu(t)\|_\infty) \|\Psi_e(t) - \nu(t)\|_X. \]

Utilizing (4.42) once again yields

\[ \int Vn_e(t) \, dx = \int \frac{n_e(t)}{|x| + \epsilon} \, dx \overset{\epsilon \to 0^+}{\longrightarrow} \int \frac{n(t)}{|x|} \, dx \quad \text{a.e. } t \in (0,T). \quad (4.45) \]

Consider equation (4.21), repeated here for convenience,

\[ \left\{ \|xG(t)\Psi(t)\|_X^2 + 2t^2 E_{\alpha,\beta}(t) \right\} \bigg|_{t_0}^{t_1} = \int_{t_0}^{t_1} 2s \left[ E_{\alpha,\beta}(s) + \epsilon \beta \int \frac{n_e(x,s)}{|x| + \epsilon}^2 \, dx \right] \, ds \]

in the limit as \( \epsilon \to 0^+ \). Expressions (4.44), (4.45) and the definitions of \( E_{\alpha,\beta}(t) \) and \( E_{\alpha,\beta}(t) \) imply that for almost every \( t \in (0,T) \),

\[ 2t^2 E_{\alpha,\beta}(t) \bigg|_{t_0}^{t_1} \overset{\epsilon \to 0^+}{\longrightarrow} 2t^2 E_{\alpha,\beta}(t) \bigg|_{t_0}^{t_1}. \]

The integrals with respect to \( s \) require some additional estimates. For these final estimates, one has the following uniform bounds with respect to \( \epsilon \):

\[ \int V(\Psi_e(x,t))n_e(x,t) \, dx \leq \|V(\Psi_e(t))\|_\infty \|n_e(t)\|_1. \]
4.4: An Approximate Conservation Law

\begin{align*}
\int V_\varepsilon(x)n_\varepsilon(x,t) \, dx &\leq \sum_{j=1}^\infty \lambda_j \int \frac{|\psi_{j,\varepsilon}(x,t)|^2}{|x|} \, dx \\
&\leq \sum_{j=1}^\infty \lambda_j \|\psi_{j,\varepsilon}(t)\|_2 \left\| \frac{\psi_{j,\varepsilon}(\cdot,t)}{|\cdot|} \right\|_2 \\
&\leq C \|\Phi\|_X \|\Psi_\varepsilon(t)\|_Y \\
&\leq C \quad \text{a.e. } t \in (0,T),
\end{align*}
(4.46)

\begin{align*}
\int \frac{n_\varepsilon(x,t)}{(|x| + \varepsilon)^2} \, dx &\leq \sum_{j=1}^\infty \lambda_j \left\| \frac{|\psi_{j,\varepsilon}(\cdot,t)|^2}{(|\cdot| + \varepsilon)^2} \right\|_1 \\
&\leq \sum_{j=1}^\infty \lambda_j \left\| \psi_{j,\varepsilon}(\cdot,t) \right\|_2 \left\| \frac{1}{|\cdot|} \right\|_2 \\
&\leq C \sum_{j=1}^\infty \lambda_j \|\nabla \psi_{j,\varepsilon}(t)\|_2 \\
&\leq C \|\Psi_\varepsilon(t)\|_Y^2 \\
&\leq C \quad \text{a.e. } t \in (0,T).
\end{align*}
(4.47)

The bounds (4.46) and (4.47) show that $|E_{\alpha,\beta}^\varepsilon(t)|$ is bounded above by a constant that
is independent of $\varepsilon$ while the previous argument illustrated that $E_{\alpha,\beta}^\varepsilon(t) \rightarrow E_{\alpha,\beta}(t)$
as $\varepsilon \rightarrow 0^+$ a.e. $t \in (0,T)$. Therefore by the dominated convergence theorem [58]
\[ \lim_{\varepsilon \rightarrow 0^+} \int_0^t 2s \left| E_{\alpha,\beta}^\varepsilon(s) - E_{\alpha,\beta}(s) \right| \, ds = 0 \]
for any $t \in (0,T)$, $T < \infty$. The estimate (4.48) shows that
\[ \lim_{\varepsilon \rightarrow 0^+} 2\epsilon \beta \int_0^t s \int \frac{n(x,s)}{|x| + \varepsilon^2} \, dx \, ds = 0. \]
This leaves the consideration of the \( \|xG(-t)\Psi(x,t)\|^2_X \) term. Since
\[
\int_{|x| \leq N} |x|^2 |G(-t)\psi_j(x,t)|^2 \, dx = \lim_{\varepsilon \to 0} \int_{|x| \leq N} |x|^2 |G(-t)\psi_{\varepsilon,j}(x,t)|^2 \, dx \leq C
\]
independent of \( N \), the sequence \( \chi_{\{x:|x| \leq N\}} |x|^2 |G(-t)\psi_j(x,t)|^2 \) is a monotone increasing sequence in \( N \) with
\[
\int \chi_{\{x:|x| \leq N\}} |x|^2 |G(-t)\psi_j(x,t)|^2 \, dx \leq C.
\]
Therefore by the monotone convergence theorem,
\[
\lim_{N \to \infty} \chi_{\{x:|x| \leq N\}} |x|^2 |G(-t)\psi_j(x,t)|^2 = |x|^2 |G(-t)\psi_j(x,t)|^2
\]
is integrable. That is, \( |x|G(-t)\psi_j(x,t) \in L^2 \). As a result, one has the estimate
\[
\int |x|^2 |G(-t)\psi_j(x,t)|^2 \, dx = \lim_{N \to \infty} \int_{|x| \leq N} |x|^2 |G(-t)\psi_j(x,t)|^2 \, dx
\]
\[
= \lim_{N \to \infty} \lim_{\varepsilon \to 0} \int_{|x| \leq N} |x|^2 |G(-t)\psi_{\varepsilon,j}(x,t)|^2 \, dx
\]
\[
\leq \lim_{\varepsilon \to 0} \int |x|^2 |G(-t)\psi_{\varepsilon,j}(x,t)|^2 \, dx.
\]
Hence, taking the limit as \( \varepsilon \to 0^+ \) in the pseudoconformal conservation law (4.21) with \( t_0 = 0 \) gives the estimate
\[
\left\{ \|xG(-t)\Psi_\varepsilon(t)\|^2_X + 2t^2 E_{\alpha,\beta}(t) \right\} \bigg|_0^t \leq \int_0^t 2s E_{\alpha,\beta}(s) \, ds.
\]
Exchanging the roles of \( 0 \) and \( t \) by specifying at time \( t \) the initial condition \( \Psi(x,t) \) the converse inequality is obtained and therefore equation (4.35) for the case \( t_0 = 0 \). The general case follows immediately from the arbitrary nature of the interval \((0,T)\). \( \square \)

This pseudoconformal conservation law allows the extraction of the time dependence of the energy \( E_{\alpha,\beta}(t) \). This estimate is then used to derive decay estimates for the rest of the Schrödinger–Poisson system and finally lift the result to the Wigner–Poisson system.
4.5 Energy Conditions that Ensure Solutions Decay

4.5.1 Order Relations

In this section it will be assumed that \( z \in \Omega \subseteq \mathbb{R}^n \). In addition, \( f(z) \) and \( g(z) \) are two functions defined and continuous on some domain \( \Omega \) and the point \( z_0 \) lies in \( \overline{\Omega} \), the closure of \( \Omega \). Suppose that as \( z \to z_0 \) in \( \Omega \) there exists a constant \( M \) which is independent of \( z \) and there exists a neighbourhood \( N_0 \) of \( z_0 \) such that

\[
|f(z)| \leq M|g(z)|
\]

for all \( z \in N_0 \cap \Omega \). In this case one says that as \( z \to z_0 \), \( f(z) \) is large \( O \) of \( g(z) \) and is denoted symbolically as

\[
f(z) = O(g(z)), \quad z \to z_0 \text{ in } \Omega.
\]

If instead for any \( \epsilon > 0 \) there exists a neighbourhood \( N_\epsilon \) of \( z_0 \) such that

\[
|f(z)| \leq \epsilon|g(z)|
\]

for all \( z \in N_\epsilon \cap \Omega \), one says that as \( z \to z_0 \), \( f(z) \) is small \( o \) of \( g(z) \). This is denoted symbolically as

\[
f(z) = o(g(z)), \quad z \to z_0 \text{ in } \Omega.
\]

There are a number of useful expressions that involve the combination of these order relations. Some of the more important formulae are collected into the following lemma.

**Lemma 4.15** For each of the following expressions, the limit as \( z \to z_0 \) in \( \Omega \) is to be understood:

(i) \( o(f) + o(f) = o(f) \); \( O(f) + O(f) = O(f) \); \( o(f) + O(f) = O(f) \)

(ii) \( O(f)O(g) = O(fg) \); \( O(f)o(g) = o(fg) \)
(iii) $O(O(f)) = O(f)$

(iv) $O(o(f)) = o(O(f)) = o(o(f)) = o(f)$

(v) If $f(z) = O(g(z))$, as $z \to z_0$ with $f$ and $g$ integrable functions then

$$\int_{z_0}^{z} f(t) \, dt = O\left(\int_{z_0}^{z} |g(t)| \, dt\right) \text{ as } z \to z_0.$$ 

**Proof.** These statements are just a simple consequence of the limit theorems applied to the definitions of $O$ and $o$. □

As an example of the interpretation of the above expressions, consider item (iii). In expanded form this reads: if $g = O(h)$ as $z \to z_0$ and $h = O(f)$ as $z \to z_0$ then $g = O(f)$ as $z \to z_0$.

Before concluding this section, notice that item (v) indicates order relations can be integrated. However, the reverse is not true. In general, order relations cannot be differentiated.

### 4.5.2 Conditions on the Initial Energy

Of primary interest is the description of the asymptotic temporal behaviour of the solution to the Schrödinger–Poisson and subsequently the Wigner–Poisson system in the presence of an external Coulomb field. Intuitively one would expect that only a mutually repulsive set of particles in the presence of an external repulsive potential would exist for arbitrarily large values of time. It is therefore significant that the proof of global existence depended neither on the sign of the self-consistent potential nor the sign of the external Coulomb field. In fact, this indicates only two outcomes are possible. For a given initial wave function $\phi$, the solution $\psi(t)$ will either tend to zero or remain bounded. Which of these two possibilities is chosen must, of course, depend critically upon the nature of the particle interactions. There exist four separate possibilities which correspond to the four possible sign configurations.
4.5: Energy Conditions that Ensure Solutions Decay

of the pair \((\alpha, \beta)\). Recall that one may interpret the system as a cloud of states that either mutually attract \((\alpha < 0)\) or repel \((\alpha > 0)\) each other and are driven externally by a Coulomb potential. Also recall that this external potential has the freedom to either attract \((\beta < 0)\) or repel \((\beta > 0)\) the system of states as a whole. The reader is referred to table 2.1.

These four cases can be grouped into two classes of behaviour. Namely the case where, as \(t \to \infty\), \(E_{\alpha, \beta}(t) \to 0\) and those cases where \(E_{\alpha, \beta}(t) \neq 0\). We will start with the simplest case: \(\alpha \geq 0, \beta \geq 0\) \([19, 37]\) which ensures that \(E_{\alpha, \beta}(t) \geq 0\). For this case we have the following lemma:

**Lemma 4.16** If \(\Phi \in \mathbb{C} \cap Z\), \(\Psi\) is a solution of the SP system \((3.15)-(3.16)\), \(\alpha \geq 0\) and \(\beta \geq 0\) then \(E_{\alpha, \beta}(t) = O(t^{-1})\).

*Proof.* By hypothesis, \(E_{\alpha, \beta}(t) \geq 0\) which implies that \(2t^2E_{\alpha, \beta}(t) \geq 0\). Letting \(f(t) = 2t^2E_{\alpha, \beta}(t)\), theorem 4.14 and lemma 4.8 yield

\[
f(t) = f(t_0) + \|xG(-t_0)\Psi(t_0)\|_X^2 - \|xG(-t)\Psi(t)\|_X^2 + \int_{t_0}^{t} \frac{f(s)}{s} ds
\]

\[
\leq 2t_0^2 E_{\alpha, \beta}(t_0) + \|xG(-t_0)\Psi(t_0)\|_X^2 + \int_{t_0}^{t} \frac{f(s)}{s} ds. \tag{4.49}
\]

Gronwall's lemma, with \(0 < t_0 \leq t\), implies

\[
f(t) = 2t^2E_{\alpha, \beta}(t) \leq \left( 2t_0^2 E_{\alpha, \beta}(t_0) + \|xG(-t_0)\Psi(t_0)\|_X^2 \right) \frac{t}{t_0}.
\]

Therefore, \(E_{\alpha, \beta}(t) = O(t^{-1})\). \(\square\)

Rather than considering all of the possible combinations of \(\alpha\) and \(\beta\), it is more instructive to consider instead whether or not the total energy is positive or negative for a given initial wave function \(\Phi\). In chapter 3, it was shown that the total energy is a conserved quantity. On a physical basis, if this total energy is negative, one typically expects the Schrödinger equation to provide states that do not decay in
4.5: Energy Conditions that Ensure Solutions Decay

time [6, 25, 43]. An example of such a solution is, of course, any multi-electron atom. In this case, the negative energy is interpreted as the amount of energy that is required to disassociate the system of particles. Alternatively, if one expects the solution to decay as \( t \to \infty \) then, in the limit of \( t \to \infty \), none of the energy can be used to maintain a particular configuration of the particles. All of the initial energy should eventually become kinetic. The first of these two situations, that negative energy solutions cannot decay, is quantified in the next proposition which is a generalization\(^6\) of an estimate given in [14]. The second situation will be quantified in proposition 4.19.

**Proposition 4.17** Let \( \Phi \in \Xi \cap \mathbb{Z} \) and \( \Psi \) be a solution of (3.15)-(3.16) with a total constant energy of

\[
E_{\text{tot}} = \frac{1}{2} \| \nabla \Psi(\cdot, t) \|^2_{\mathcal{X}} + E_{\alpha, \beta}(t). \tag{4.50}
\]

If \( E_{\text{tot}} < 0 \) then

\[
\sum_{j=1}^{\infty} \lambda_j \| \psi_j(\cdot, t) \|^2_p \not\to 0 \text{ as } t \to \infty.
\]

for any \( 2 \leq \ p \leq \infty \).

**Proof.** By the definition of \( E_{\alpha, \beta} \) earlier in this chapter,\(^7\)

\[
|E_{\alpha, \beta}(t)| \leq \frac{1}{2} \int V n \, dx + |\beta| \int \frac{n}{|x|} \, dx.
\]

To estimate the Coulomb term the integral in broken into \(|x| < 1 \) and \(|x| \geq 1 \) as

\[
\int \frac{n}{|x|} \, dx = \int_{|x| < 1} \frac{n}{|x|} \, dx + \int_{|x| \geq 1} \frac{n}{|x|} \, dx := T_1 + T_2. \tag{4.51}
\]

\(^6\) Reference [14] proves the case \( p = \infty \).

\(^7\) Recall that the \( \alpha \) is hidden in the definition of \( V \).
Applying the Minkowski and Hölder inequalities to the $T_1$ term gives

$$T_1 = \sum_{j=1}^{\infty} \lambda_j \int_{|x|<1} \frac{|\psi_j(x,t)|^2}{|x|} \, dx$$

$$\leq \sum_{j=1}^{\infty} \lambda_j \|\psi_j\|_2 \|\psi_j\|_\infty \left( \int_{|x|<1} \frac{dx}{|x|^2} \right)^{1/2}$$

$$= C \sum_{j=1}^{\infty} \lambda_j \|\psi_j\|_2 \|\psi_j\|_\infty.$$

Using the conservation of probability and the Cauchy–Schwarz inequality yields

$$T_1 \leq C \left( \sum_{j=1}^{\infty} \lambda_j \|\psi_j\|_2^2 \right)^{1/2} \left( \sum_{j=1}^{\infty} \lambda_j \|\psi_j\|_\infty^2 \right)^{1/2}$$

$$= C \|\Phi\|_X \left( \sum_{j=1}^{\infty} \lambda_j \|\psi_j(\cdot,t)\|_\infty^2 \right)^{1/2}.$$  \hfill (4.52)

Since $\|\nabla \psi(\cdot,t)\|_X$ is uniformly bounded in $t$,

$$T_1 \leq \int \frac{n}{|x|} \, dx$$

$$\leq \sum_{j=1}^{\infty} \lambda_j \|\psi_j\|_2 \left( \frac{\psi_j}{|\cdot|} \right) \|\psi_j\|_2$$

$$\leq \|\nabla \psi(\cdot,t)\|_X \left( \sum_{j=1}^{\infty} \lambda_j \|\psi_j(\cdot,t)\|_2^2 \right)^{1/2}$$

$$\leq C \left( \sum_{j=1}^{\infty} \lambda_j \|\psi_j(\cdot,t)\|_2^2 \right)^{1/2}.$$  \hfill (4.53)

The estimates (4.52) and (4.53) are combined by using the Riesz–Thorin interpolation theorem to give the estimate

$$T_1 \leq C_p \left( \sum_{j=1}^{\infty} \lambda_j \|\psi_j(\cdot,t)\|_p^2 \right)^{1/2}.$$  \hfill (4.54)

where $2 \leq p \leq \infty$. 
Similarly, for the $T_2$ term one obtains the estimate

$$T_2 = \sum_{j=1}^{\infty} \lambda_j \int_{|x| \geq 1} \frac{|\psi_j(x, t)|^2}{|x|} \, dx$$

$$\leq \sum_{j=1}^{\infty} \lambda_j \|\psi_j\|^a_p \|\psi_j^{2-a}\|_q \left( \int_{|x| \geq 1} \frac{dx}{|x|^r} \right)^{1/r}$$

$$= C_r \sum_{j=1}^{\infty} \lambda_j \|\psi_j\|^a_{ap} \|\psi_j^{2-a}\|_{(2-a)q}$$

In this case, $p \geq 1, q \geq 1, r > 3, 0 \leq a \leq 2$ and $p^{-1} + q^{-1} + r^{-1} = 1$. Letting $p = 2/a$ restricts the choice of $a$ to $a \leq 2(1 - 1/r)$. Taking $a = 3/2$ yields the estimate for any $4 \leq r \leq \infty$,

$$T_2 \leq C_r \sum_{j=1}^{\infty} \lambda_j \|\psi_j\|^2 \|\psi_j\|^{1/2} \frac{1}{r^3}$$

$$= C_r \sum_{j=1}^{\infty} \lambda_j^{3/4} \|\psi_j\|^2 \lambda_j^{1/4} \|\psi_j\|^{1/2} \frac{1}{2r^4}$$

$$\leq C_r \left( \sum_{j=1}^{\infty} \lambda_j \|\psi_j\|^2 \right)^{3/4} \left( \sum_{j=1}^{\infty} \lambda_j \|\psi_j\|^{2} \right)^{1/4}$$

$$= C_r \|\Phi\|_{X}^{3/2} \left( \sum_{j=1}^{\infty} \lambda_j \|\psi_j(\cdot, t)\|^2 \right)^{1/4} \quad (4.55)$$

Reformulating (4.55) produces

$$T_2 \leq C_p \|\Phi\|_{X}^{3/2} \left( \sum_{j=1}^{\infty} \lambda_j \|\psi_j(\cdot, t)\|^2 \right)^{1/4} \quad (4.56)$$

where $2 \leq p \leq \infty$.

The self-consistent term of $E_{\alpha,\beta}(t)$ requires item (i) of theorem 3.23 which states $V \in L^\infty([0, \infty); L^p)$ for any $3 < p \leq \infty$. Consequently, there exists a constant $C_\varepsilon$ such that

$$\|V(\cdot, t)\|_{3+\varepsilon} \leq C_\varepsilon \quad (4.57)$$
4.5: Energy Conditions that Ensure Solutions Decay

for all $t \in [0, \infty)$ and $\epsilon > 0$. Using (4.57) and the Hölder inequality gives the result

$$\left| \frac{1}{2} \int V|\psi_j|^2 \, dx \right| = C \left\| V|\psi_j|^2 \right\|_1$$

$$\leq C \left\| V \right\|_{3+\epsilon} \left\| |\psi_j|^a \right\|_p \left\| |\psi_j|^{2-a} \right\|_q$$

$$\leq C \epsilon \left\| \psi_j \right\|_2 \left\| \psi_j \right\|_{2-a} \frac{2(3+\epsilon)(2-\epsilon)}{4+2\epsilon-(3+\epsilon)a}$$

$$\leq C \epsilon \left\| \psi_j \right\|_2 \left\| \psi_j \right\|_{2-a} \frac{2(3+\epsilon)(2-\epsilon)}{4+2\epsilon-(3+\epsilon)a}.$$  \hspace{1cm} (4.58)

The following restrictions are observed: $p > 1$, $q > 1$ and $p^{-1} + q^{-1} = (2+\epsilon)/(3+\epsilon)$ having chosen $p = 2/a$. This choice further restricts the range of $a$ to $0 < a < (4+2\epsilon)/(3+\epsilon)$. Summing (4.58) over the $\lambda_j$ and using the Minkowski inequality gives

$$\left| \frac{1}{2} \int Vn \, dx \right| \leq C \epsilon \sum_{j=1}^{\infty} \lambda_j \left\| \psi_j \right\|_2 \left\| \psi_j \right\|_{2-a} \frac{2(3+\epsilon)(2-\epsilon)}{4+2\epsilon-(3+\epsilon)a}$$

$$\leq C \epsilon \left( \sum_{j=1}^{\infty} \lambda_j \left\| \psi_j \right\|_2 \right)^{a/2} \left( \sum_{j=1}^{\infty} \lambda_j \left\| \psi_j \right\|_{2-a} \frac{2(3+\epsilon)(2-\epsilon)}{4+2\epsilon-(3+\epsilon)a} \right)^{1-a/2}$$

$$= C \epsilon \left\| \Phi \right\|_X \left( \sum_{j=1}^{\infty} \lambda_j \left\| \psi_j(\cdot, t) \right\|_{2-a} \frac{2(3+\epsilon)(2-\epsilon)}{4+2\epsilon-(3+\epsilon)a} \right)^{1-a/2}.$$  \hspace{1cm} (4.59)

Consider the function $f(\epsilon, a) = 2(3+\epsilon)(2-a)/[4+2\epsilon-(3+\epsilon)a]$ on the domain $\epsilon > 0$ and $0 < a \leq (4+2\epsilon)/(3+\epsilon)$ which is illustrated in figure 4.4. The boundary of the domain consists of four segments: $C_1 : a = 0, 0 < \epsilon \leq \infty$; $C_2 : \epsilon \to \infty, 0 \leq a \leq 2$, $C_3 : a = (4+2\epsilon)/(3+\epsilon), 0 < \epsilon \leq \infty$ and $C_4 : \epsilon \to 0^+, 0 \leq a \leq 4/3$. Along $C_1$, $f = 2(3+\epsilon)/(2+\epsilon)$ which approaches 3 as $\epsilon \to 0^+$ and reaches 2 as $\epsilon \to \infty$. Along $C_2$, $f = 2$ except at the point $a = 2$ where $f$ becomes unbounded. Along $C_3$, $f = \infty$. The segment $C_4$ is not part of the domain so consider instead
4.5: Energy Conditions that Ensure Solutions Decay

Figure 4.4: An analysis of \( f(\epsilon, a) = \frac{2(3+\epsilon)(2-a)}{4+2a-(3+\epsilon)a} \).

This surface illustrates the behaviour of the function \( f(\epsilon, a) \) on the domain \((\epsilon, a) = (0, \infty) \times [0, (4+2\epsilon)/(3+\epsilon)]. f(\epsilon, a) \geq 2\) for all values in the domain and is a convex function in both variables.

The segment mapped out by the parametric path

\[
C_{\epsilon_0} : \begin{cases} \epsilon = \epsilon_0 + t, \\ a = \frac{4 + 2\epsilon_0}{(3 + \epsilon_0)(1 + t)} \end{cases}
\]

with \( t \geq 0 \) for any \( \epsilon_0 > 0 \). This curve is also depicted in figure 4.4. Along \( C_{\epsilon_0} \), \( f \) attains the value 2 as \( t \to \infty \) and becomes unbounded as \( t \to 0^+ \). This analysis infers that, by letting \( \epsilon_0 = 1 \) and \( t \to \infty \), the bound (4.59) can be expressed as

\[
\left| \frac{1}{2} \int Vn \, dx \right| \leq C_p \| \Phi \|_{L^p}^p \left( \sum_{j=1}^{\infty} \lambda_j \| \psi_j(\cdot, t) \|_{L^p}^2 \right)^{1 - \alpha_p/2} \tag{4.60}
\]
where \(2 \leq p \leq \infty\) and
\[
a_p = \frac{5p - 18 + \sqrt{169p^2 - 756p + 900}}{12(p - 2)}.
\]
The function \(a_p\) is monotonically increasing with \(a_p \to 0^+\) as \(p \to 2^+\) and \(a_p \to 3/2\) as \(p \to \infty\).

Combining the expressions (4.51), (4.54), (4.56) and (4.60) gives the bound
\[
|E_{\alpha, \beta}(t)| \leq C_p |\beta| \left( \sum_{j=1}^{\infty} \lambda_j \| \psi_j(\cdot, t) \|_p^2 \right)^{1/2} + C_p |\beta| \| \Phi \|_X^3 \left( \sum_{j=1}^{\infty} \lambda_j \| \psi_j(\cdot, t) \|_p^2 \right)^{1/4}
+ C_p \| \Phi \|_X^{3/2} \left( \sum_{j=1}^{\infty} \lambda_j \| \psi_j(\cdot, t) \|_p^2 \right)^{1 - a_p/2},
\]
where we can choose any \(p \in (2, \infty]\). The case \(p = 2\) has been eliminated since conservation of probability gives
\[
\sum_{j=1}^{\infty} \lambda_j \| \psi_j(\cdot, t) \|_2^2 = \sum_{j=1}^{\infty} \lambda_j \| \varphi_j \|_2^2 = 1 \neq 0.
\]
Suppose that \(\sum_j \lambda_j \| \psi_j(\cdot, t) \|_p^2 \to 0\) for some \(2 < p \leq \infty\) as \(t \to \infty\). This implies that the total energy expression (4.50) becomes, in the limit as \(t \to \infty\),
\[
E_{\text{tot}} = \frac{1}{2} \| \nabla \Psi(\cdot, t) \|_X^2
\]
which is a contradiction since we have assumed \(E_{\text{tot}} < 0\). □

To see that there do exist initial wave functions with \(E_{\text{tot}} < 0\) pick \(\lambda_j = \delta_{i,j}\) and for some \(\xi > 0\) consider the spherically symmetric wave function
\[
\varphi_1(x) = \left( \frac{\xi^3}{\pi} \right)^{1/2} e^{-\xi|x|}.
\]
It is an easy exercise to establish that for this initial wave function, \(\Phi \in \Xi \cap Z\), \(\| \Phi \|_2^2 = 1\) and as in [14] one can determine that
\[
V(x) = \alpha \left( \frac{1}{|x|} \int_0^{|x|} s^2 |\varphi_1(s)|^2 \, ds + \int_{|x|}^{\infty} s |\varphi_1(s)|^2 \, ds \right)
= \frac{\alpha}{4\pi} \left[ \frac{1}{|x|} - e^{-2\xi|x|} \left( \xi + \frac{1}{|x|} \right) \right].
\]
As a result, the total energy is given by the expression

\[ E_{\text{tot}} = \frac{1}{2} \| \nabla \Phi \|_X^2 + \frac{1}{2} \int V n \, dx + \beta \int \frac{n}{|x|} \, dx \]

\[ = \frac{1}{2} \xi^2 + \frac{5\alpha}{64\pi} \xi + \beta \xi. \]

Thus, if \( \beta \leq -5\alpha/64\pi \) then \( E_{\text{tot}} \) is negative for any \( \xi \in (0, -5\alpha/32\pi - 2\beta) \). If \( \xi \) is chosen in this range, proposition 4.17 concludes that \( \| \psi(\cdot,t) \|_p \neq 0 \) as \( t \to \infty \) for any \( 2 < p \leq \infty \). The bound \( \beta \leq -5\alpha/64\pi \) has two physical interpretations based upon the sign of \( \alpha \) and \( \beta \). One obtains a bound state (solutions do not decay in time) provided the initial wave function is sufficiently wide \( \xi \in (0, -5\alpha/32\pi - 2\beta) \) and either of the two following mutually exclusive cases hold:

Case 1: The particles repel each other (\( \alpha > 0 \)) but the external Coulomb potential has a sufficiently large attraction (\( \beta \leq -5\alpha/64\pi < 0 \)) so as to capture the system as a whole.

Case 2: The particles attract each other (\( \alpha < 0 \)) in the presence of either an external attractive Coulomb potential (\( \beta < 0 \)) or an external repulsive Coulomb potential without enough strength (\( \beta \leq -5\alpha/64\pi > 0 \)) to disperse the system of particles.

If \( \xi > -5\alpha/32\pi - 2\beta \) then the initial wave function has positive total energy and consequently the solution may not decay in time. Figure 4.5 depicts the energy density of the Coulomb and self-consistent energy densities for the values \( \xi = 1/2, \alpha = 32\pi/5 \) and \( \beta = \pm 1 \). If \( \beta = 1 \) then both \( \alpha \) and \( \beta \) are positive and by lemma 4.16, \( E_{\alpha,\beta} \to 0 \) as \( t \to \infty \). If \( \beta = -1 \) then \( E_{\text{tot}} = -1/8 \). Hence, by proposition 4.17, the solutions cannot go to zero.

The preceding discussion dealt with negative total energy solutions. We will now show that if one expects a solution to decay, then as \( t \to \infty \), all of the energy in the system must become kinetic. Illustrating this point requires the following lemma:
Lemma 4.18 If $\Phi \in \Xi$ and $G(-t)$ is the unitary operator given in lemma 4.4 then $\psi_j \in L^p$ for all $j$ and for $2 \leq p < 6$

$$\sum_{j=1}^{\infty} \lambda_j \|\psi_j(\cdot, t)\|_p^2 \leq C_p \|\Phi\|_\infty^{2a} \|xG(-t)\psi(\cdot, t)\|_\infty^{2(1-a)} t^{2(a-1)}, \quad t > 0,$$

where $1 - a = 3(1/2 - 1/p)$.

Proof. This is a corollary of lemma 4.6. Since $\Phi \in \Xi$, theorem 4.14 implies that $\Psi \in \Xi$. Therefore applying lemma 4.6 to each of the $\psi_j$ gives

$$\|\psi_j(\cdot, t)\|_p^2 \leq C_p \|G(-t)\psi_j(\cdot, t)\|_2^{2a} \|xG(-t)\psi_j(\cdot, t)\|_2^{2(1-a)} t^{2(a-1)}.$$

Lemma 4.4 furnishes $\|G(-t)\psi_j(\cdot, t)\|_2 = \|\psi_j(\cdot, t)\|_2 = \|\psi_j\|_2$. Hence, summing over
the $\lambda_j$ and using the Cauchy–Schwarz inequality yields

$$\sum_{j=1}^{\infty} \lambda_j \|\psi_j(t)\|_p^2 \leq C_p \sum_{j=1}^{\infty} \left( \frac{\lambda_j^{1/2}}{\|\varphi_j\|_2} \right)^{2\alpha} \left( \frac{\lambda_j^{1/2}}{\|xG(-t)\psi_j(t)\|_2} \right)^{2(1-\alpha)} t^{2(\alpha-1)}$$

$$\leq C_p \left[ \sum_{j=1}^{\infty} \left( \lambda_j^{1/2} \|\varphi_j\|_2 \right)^2 \right]^\alpha \left[ \sum_{j=1}^{\infty} \left( \lambda_j^{1/2} \|xG(-t)\psi_j(t)\|_2 \right)^2 \right]^{1-\alpha} t^{2(\alpha-1)}$$

$$= C_p \|\Phi\|_\infty^2 \|xG(-t)\Psi(t)\|_X^{2(1-\alpha)} t^{2(\alpha-1)}. \quad \Box$$

The final result of this section establishes that if the self-consistent energy is positive ($\alpha > 0$), then a solution will decay as $t \to \infty$ if and only if the total energy of the system becomes kinetic. Alternatively, a solution will decay if and only if the energy contained in the configuration of the system, $E_{\alpha,\beta}$, vanishes as $t \to \infty$. This extends a theorem of reference [19].

**Proposition 4.19** If $\Phi \in \Xi \cap Z$, $\alpha > 0$ and $\Psi$ is a solution of the SP system (3.15)–(3.16) then the following statements are equivalent:

(i) $\lim_{t \to \infty} E_{\alpha,\beta}(t) \to 0$

(ii) $\lim_{t \to \infty} \int \frac{n(x,t)}{|x|} dx \to 0$

(iii) $\lim_{t \to \infty} \sum_{j=1}^{\infty} \lambda_j \|\psi_j(\cdot, t)\|_p^2 \to 0$ for any $2 < p < 6$

(iv) $\lim_{t \to \infty} \Psi(t) \to 0$ in $X_{0,\text{loc}} \left( \Gamma = \{\gamma_j\}_{j \in \mathbb{N}} : \gamma_j \in L^2_{\text{loc}}(\mathbb{R}^3) \forall j \right)$.

**Proof.** (iii) $\Rightarrow$ (i): This follows from estimate (4.61) of proposition 4.17.

(i) $\Rightarrow$ (iii): This requires an auxiliary calculation. Let $\zeta(t) = \|x\Psi(t)\|_X^2$. By multiplying equation (3.15) by the factor $|x|\overline{\psi_j}$, integrating over $\mathbb{R}^3$ and then taking the imaginary part gives

$$\frac{d}{dt} \left( \|x\psi_j(t)\|_X^2 \right) = 2\text{Im} \int \nabla \left( \frac{|x|^2}{2} \overline{\psi_j} \right) \cdot \nabla \psi_j \, dx.$$
4.5: Energy Conditions that Ensure Solutions Decay

Summing over the $\lambda_j$ and computing the gradient yields

$$\frac{d\zeta}{dt} = \frac{d}{dt} \left( \|x\Psi(t)\|_X^2 \right) = 2 \text{Im} \sum_{j=1}^{\infty} \lambda_j \int x\overline{\psi}_j \cdot \nabla \psi_j \, dx. \tag{4.62}$$

To obtain the second derivative $\zeta''$, the pseudoconformal conservation law of theorem 4.14, equation (4.62) and the conservation of energy from proposition 3.16 are used in this order. Explicitly,

$$\|xG(-t)\Psi\|_X^2 = \|x\Psi\|_X^2 - 2t \text{Im} \sum_{j=1}^{\infty} \lambda_j \int x\overline{\psi}_j \cdot \nabla \psi_j \, dx + t^2 \|\nabla \Psi\|_X^2$$

$$= \zeta(t) - t \frac{d\zeta}{dt} + t^2 \|\nabla \Psi\|_X^2$$

$$= \zeta(t) - t \frac{d\zeta}{dt} + 2t^2 E_{\text{tot}} - 2t^2 E_{\alpha,\beta}(t). \tag{4.63}$$

Taking the derivative of expression (4.63) with respect to $t$ yields

$$\frac{d}{dt} \left( \|xG(-t)\Psi\|_X^2 \right) = -t \frac{d^2\zeta}{dt^2} + 4t E_{\text{tot}} - 4t E_{\alpha,\beta} - 2t^2 \frac{dE_{\alpha,\beta}}{dt}$$

while the pseudoconformal conservation law gives

$$\frac{d}{dt} \left( \|xG(-t)\Psi\|_X^2 \right) = -2t^2 \frac{dE_{\alpha,\beta}}{dt} - 2t E_{\alpha,\beta}.$$

Equating these two expressions and using the conservation of energy

$$E_{\text{tot}} = \|\nabla \Psi(t)\|_X^2 / 2 + E_{\alpha,\beta}$$

yields

$$\frac{d^2\zeta}{dt^2} = 2E_{\text{tot}} + \|\nabla \Psi(t)\|_X^2. \tag{4.64}$$

Since $E_{\alpha,\beta}(t) \to 0$, this implies $\|\nabla \Psi(t)\|_X^2 \to 2E_{\text{tot}}$ and hence expression (4.64) implies $\zeta'' = 4E_{\text{tot}} + o(1)$. Integrating with respect to $t$, $\zeta' = 4E_{\text{tot}} t + o(t)$ and $\zeta = 2E_{\text{tot}} t^2 + o(t^2)$. Relation (4.63) yields the conclusion

$$\|xG(-t)\Psi\|_X^2 = o(t^2)$$
and consequently if $0 \leq a < 1$, 
\[ \| xG(-t) \Psi \|_X^{2(1-a)} = o \left( t^{2(a-1)} \right). \]

Using the estimate of lemma 4.18 and item (ii) of lemma 4.15 gives 
\[ \sum_{j=1}^{\infty} \lambda_j \| \psi_j(\cdot, t) \|_p^2 = O(1) o \left( t^{2(1-a)} \right) O \left( t^{2(a-1)} \right) = o(1) \]
where $2 < p < 6$. The fact that $a \neq 1$ forces $p \neq 2$.

(ii) $\iff$ (iv): This equivalence follows by taking any $R > 0$ and using the fact that $\| \nabla \psi(\cdot, t) \|_X$ is uniformly bounded to obtain the estimates
\[ \sum_{j=1}^{\infty} \lambda_j \int_{|x|<R} |\psi_j(x, t)|^2 \, dx \leq R \int \frac{n(x, t)}{|x|} \, dx \] (4.65)
(for the $(ii) \Rightarrow (iv)$ implication) and 
\[ \int \frac{n(x, t)}{|x|} \, dx = \sum_{j=1}^{\infty} \lambda_j \int_{|x|<R} \frac{|\psi_j(x, t)|^2}{|x|} \, dx + \sum_{j=1}^{\infty} \lambda_j \int_{|x|\geq R} \frac{|\psi_j(x, t)|^2}{|x|} \]
\[ \leq 2\| \nabla \psi(\cdot, t) \|_X \sum_{j=1}^{\infty} \lambda_j \int_{|x|<R} |\psi_j(x, t)|^2 \, dx + \frac{1}{R} \| \psi(\cdot, t) \|_X^2 \]
\[ \leq C \sum_{j=1}^{\infty} \lambda_j \int_{|x|<R} |\psi_j(x, t)|^2 \, dx + \frac{1}{R} \| \psi(\cdot, t) \|_X^2 \]
(for the $(iv) \Rightarrow (ii)$ implication).

(iii) $\Rightarrow$ (ii): This follows from equations (4.51), (4.54) and (4.56) of proposition 4.17.

(ii) $\Rightarrow$ (iii): For brevity this step uses the notation:
\[ V_{self}(t) = \frac{1}{2} \int V(x, t)n(x, t) \, dx \quad \text{and} \quad V_{coul}(t) = \beta \int \frac{n(x, t)}{|x|} \, dx. \]

Since $\alpha > 0$, the self-consistent energy $V_{self}(t) > 0$.

Case 1: ($\beta > 0$)

Since $\beta > 0$, $V_{coul}(t) > 0$ and therefore $E_{\alpha, \beta}(t) > 0$. From lemma 4.16, $E_{\alpha, \beta}(t) = O(t^{-1}) \to 0$ as $t \to \infty$ which is item (i). However, the implication (i) $\Rightarrow$ (iii) has already been established above.
4.5: Energy Conditions that Ensure Solutions Decay

Case 2: ($\beta < 0$)

Consider the function

$$f(t) = \|xG(-t)\Psi(\cdot, t)\|_X^2 + 2t^2V_{\text{coul}}(t)$$  \hspace{1cm} (4.66)

for $t \geq 0$ with the property $f(0) = \|x\Phi\|_X^2 > 0$. Since $\beta < 0$, $V_{\text{coul}}(t) < 0$. There are two subcases to consider.

Subcase 1: ($f(t) \geq 0$, $t \in [0, \infty)$)

If $f(t)$ remains positive for all $t$ then the pseudoconformal conservation law yields the estimate

$$f(t) + 2t^2V_{\text{self}}(t) = f(t_0) + 2t_0^2V_{\text{self}}(t_0) + \int_{t_0}^{t} 2s [V_{\text{self}}(s) + V_{\text{coul}}(s)] \, ds$$

$$\leq f(t_0) + 2t_0^2V_{\text{self}}(t_0) + \int_{t_0}^{t} 2sV_{\text{self}}(s) \, ds$$  \hspace{1cm} (4.67)

for any $t_0 > 0$. Identifying $g(t) = 2t^2V_{\text{self}}(t) > 0$ and using the fact that $f(t) > 0$ gives the inequality

$$g(t) \leq f(t_0) + 2t^2_0V_{\text{self}}(t_0) + \int_{t_0}^{t} \frac{g(s)}{s} \, ds.$$  

Utilizing Gronwall's inequality gives

$$g(t) = 2t^2V_{\text{self}}(t) \leq \left[ f(t_0) + 2t_0^2V_{\text{self}}(t_0) \right] \frac{t}{t_0}$$

and hence, from expression (4.67), the decay estimate $f(t) = O(t)$. Using lemma 4.18 gives the additional expression

$$C_p t^2 \|\Phi\|_X^{2/3} \left( \sum_{j=1}^{\infty} \lambda_j \|\psi_j(\cdot, t)\|_p^2 \right)^{2p/3} \leq \|xG(-t)\Psi(\cdot, t)\|_X^2$$  \hspace{1cm} (4.68)

for all $2 < p < 6$. Applying the estimate (4.68) to (4.66) and using the fact that both $V_{\text{coul}}(t) \to 0$ and $f(t) = O(t)$ as $t \to \infty$ gives the decay estimate

$$\sum_{j=1}^{\infty} \lambda_j \|\psi_j(\cdot, t)\|_p^2 = O \left( t^{\frac{3(2-p)}{2p}} \right).$$
On the restriction $2 < p < 6$, $-1 < 3(2 - p)/2p < 0$ and therefore,
\[ \sum_{j=1}^{\infty} \lambda_j \| \psi_j(\cdot, t) \|^2_p \to 0 \]
as $t \to \infty$ as required.

If $f(t)$ is not always positive then there will exist some time $t$ for which $f(t) < 0$. In addition there may exist interval(s) $I = [t_0, t_1)$ where $f(t_0) = 0$, $0 < t_0 \leq t_1 \leq \infty$ and $f \geq 0$ throughout the interval. These two separate situations are dealt with separately.

**Subcase 2a: ($f(t) \leq 0$ for some $t > 0$)**

Suppose at some time $t$, $f(t) \leq 0$ so that
\[ C_p t^2 \| \Phi \|_{X^{-2/3}}^2 \left( \sum_{j=1}^{\infty} \lambda_j \| \psi_j(\cdot, t) \|^2_p \right)^{\frac{2p}{3p-2}} \leq \| x G(-t) \psi(\cdot, t) \|^3_X \leq -2t^2 V_{coul}(t) \]
by using the estimate (4.68) and the definition (4.66). Since $V_{coul}(t) \to 0$ and $2p/(3p - 6) > 1$ for $2 < p < 6$, item (iii) is established once again.

**Subcase 2b: ($f(t) \geq 0$ for some interval $I = [t_0, t_1)$)**

In this last case one supposes that there exists an interval $I = [t_0, t_1)$ where $f(t_0) = 0$, $0 < t_0 \leq t_1 \leq \infty$ and $f \geq 0$ throughout the interval. For any time $t$ in the interval $I$, the pseudoconformal conservation law gives the estimate
\[ f(t) + 2t^2 V_{self}(t) \leq f(t_0) + 2t_0^2 V_{self}(t_0) + \int_{t_0}^{t} 2s V_{self}(s) ds. \] (4.69)
As in the first subcase, one lets $g(t) = 2t^2 V_{self}(t) > 0$ and obtains the inequality
\[ g(t) \leq 2t_0^2 V_{self}(t_0) + \int_{t_0}^{t} \frac{g(s)}{s} ds. \]

In this case Gronwall's inequality gives
\[ g(t) = 2t^2 V_{self}(t) \leq 2t_0 t V_{self}(t_0) \] (4.70)
for any \( t \in [t_0, t_1] \). Also notice that since \( f \geq 0 \), one has

\[
\|xG(-t_0)\Psi(\cdot, t_0)\|_X^2 \geq -2t^2 V_{\text{coul}}(t).
\]

In addition, \( \beta < 0 \), so that the right hand side is a positive quantity. Taking square roots gives the estimate

\[
\|xG(-t_0)\Psi(\cdot, t_0)\|_X \geq \left[ -2t^2 V_{\text{coul}}(t) \right]^{1/2}. \tag{4.71}
\]

At this point an upper bound on the self-consistent energy, \( V_{\text{self}}(t) \), is required. In the derivation of equation (4.60) the estimate

\[
V_{\text{self}}(t) = \left| \frac{1}{2} \int V n \, dx \right| \leq C_n \| \Phi \|_X^2 \left( \sum_{j=1}^{\infty} \lambda_j \| \psi_j(\cdot, t) \|_{L^2(\mathbb{R})}^2 \frac{2(3 + \epsilon)(2 - a)}{3 + 2 \epsilon - (3 + \epsilon) a} \right)^{1-a/2} \tag{4.72}
\]

was considered along the path \( a = 3/(2 \epsilon) \). Considering the path \( a = 3a_0/(3 + \epsilon) \) with \( 0 \leq a_0 \leq 4/3 \) and solving the expression

\[
2(3 + \epsilon)(2 - a) = 4 + 2 \epsilon - (3 + \epsilon) a
\]

for \( \epsilon \) with the \( a \) variable defined by this new path gives

\[
\epsilon = \frac{3}{2} a_0 - 2 \frac{p - 3}{p - 2}.
\]

Therefore

\[
a = \frac{6a_0(p - 2)}{2p + a_0(3p - 6)} \quad \text{and} \quad 1 - \frac{a}{2} = \frac{2p}{2p + a_0(3p - 6)}.
\]

By taking \( a_0 = 1 \), equation (4.72) becomes the estimate

\[
\left| \frac{1}{2} \int V n \, dx \right| \leq C_p \| \Phi \|_{X}^2 \left( \sum_{j=1}^{\infty} \lambda_j \| \psi_j(\cdot, t) \|_{L^2(\mathbb{R})}^2 \right)^{\frac{2p}{3p-5}}
\]

\(^8\) Recall \( \epsilon_0 = 1 \).
where \(2 < p < 6\). By using lemma 4.18 the final form of the required upper bound is obtained

\[
V_{\text{self}}(t) = \left| \frac{1}{2} \int Vn \, dx \right| \leq C_p \|\Phi\|_X^{2(3-p)/p} \|\Phi\|_X^{4p/3-p} \|xG(-t)\Psi(\cdot, t)\|_X^{4(2-p)/3-p} t^{(1-s)/3-p}.
\]

The application of the estimate (4.73) as \(p \to 6^-\) at \(t = t_0\) to the estimate (4.70) and then using the estimate (4.71) yields

\[
tV_{\text{self}}(t) \leq t_0 V_{\text{self}}(t_0)
\]

\[
\leq C t_0 \|xG(-t_0)\Psi(\cdot, t_0)\|_X
\]

\[
\leq C t_0 \left[ -2t_0^2 V_{\text{coul}}(t_0) \right]^{1/2}
\]

for any \(t \in [t_0, t_1)\). Estimate (4.68) and the expressions (4.66), (4.69), (4.74) give the result

\[
C_p t^2 \|\Phi\|_X^{2/3} \left( \sum_{j=1}^{\infty} \lambda_j \|\psi_j(\cdot, t)\|_p^2 \right)^{2p/(3p-1)} \leq \|xG(-t)\Psi(\cdot, t)\|_X^2
\]

\[
= \left[ f(t) + 2t^2 V_{\text{self}}(t) \right] - 2t^2 [V_{\text{coul}}(t) + V_{\text{self}}(t)]
\]

\[
\leq f(t_0) + 2t_0^2 V_{\text{self}}(t_0) + \int_{t_0}^t 2s V_{\text{self}}(s) \, ds - 2t^2 V_{\text{coul}}(t)
\]

\[
\leq C t_0^2 \left[ -2t_0^2 V_{\text{coul}}(t_0) \right]^{1/2} + 2C(t - t_0) t_0 \left[ -2t_0^2 V_{\text{coul}}(t_0) \right]^{1/2} - 2t^2 V_{\text{coul}}(t).
\]

The second step required \(V_{\text{self}}(t) \geq 0\) and the last step used the fact that \(f(t_0) = 0\). Hence,

\[
\left( \sum_{j=1}^{\infty} \lambda_j \|\psi_j(\cdot, t)\|_p^2 \right)^{2p/(3p-1)} \leq C \left\{ \frac{t_0^2}{t} \left[ -2V_{\text{coul}}(t_0) \right]^{1/2} - V_{\text{coul}}(t) \right\}
\]

for \(t \in [t_0, t_1)\) which completes the last subcase of the last implication. \(\square\)

It is worth noting that only the \((ii) \Rightarrow (iii)\) implication required \(\alpha > 0\). In particular, both the equivalences \((i) \Leftrightarrow (iii)\) and \((ii) \Leftrightarrow (iv)\) remain true for any
4.6: Decay Estimates for the SP System

\( \alpha \in \mathbb{R} \). In the next section the decay estimates for the SP system are summarized for the case where \( E_{\alpha,\beta}(t) \to 0 \) as \( t \to \infty \).

4.6 Decay Estimates for the SP System

**Theorem 4.20** If \( \Phi \in \Xi \cap Z, \Psi \) is a solution of the SP system (3.15)-(3.16) and \( \alpha, \beta \) are chosen so that \( E_{\alpha,\beta}(t) > 0 \) for all \( t > 0 \), then the following decay estimates hold:

(i) \( \|V\|_r = O(t^{-\frac{1}{2}+\frac{3}{p}}), \ 3 < r < \infty \)

(ii) \( \|\nabla V\|_q = O(t^{-\frac{1}{2}+\frac{3}{p}}), \ 3/2 < q \leq \infty \)

(iii) \( \|\Delta V\|_p = |\alpha||n(\cdot, t)|_p = O(t^{-\frac{1}{2}+\frac{3}{p}}), \ 1 \leq p \leq 3 \)

(iv) \( \sum_{j=1}^{\infty} \lambda_j \|\psi_j(\cdot, t)\|_p^2 = O(t^{-\frac{1}{2}+\frac{3}{p}}), \ 2 \leq p \leq 6 \).

**Proof.** Let \( f(t) = 2t^2 E_{\alpha,\beta}(t) > 0 \) and use the pseudoconformal conservation law to make the estimate

\[
f(t) \leq 2t^2 E_{\alpha,\beta}(t_0) + \|zG(-t_0)\Psi(t_0)\|_X^2 + \int_{t_0}^{t} \frac{f(s)}{s} \, ds.
\]

From Gronwall's inequality, for any \( 0 < t_0 \leq t \),

\[
f(t) \leq \left(2t_0^2 E_{\alpha,\beta}(t_0) + \|zG(-t_0)\Psi(t_0)\|_X^2 \right) \frac{t}{t_0}
\]

and consequently

\[
E_{\alpha,\beta}(t) = O(t^{-1}). \quad (4.75)
\]

Substituting this dependence back into the pseudoconformal conservation law (theorem 4.14), gives

\[
\|zG(-t)\Psi(t)\|_X = O(t^{1/2}).
\]
Utilizing lemma 4.18 establishes
\[ \sum_{j=1}^{\infty} \lambda_j \| \psi_j (\cdot, t) \|^2_p \leq C_p \| \Phi \|_{\mathcal{X}}^{2p} \| x G(-t) \Psi (\cdot, t) \|_{\mathcal{X}}^{2(1-a)} t^{2(a-1)} \]

\[ = O(1) O\left( t^{1-a} \right) O\left( t^{2(a-1)} \right) \]

\[ = O\left( t^{a-1} \right) \]

\[ = O\left( t^{-\frac{3(p-1)}{2p}} \right) \]

for all \( 2 \leq p < 6 \). For the case \( p = 6 \), the \( L^6 \) estimate \( \| f \|_6 \leq C \| \nabla f \|_2 \) is required to convey
\[ \sum_{j=1}^{\infty} \lambda_j \| \psi_j \|^2_6 \leq C \sum_{j=1}^{\infty} \lambda_j \| \nabla \psi_j \|^2_2 = C \| \nabla \Psi \|_{\mathcal{X}}^2. \]

However, the conservation of energy implies \( \| \nabla \Psi \|_{\mathcal{X}}^2 = E_{\text{tot}} - E_{\alpha, \beta}(t) \) and the decay estimate (4.75) gives \( E_{\alpha, \beta}(t) = O(t^{-1}) \). This completes the proof of item (iv). Item (iii) is a direct consequence of item (iv) since the definition of \( n(t) \) reveals
\[ \| n(\cdot, t) \|_p \leq \sum_{j=1}^{\infty} \lambda_j \| | \psi_j (\cdot, t) | |^2_p \]

\[ = \sum_{j=1}^{\infty} \lambda_j \| \psi_j \|_{2p}^2 \]

\[ = O\left( t^{-\frac{3(p-1)}{2p}} \right) \]

for any \( 1 \leq p \leq 3 \).

Item (ii) is produced by applying lemma 3.22 which gives the estimate
\[ \| \nabla V(t) \|_q = \left\| \int \frac{\Delta V(y, t)}{|y - \cdot|^2} \, dy \right\|_q \leq C \| \Delta V(t) \|_p \]

provided \( p > 1 \), \( q^{-1} = p^{-1} - 1/3 > 0 \) and, from item (iii), \( p \leq 3 \). This gives the asymptotic behaviour
\[ \| \nabla V(t) \|_q \leq C \| \Delta V(t) \|_{\frac{3a}{3+a}} = O\left( t^{-\frac{2q-3}{3q}} \right) \]
for all \( q \in (3/2, \infty) \). The case \( q = \infty \) follows from the GN inequality (lemma 3.7) applied to \( \nabla V \). This gives the estimate

\[
\|\nabla V\|_p \leq C\|D^2 V\|_\infty \|\nabla V\|_q^{1-a}
\]

\[
= C\|n\|_r^a \|\nabla V\|_q^{1-a}
\]

where \( p^{-1} = (r^{-1} - 1/3)a + (1-a)q^{-1}, \) \( 1 \leq p, r \leq \infty \) and \( 0 \leq a \leq 1 \) provided \( 1 - 3/r \) is not a nonnegative integer. We have used the fact that, provided \( r > 3/2 \), the mixed second order partial derivatives \( D^2 V \) can be estimated in \( L^r(\mathbb{R}^3) \) by \( \|\Delta V\|_r = C\|n\|_r \). The desired estimate is furnished by taking \( p = \infty, q \to \infty \) and \( r \to 3^- \). With this choice \( 1 - 3/r \to 0 \), which is a nonnegative integer and therefore an exceptional case of the GN inequality. Therefore \( a \) is restricted to the range \( 0 < a < 1 \). However, for any value of \( a \) in this range, the choices of \( p, q \) give the estimate

\[
\|\nabla V(\cdot, t)\|_\infty \leq C\|n(\cdot, t)\|_3.
\]

Item (iii) with \( r = 3 \) yields

\[
\|\nabla V(\cdot, t)\|_\infty = O\left(t^{-1}\right).
\]

Item (i) is attained in a similar manner by using the estimate

\[
\|V(t)\|_r = \left\|\int \frac{\Delta V(y, t)}{|y - \cdot|} \, dy\right\|_r \leq C\|\Delta V(t)\|_p
\]

provided \( p > 1, r^{-1} = p^{-1} - 2/3 > 0 \) and, from item (iii), \( p \leq 3 \). In this case, the valid range of \( p \) is \( 1 < p < 3/2 \) and therefore

\[
\|V(t)\|_r \leq C\|\Delta V(t)\|_{3/2}^{1/2} = O\left(t^{-r/3}\right)
\]

for all \( r \in (3, \infty) \). The case \( r = \infty \) is reached through theorem 3.23 item (i) with \( p = \infty \) which states that \( V \in L^\infty([0, \infty); L^\infty) \). This fact along with item (iii) above for the case \( p = 3/2 \) give the result. □
4.6: Decay Estimates for the SP System

Table 4.1: A comparison of SP decay rates.

The asymptotic behaviour for $\beta = 0$ [37] (no external potential) are compared to the situation $\beta \neq 0$ where $\alpha, \beta$ are chosen to ensure that $E_{\alpha, \beta}(t) > 0$. The $\beta = 0$ case must have $\alpha > 0$.

The case $\alpha > 0$, $\beta = 0$, which is analysed in [37], is shown to behave as

$$
\|\nabla V\|_q = O\left(t^{-1+\frac{1}{q}}\right); \quad 2 \leq q \leq \infty.
$$

This is due to the fact that if $\alpha > 0$ and $\beta = 0$, then $E_{\alpha, \beta}(t) = O(t^{-1})$ allows one to conclude that

$$
\|\nabla V(., t)\|_2 = O(t^{-1/2}). \quad (4.76)
$$

If $\beta \neq 0$ one cannot infer the estimate (4.76). Hence the reported decrease in the strength for the decay estimates of theorem 4.20.

The results for the asymptotic behaviour are compared in table 4.1 with those obtained in [37] who analyse the case $\alpha > 0$, $\beta = 0$. These asymptotic behaviour results of the SP system are inherited by the corresponding WP system. Lifting
these results so as to obtain asymptotic behaviour for the WP system is the topic of the next section.

4.7 Decay Estimates for the WP System

This is the last section that deals with the topic of asymptotic behaviour. It is possible to strengthen the decay estimates listed here. However, this is typically accomplished by assuming more regularity in the initial conditions. Progress has been made in this direction for the SP system. The interested reader is referred to the work of Hayashi [35, 36].

To transfer the results of the previous section to the WP system recall that the solution of the WP system is given by

\[ z(r, s, t) = \sum_{j=1}^{\infty} \lambda_j \overline{\psi}_j(r, t)\psi_j(s, t). \]

In terms of the \( \{\psi_j\}_{j \in \mathbb{N}} \) we obtain the estimate

\[
\|z(\cdot, \cdot, t)\|_{L^p(\mathbb{R}^3 \times \mathbb{R}^3)} = \left\| \sum_{j=1}^{\infty} \lambda_j \overline{\psi}_j(\cdot, t)\psi_j(\cdot, t) \right\|_{L^p(\mathbb{R}^3 \times \mathbb{R}^3)} \\
\leq \sum_{j=1}^{\infty} \lambda_j \left( \int \int |\overline{\psi}_j(r, t)|^p |\psi_j(s, t)|^p \, dr \, ds \right)^{1/p} \\
= \sum_{j=1}^{\infty} \lambda_j \|\psi_j(\cdot, t)\|_{L^p}^2
\]

which allows the determination of the asymptotic behaviour of \( z \). This is stated as a proposition:

**Proposition 4.21** Under the assumptions of theorem 4.20,

\[
\|z(\cdot, \cdot, t)\|_{L^p(\mathbb{R}^3 \times \mathbb{R}^3)} = O \left( t^{-\frac{3}{2} + \frac{\gamma}{p}} \right), \quad 2 \leq p \leq 6.
\]
Proof. A simple application of item (iv) of theorem 4.20 to the expression (4.77) yields the result. □

As in chapter 3, the properties of the Wigner function can be lifted from those of \(z\) using the fact that \(\rho_w\) and \(z\) are connected through the relationship

\[
\rho_w(x, k, t) = \mathcal{F}^{-1}\mathcal{T}^{-1}z(r, s, t).
\]

Recall that the \(\mathcal{T}^{-1}\) denotes the coordinate transformation \((r, s) \to (x, \eta)\). In detail, one has the expression

\[
\rho_w(x, k, t) = \sum_{j=1}^{\infty} \lambda_j \int e^{2\pi ik \cdot \eta} \overline{\psi_j}(x + \eta/2, t) \psi_j(x - \eta/2, t) \, d\eta
\]

so that

\[
\|\rho_w(x, \cdot, t)\|_{L^p(\mathbb{R}^2_+)} \leq \sum_{j=1}^{\infty} \lambda_j \left\| \mathcal{F}_\eta \left[ \overline{\psi_j}(x + \eta/2, t) \psi_j(x - \eta/2, t) \right] (k) \right\|_{L^p(\mathbb{R}^2_+)}
\]

\[
\leq \sum_{j=1}^{\infty} \lambda_j \left\| \overline{\psi_j}(x + \eta/2, t) \psi_j(x - \eta/2, t) \right\|_{L^4(\mathbb{R}^2_+)}
\]

\[
= \sum_{j=1}^{\infty} \lambda_j \|\psi_j(\cdot, t)\|_{L^2(\mathbb{R}^2)}^2
\]

provided (by the Hausdorff-Young inequality) that \(q^{-1} + p^{-1} = 1, \ p \geq 2\). These estimates allow us to summarize the asymptotic behaviour of the WP system.

**Theorem 4.22** Under the assumptions of theorem 4.20 the solution \((\rho_w, n, V_{\text{eff}})\) of the WP system (3.1.a)-(3.1.e) has the following properties

(i) \(\|\rho_w(x, \cdot, t)\|_{L^p(\mathbb{R}^2_+)} = O(t^{-\frac{3}{2p}}), \ 3/2 \leq p \leq \infty\)

(ii) \(\|\Theta(V_{\text{eff}})\rho_w(\cdot, \cdot, t)\|_{L^2(\mathbb{R}^2_+ \times \mathbb{R}^2_+)} = O(t^{-\frac{1}{2}})\)

(iii) \(\|n(\cdot, t)\|_r = O(t^{-\frac{3}{2} + \frac{r}{2}}), \ 1 \leq r \leq 3\).

The effective potential \(V_{\text{eff}}\) is defined as \(V_{\text{eff}} = V + \beta V_0\) and \(V\) satisfies the properties of theorem 4.20.
4.7: Decay Estimates for the WP System

The asymptotic behaviour for $\beta = 0$ [37] (no external potential) are compared to the situation $\beta \neq 0$ where $\alpha, \beta$ are chosen to ensure that $E_{\alpha, \beta}(t) > 0$. The $\beta = 0$ case must have $\alpha > 0$.

**Proof.** Item (iii) is a restatement of theorem 4.20 item (iii). Item (i) is a result of item (iv) in theorem 4.20 applied to the expression (4.78). This leaves item (ii). As in chapter 3, consider the auxiliary estimate

$$
\|V_{\text{eff}}(\cdot, t)z(\cdot, t)\|_{L^2(\mathbb{R}^3 \times \mathbb{R}^3)}^2 = \int \int \sum_{j=1}^{\infty} \left( \frac{\beta}{4\pi|\tau|} + V(r, t) \right) \overline{\psi_j}(r, t)\psi_j(s, t) \, dr \, ds
$$

$$
\leq \int \sum_{j=1}^{\infty} \lambda_j \left( \frac{\beta}{4\pi|\tau|} + V(r, t) \right) \overline{\psi_j}(r, t) \right|^2 \, dr
\times \int \sum_{j=1}^{\infty} \lambda_j |\psi_j(s, t)|^2 \, ds
\leq \left( C\|\nabla\psi(\cdot, t)\|_X^2 + \|V(\cdot, t)\|_\infty\|\psi(\cdot, t)\|_X^2 \right) \|\psi(\cdot, t)\|_X^2
= \left[ O(t^{-1}) + O(t^{-1}) \right] O(1)
= O(t^{-1}).
$$

However, under the Fourier transform,

$$
\|\Theta(V_{\text{eff}})\rho_w\|_{L^1(\mathbb{R}^3 \times \mathbb{R}^3)} = \|[V_{\text{eff}}(\cdot, t) - V_{\text{eff}}(\cdot, t)]z(\cdot, t)\|_{L^2(\mathbb{R}^3 \times \mathbb{R}^3)} = O(t^{-1/2})
$$

which completes the proof. □
4.7: Decay Estimates for the WP System

It is informative to compare the decay estimates with those obtained in [37] which considers the case \( \alpha > 0, \beta = 0 \). Table 4.2 compares the decay properties of the WP system (3.15)–(3.17) to the corresponding problem without an external potential \( (\beta = 0) \). The results of this latter case originate with the paper by Illner, Lange and Zweifel [37].
Chapter 5

Discussion & Conclusions

The analysis of the Wigner–Poisson (WP) system with the addition of an external Coulomb potential was broken into two separate problems. The question of existence and uniqueness of solutions was examined in the first half of the dissertation while the second half was concerned with the asymptotic behaviour of admissible solutions. In both cases, a transformation was introduced that reduces the WP system to the problem of analyzing a countably infinite set of coupled Schrödinger equations. This reduced set of equations is referred to as the Schrödinger–Poisson (SP) system.

The question of existence and uniqueness for the WP system without an external potential has been previously analyzed [10, 14, 37]. It was found that there exists a unique global solution independent of whether or not the particles attract each other. These results are obtained by first proving the existence of a unique solution for the corresponding SP problem.

By specifying that the initial sequence of wave functions is sufficiently regular ($\Phi(z) \in Z$) it was found that there exists a unique global solution to the SP problem with an external potential. The proof does not depend on whether or not the Coulomb field is attractive or repulsive in nature. Consequently, there exists a unique global solution to the WP problem if the initial Wigner function is taken to
be a valid Wigner distribution and is sufficiently regular \( \rho_{\text{w},t} \in L^2(\mathbb{R}_x^3 \times \mathbb{R}_k^3) \). Some of the techniques used in this dissertation were used to extend the regularity results for the case without an external field. With these extensions, there is seen to be a slight loss in the regularity of both the SP and WP problems with the addition of an external potential.

These results were arrived at by reducing the WP problem to the SP problem and then stating the SP problem as an abstract Cauchy problem where the external potential was treated as part of the unperturbed evolution operator. The perturbed portion of the evolution operator was taken to be the self-consistent potential. It is shown, with the use of the Kato–Rellich theorem, that the unperturbed operator is self-adjoint on the space \( X \). The fact that the unperturbed operator has a spectrum that is bounded from below is used to establish a norm equivalence argument which is itself used to extend the operator to the space \( Y \). Moreover, the self-adjointness property generates a \( C_0 \) group of operators on the Hilbert space \( Y \). Existence of a unique local solution then depends upon whether or not the perturbed portion of the operator (the self-consistent potential) is locally Lipschitz on the space \( Y \). Illustration of this fact follows directly from the arguments found in [37]. A contractive mapping argument is then used to show that there exists a unique local solution \( \Psi \in C([0,T);Y) \). The solution is then shown to be global \( (T = \infty) \) through the use of the probability and energy conservation laws. Since \( Y \) is a reflexive Banach space, the Lipschitz continuity is enough to allow one to conclude that if \( \Phi \in Z \) then \( \Psi \in C^1([0,\infty);X) \). Other regularity properties of the solution are then found by using various Sobolev estimates together with the conservation laws. These results are then lifted back to the WP problem where it is shown, provided \( \rho_{\text{w},t} \in L^2(\mathbb{R}_x^3 \times \mathbb{R}_k^3) \), there exists a unique global solution \( \rho_{\text{w}} \in C([0,\infty);L^2(\mathbb{R}_x^3 \times \mathbb{R}_k^3)) \). By further restricting the regularity of the initial Wigner function to \( \rho_{\text{w},t} \in H^2(\mathbb{R}_x^3 \times \mathbb{R}_k^3) \), it is
proved that \( \| k \cdot \nabla z \psi \|_{L^2(\mathbb{R}^3 \times \mathbb{R}^2)} \) remains exponentially bounded.

From this point forward, the asymptotic behaviour of the solutions is considered. Ginibre and Velo [26, 27] pioneered the use of the pseudoconformal conservation law as a technique for exhibiting the asymptotic temporal behaviour for nonlinear Schrödinger equations. This technique was used by Dias and Figueira [18, 19] to illustrate how an external Coulomb potential can be regularized to obtain this pseudoconformal law for all values of the regularization parameter. By using the regularity properties of existence proof together with a weak compactness argument, the regularization parameter can then be removed. Illner, Lange and Zweifel [37] consider the WP problem and the corresponding SP problem in the case of no external field. They showed that if the particles repel each other then the solution will decay in time. Chadam and Glassey [14] illustrated that if the total energy is negative then the solution will not decay in the sense of \( L^\infty \).

In this dissertation, it was shown that if the configurational energy is positive definite, then the configurational energy must decay as \( E_{\alpha, \beta} = O(t^{-1}) \). The decay results of [37] are a special case of this condition. By generalizing an argument of Dias and Figueira [19], it is shown that this condition is equivalent to having the solution decay in \( L^p \) for the range \( 2 < p < 6 \). The nonexistence result of [14] is also generalized. If the total energy of the SP system is negative then the solution cannot decay in the sense of \( L^p \) for any \( 2 < p \leq \infty \). Decay estimates for the SP problem are exhibited in those situations were it is guaranteed that the solution decays. Alternatively, if the configurational energy is positive for all time, \( E_{\alpha, \beta} = O(t^{-1}) \), \( 2 \leq p \leq 6 \).

In the case where the SP problem decays, results for the decay behaviour of the WP system were calculated. That is, \( \| \rho_u(x, \cdot, t) \|_{L^p(\mathbb{R}^3)} = O(t^{-\frac{1}{3}}) \), \( 3/2 \leq p \leq \infty \).
Most of these results are a consequence of repeated applications of the pseudoconformal conservation law. The negative energy result is produced by a generalization of the Sobolev estimates used by Chadam and Glassey [14] with the regularity properties that were derived in the proof of existence an uniqueness. The equivalent characterization of solutions that decay in $L^p$ for $2 < p < 6$ to other notions of asymptotic decay is essentially variations of the work of Dias and Figueira [19]. Only one of the inferences in this proof involves the attractive or repulsive nature of the particle interactions. Decay estimates for the SP system are obtained in essentially the same manner as in [37] where the condition that the particles repel each other is replaced by the condition that the configurational energy remain positive for all times. These two conditions are equivalent in the case without an external field. Decays results for the WP system were calculated as in [37] by using the isometry properties of the Fourier transform on $L^2$ as well as various Sobolev estimates.
Bibliography


Appendix A

Notation and Definitions

This appendix starts with the definition of some sequence spaces. The Banach space consisting of complex valued sequences $a = \{a_n\}_{n \in \mathbb{N}}$ such that $|a_n|^p$ is summable for $1 \leq p < \infty$ is denoted by $l^p$. For the case $p = \infty$, the corresponding condition is $\sup\{|a_n| : n \in \mathbb{N}\} < \infty$. The norm is written as

$$\|a\|_p = \left\{ \begin{array}{ll}
\left( \sum_{n=1}^{\infty} |a_n|^p \right)^{1/p} & 1 \leq p < \infty, \\
\sup_{n \in \mathbb{N}} |a_n| & p = \infty.
\end{array} \right.$$ 

The sets $l^p \subset l^\infty$.

The Banach spaces $L^p$ can similarly be defined. $L^p(\mathbb{R}^d)$ ($1 \leq p \leq \infty$) denotes the Banach space consisting of complex valued measurable functions $u = u(x)$ on $\mathbb{R}^d$ such that $|u|^p$ is integrable for $1 \leq p < \infty$. For $p = \infty$, the condition is: $^1 \text{ess sup}\{|u(x)| : x \in \mathbb{R}^d\} < \infty$. The norm is written as

$$\|u\|_p = \left\{ \begin{array}{ll}
\left( \int_{\mathbb{R}^d} |u(x)|^p \, dx \right)^{1/p} & 1 \leq p < \infty, \\
\text{ess sup}\{|u(x)| : x \in \mathbb{R}^d\} & p = \infty.
\end{array} \right.$$ 

The space $l^p = L^p(\mathbb{R}, d\mu)$, where $\mu$ is the measure with mass one at each positive integer and zero everywhere else. Many of the standard facts and properties of the

---

$^1$ This is the sup\{|u(x)| : x \in \mathbb{R}^d\}, except for some set or measure zero.
IP and \( l^p \) spaces are collected in appendix B.

Let \( \Omega \) be a fixed domain in \( \mathbb{R}^d \) and denote by \( C^m(\Omega) \) the set of all \( m \)-times continuously differentiable complex valued functions on \( \Omega \). \( C^m_0(\Omega) \) denotes the subspace of \( C^m(\Omega) \) consisting of those functions with compact support in \( \Omega \). In a similar fashion, \( C(I; B) \) denotes the space of \( B \)-valued continuous functions on \( I \) for any interval \( I \in \mathbb{R} \) and any Banach space \( B \) with the norm \( \| \cdot \|_B \). Furthermore, \( C^k(I; B) \) is the space of \( k \)-times continuously differentiable functions from \( I \) to \( B \).

Let \( n \) be a positive integer, \( n \in \mathbb{N} \). We define \( \alpha \) to be a multi-index if \( \alpha = (\alpha_1, \alpha_2, \ldots, \alpha_n) \in \{ \mathbb{N} \cup \{0\} \}^n \). Moreover, derivatives are denoted as \( D^\alpha = \partial_1^{\alpha_1} \cdots \partial_n^{\alpha_n} \), where \( \partial_j = \partial/\partial x_j \) (\( j = 1, 2, \ldots, n \)). For \( u \in C^m(\Omega) \) and \( 1 \leq p < \infty \), a norm for \( u \) is defined by the expression

\[
\|u\|_{m,p} = \left( \int_\Omega \left( \sum_{|\alpha| \leq m} |D^\alpha u|^p \, dx \right)^{1/p} \right),
\]

where \( |\alpha| = \alpha_1 + \alpha_2 + \ldots + \alpha_n \). If \( p = 2 \) and \( u, v \in C^m(\Omega) \) this norm generates an inner product defined by

\[
(u, v)_m = \int_\Omega \sum_{|\alpha| \leq m} D^\alpha u \overline{D^\alpha v} \, dx
\]

with the Reed–Simon convention [55] that the inner product is linear in the second index. In the special case, \( m = 0 \), the inner product will not carry a subscript, i.e. \( (u, v) := (u, v)_0 \). Taking \( \tilde{C}^m_p(\Omega) \) to be the subset of \( C^m(\Omega) \) consisting of those functions \( u \) for which \( \|u\|_{m,p} < \infty \), the spaces \( W^{m,p}(\Omega) \) and \( W^{m,p}_0(\Omega) \) denote the completion in the norm \( \| \cdot \|_{m,p} \) of \( \tilde{C}^m_p(\Omega) \) and \( \tilde{C}^m_0(\Omega) \) respectively. For the case \( p = 2 \), the Hilbert space \( W^{m,2}(\Omega) \) is denoted by \( H^m(\Omega) \).

There is another characterization of the Hilbert spaces \( H^m(\Omega) \). However, it requires a definition of the Fourier transform. For \( f : \mathbb{R}^d \to \mathbb{C} \), \( \hat{f} = \mathcal{F}f \) and \( \hat{f} = \mathcal{F}^{-1}f \) denote the Fourier transform and the inverse Fourier transform of \( f \).
respectively. Normalization is defined via the expressions

\[ \begin{align*}
    \hat{f}(\xi) &= \frac{1}{(2\pi)^{s/2}} \int_{\mathbb{R}^s} e^{-ix \cdot \xi} f(x) \, dx \\
    \hat{f}(x) &= \frac{1}{(2\pi)^{s/2}} \int_{\mathbb{R}^s} e^{ix \cdot \xi} f(\xi) \, d\xi.
\end{align*} \]

Parseval's relation \( \|D^\alpha u\|_2 = \|\xi_1^{\alpha_1} \cdots \xi_s^{\alpha_s} \hat{u}(\xi)\|_2 \) yields

\[ \|u\|^2_{m,2} = \frac{1}{(2\pi)^{s/2}} \int_{\Omega} \left( \sum_{|\alpha| \leq m} \xi_1^{2\alpha_1} \cdots \xi_s^{2\alpha_s} \right) |\hat{u}(\xi)|^2 \, d\xi. \]

However, one may find constants \( C_1, C_2, \) independent of the value of \( \xi \) such that [41]

\[ \frac{1}{C_1} (1 + |\xi|^2)^m \leq \sum_{|\alpha| \leq m} \xi_1^{2\alpha_1} \cdots \xi_s^{2\alpha_s} \leq C_2 (1 + |\xi|^2)^m, \quad \xi \in \mathbb{R}^s. \]

Therefore \( u \in H^m(\Omega) \) if and only if \( (1 + |\xi|^2)^{m/2} \hat{u}(\xi) \in L^2(\Omega). \)
Appendix B

Some Classical Analysis

The purpose of this appendix is to present some of the basic topological results for the $l^p$ and $L^p$ spaces. Supplementary material can be found in the book by Weidmann [66] or any text on Lebesgue integration theory, for example the books by W. Rudin [57, 58]. The elements of the Banach spaces $l^p$ and $L^p$ satisfy a number of fundamental inequalities. These results are presented first, as they are used to obtain many of the estimates in this dissertation.

B.1 Useful Inequalities

The following standard results from $l^p, L^p$ theory are used throughout the work. One can find most of the proofs in Reed & Simon [56] or the book by Rudin [57]. Inequalities that deal with the sequence spaces $l^p$ are presented first.

Proposition B.1 (Cauchy–Schwarz–Bunyakowski inequality). If $s = \{s_j\}_{j \in \mathbb{N}}$ and $t = \{t_j\}_{j \in \mathbb{N}}$ are in $l^2$ then $\sum_{j=1}^{\infty} s_j t_j$ is absolutely convergent and

$$\left| \sum_{j=1}^{\infty} s_j t_j \right| \leq \left( \sum_{j=1}^{\infty} s_j^2 \right)^{1/2} \left( \sum_{j=1}^{\infty} t_j^2 \right)^{1/2}$$

with equality if and only if the sequences are proportional. That is, there exist numbers $\alpha, \beta$ such that $\alpha s_j = \beta t_j$ for all $j \in \mathbb{N}$. 
Proposition B.2 (Minkowski’s inequality). If \( f, g \in L^p \) with \( 1 \leq p \leq \infty \) then
\[
\|f + g\|_p \leq \|f\|_p + \|g\|_p.
\]
Equality holds if and only if the sequences \( f \) and \( g \) are proportional.

Proposition B.3 (Hölder’s inequality). Let \( f = \{f_j\}_{j \in \mathbb{N}} \in L^p \) and \( g = \{g_j\}_{j \in \mathbb{N}} \in L^q \) where \( 1 \leq p \leq \infty \) and \( 1 \leq q \leq \infty \). If \( p^{-1} + q^{-1} = r^{-1} \) and \( 1 \leq r \leq \infty \) then the product \( fg = \{f_j g_j\}_{j \in \mathbb{N}} \in L^r \) and
\[
\|fg\|_r \leq \|f\|_p \|g\|_q
\]
with equality if and only if there exist positive constants \( \alpha, \beta \) such that \( \alpha |f_j|^p = \beta |g_j|^q \) for all \( j \in \mathbb{N} \).

The rest of the inequalities deal directly with the \( L^p \) spaces defined in appendix A. Many of the fundamental properties have been consolidated into a single proposition.

Proposition B.4
(i) (Duality). If \( 1 \leq p < \infty \) then the dual space of \( L^p \) denoted by \( (L^p)^* \) can be identified with \( L^q \) where \( p^{-1} + q^{-1} = 1 \).
(ii) (Minkowski’s inequality). If \( f, g \in L^p \) with \( 1 \leq p \leq \infty \) then
\[
\|f + g\|_p \leq \|f\|_p + \|g\|_p.
\]
The equality holds if and only if \( f(x) = kg(x) \) a.e.\(^1\) for some real \( k \geq 0 \).
(iii) (Hölder’s inequality). Let \( p, q \) and \( r \) be positive numbers satisfying \( p, q, r \geq 1 \) and \( p^{-1} + q^{-1} = r^{-1} \). If \( f \in L^p \) and \( g \in L^q \) then the product \( fg \in L^r \) and
\[
\|fg\|_r \leq \|f\|_p \|g\|_q
\]
\(^1\) The term “almost everywhere” and typically denoted as a.e., is commonly used to designate the phrase: “except for a set whose measure is zero.”
with equality if and only if $|\alpha f(x)|^p = |\beta g(x)|^q$ a.e. with $\alpha, \beta$ positive constants.

(iv) If $0 < \lambda < 1$ and $p, q, r$ are positive numbers satisfying $p, q, r \geq 1, \ r^{-1} = \lambda p^{-1} + (1 - \lambda)q^{-1}$ then $L^p \cap L^q \subset L^r$ and $^2$

$$\|f\|_r \leq \|f\|_p^\lambda \|f\|_q^{1-\lambda}.$$  

(v) (The Hausdorff-Young inequality). Let $f \in L^p$ where $1 \leq p \leq 2$ with $p^{-1} + q^{-1} = 1$ then the Fourier transform is a bounded map from $L^p(\mathbb{R}^d)$ to $L^q(\mathbb{R}^d)$ with

$$\|\hat{f}\|_q \leq (2\pi)^{s/2-s/p}\|f\|_p.$$  

(vi) (Young's inequality). Let $f \in L^p$ and $g \in L^q$ where $1 \leq p \leq \infty$ and $1 \leq q \leq \infty$. If $p^{-1} + q^{-1} = 1 + r^{-1}$ and $1 \leq r \leq \infty$ then the convolution of $f$ an $g$ denoted by $f \ast g$ is an element of $L^r$ and

$$\|f \ast g\|_r \leq \|f\|_p \|g\|_q.$$  

(vii) (The Riesz-Thorin interpolation theorem). Let $p_0, p_1, q_0, q_1 \in [1, \infty]$ and let $T$ be a linear transform from $L^{p_0} \cap L^{p_1}$ to $L^{q_0} \cap L^{q_1}$ which satisfies

$$\|Tf\|_{q_i} \leq M_i\|f\|_{p_i}$$

for all $f$ and $i = 0, 1$. Then for each $f \in L^{p_0} \cap L^{p_1}$ and $0 < t < 1$, $Tf \in L^q$ and

$$\|Tf\|_q \leq M_1^tM_0^{1-t}\|f\|_p$$

where

$$p^{-1} = tp_1^{-1} + (1-t)p_0^{-1}, \quad q^{-1} = tq_1^{-1} + (1-t)q_0^{-1}.$$  

$^2$ The proof of this result can be found in Folland [23] p. 177 or derived directly from item (iii).
B.2 Properties of the Fourier Transform

The Fourier transform, when it exists, is typically defined as the operation

$$\hat{f}(\xi) = \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} e^{-ix \cdot \xi} f(x) \, dx.$$  

As a starting point, define the space $M_0(\mathbb{R}^n)$ as the set of all functions $f(\mathbb{R}^n)$ such that there exists some $\varphi \in C_0^\infty(\mathbb{R}^n)$ with $\hat{\varphi} = f$. This definition implies that provided $f \in M_0(\mathbb{R}^n)$, it can be written as

$$f(x) = \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} e^{-ix \cdot \xi} \varphi(\xi) \, d\xi, \quad \varphi \in C_0^\infty(\mathbb{R}^n).$$

Because $\varphi$ has compact support, differentiation under the integral sign is well defined and yields the expression

$$D^\nu f(x) = \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} (-i\xi_1)^{\nu_1} \ldots (-i\xi_n)^{\nu_n} e^{-i\xi \cdot x} \varphi(\xi) \, d\xi.$$  

Also, for $f \in M_0(\mathbb{R}^n)$, the Fourier transform is defined to be

$$\hat{f}(\xi) = \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} e^{ix \cdot \xi} f(x) \, dx = \varphi(\xi), \quad \xi \in \mathbb{R}^n.$$  

For any $f, g \in M_0(\mathbb{R}^n)$ the following properties of the Fourier transform, stated without proof, must hold.

**Proposition B.5**

(i) For any $f, g \in M_0(\mathbb{R}^n)$, $(f * g)(\xi) = (2\pi)^{n/2} \hat{f}(\xi) \hat{g}(\xi)$.

(ii) If $f(x) = (2m)^{-s/2} e^{-|x|^2/4m}$ then $\hat{f}(\xi) = e^{-m|\xi|^2}$.

(iii) For any $f, g \in M_0(\mathbb{R}^n)$,

$$\int_{\mathbb{R}^n} \hat{f}(x) g(x) \, dx = \int_{\mathbb{R}^n} f(x) \hat{g}(x) \, dx.$$  

(iv) For each $y \in \mathbb{R}^d$, 

$$f(y) = \lim_{m \to \infty} \left( \frac{m}{\pi} \right)^{d/2} \int_{\mathbb{R}^d} e^{-m|z-y|^2} f(z) \, dz.$$ 

(v) (Parseval's relation). For any $f \in M_0(\mathbb{R}^d)$, $\|f\|_2 = \|\hat{f}\|_2$.

Extending these properties to the space $L^2(\mathbb{R}^d)$ is accomplished in the following manner. First, one shows that $M_0$ is dense in $L^2$ so that $f \to \hat{f}$ is a densely defined bounded linear operator from $M_0 \subset L^2 \to L^2$. The Fourier transform $\hat{f} \in L^2$ for any $f \in L^2$ is obtained by continuous extension. With this extension, items (i) through (v) above become valid for all of $L^2(\mathbb{R}^d)$. The final section of this appendix details the first step of this extension, showing that $C^\infty_0(\mathbb{R}^d)$ is dense in $L^2(\mathbb{R}^d)$.

B.3 Results from Classical Analysis

Starting with some fundamental definitions, let $A$ and $B$ be subsets of a normed Hilbert space $\mathcal{H}$. The set $A$ is said to be dense relative to $B$ if $B \subset \overline{A}$ holds. If $A \subset B$, then $A$ is said to be a dense subset of $B$ or, $A$ is dense in $B$. If $A$ is dense relative to $\mathcal{H}$, then it is said that $A$ is dense.

Lemma B.6 If $A_1$ is dense relative to $A_2$ and $A_2$ is dense relative to $A_3$ then $A_1$ is dense relative to $A_3$.

Proof. $A_2 \subset \overline{A}_1$ and $A_3 \subset \overline{A}_2$ is given therefore, $A_3 \subset \overline{A}_2 \subset \overline{A}_1 = \overline{A}_1$. □

Lemma B.6 shows that by choosing an intermediary space in a judicious fashion, one may prove that a particular set is dense in another. Consider the subspace $L^2_0$ of $L^2$, defined on some measurable subset $M$ of $\mathbb{R}^d$, as

$$L^2_0(M) := \{ f \in L^2(M) : \text{there exists a } K > 0 \text{ such that} \]

$$|f(x)| \leq K \text{ a.e. } \in M, 
\text{and } f(x) = 0 \text{ a.e. } \in \{ x \in M : |x| > K \} \}.$$
Theorem B.7 $L^2_0(M)$ is dense in $L^2(M)$. 

Proof. Let $f \in L^2(M)$ and for all $n \in \mathbb{N}$, let 

$$f_n(x) = \begin{cases} 
  f(x) & \text{if } |x| \leq n \text{ and } |f(x)| \leq n \\
  0 & \text{otherwise.} 
\end{cases}$$

With this construction, each of the $f_n(x) \in L^2_0(M)$ and $|f_n(x)| \leq |f(x)|$ for all $n \in \mathbb{N}$ and for all $x \in M$. Also, for any fixed value of $x$, choosing $n$ such that $n > \max\{|x|, |f(x)|\}$, shows that $|f_n(x) - f(x)| = 0$. i.e. $f_n(x) \to f(x)$ as $n \to \infty$. Therefore, by Lebesgue's dominated convergence theorem,

$$\|f_n - f\|^2 = \int_M |f_n - f|^2 \, dx \to 0$$

as $n \to \infty$. Hence, $f_n \to f$. \qed

An interval in $\mathbb{R}^d$ is defined as a subset $\mathcal{J}$ of $\mathbb{R}^d$ of the form 

$$\mathcal{J} = \{x = (x_1, \ldots, x_s) \in \mathbb{R}^d : a_j \leq x_j < b_j, \ j = 1, 2, \ldots, s\}$$

with $a_j, b_j \in \mathbb{R}$ and any combination of the signs $<$ and $\leq$ are permitted. A function $f : \mathbb{R}^d \to \mathbb{C}$ is called a step function if there are finitely many intervals $\mathcal{J}_1, \ldots, \mathcal{J}_n$ and complex numbers $c_1, \ldots, c_n$ such that

$$f(x) = \sum_{j=1}^{n} c_j \chi_{\mathcal{J}_j}(x)$$

where $\chi_A(x)$ denotes the characteristic function of the set $A$.

Theorem B.8 The set $T(\mathbb{R}^d)$ of step functions on $\mathbb{R}^d$ is a dense subspace of $L^2(\mathbb{R}^d)$.

Proof. $T(\mathbb{R}^d)$ is obviously a vector space and moreover, $T(\mathbb{R}^d) \subset L^2_0(\mathbb{R}^d)$. Therefore, by theorem B.7, it is sufficient to show that $T(\mathbb{R}^d)$ is dense in $L^2_0(\mathbb{R}^d)$. Choose a function $f \in L^2_0(\mathbb{R}^d)$ so that $f$ is integrable and there exists a sequence of functions $f^n$
\{f_j\}_{j=1}^\infty$ from $T(\mathbb{R}^*)$ such that $f_j(x) \to f(x)$ a.e. in $\mathbb{R}^*$. Moreover,

$$\int_{\mathbb{R}^*} |f_j(x) - f(x)| \, dx \to 0$$

as $j \to \infty$. If, for $K \geq 0$, $f$ satisfies the condition $|f(x)| \leq K$ a.e., then it may assumed that $|f_n(x)| \leq K$ for all $x \in \mathbb{R}^*$, and for all $n \in \mathbb{N}$. Hence,

$$\|f_n - f\|^2 = \int_{\mathbb{R}^*} |f_n(x) - f(x)|^2 \, dx \leq \int_{\mathbb{R}^*} (|f_n(x)| + |f(x)|)|f_n(x) - f(x)| \, dx \leq 2K \int_{\mathbb{R}^*} |f_n(x) - f(x)| \, dx \to 0$$

as $n \to \infty$. In other words, $f_n \to f$. \qed

**Theorem B.9** The set of infinitely differentiable functions with compact support $C_0^\infty(\mathbb{R}^*)$ is a dense subspace of $L^2(\mathbb{R}^*)$.

**Proof.** Theorem B.8 indicates that it is enough to show that $C_0^\infty(\mathbb{R}^*)$ is dense relative to $T(\mathbb{R}^*)$. This can be accomplished if it can be shown that for every interval $J$ the characteristic function $\chi_J$ is in the closure of $C_0^\infty(\mathbb{R}^*)$. In other words, it must be shown that the characteristic function of any interval $J$ can be approximated arbitrarily well by some function in $C_0^\infty(\mathbb{R}^*)$. Define for any $\epsilon > 0$, the function $\delta_\epsilon : \mathbb{R}^* \to [0, \infty)$ by

$$\delta_\epsilon(x) = \left[\int_{\mathbb{R}^*} \tilde{\delta}_\epsilon(x) \, dx\right]^{-1} \tilde{\delta}_\epsilon(x)$$

where

$$\tilde{\delta}_\epsilon(x) = \begin{cases} \exp\left(\frac{1}{|x|^2 - \epsilon^2}\right) & \text{for } |x| < \epsilon \\ 0 & \text{for } |x| \geq \epsilon. \end{cases}$$

For $s = 1$ and $j \geq 1$, the $j^{th}$ derivative of $\delta_\epsilon$ is

$$\frac{d^j}{dx^j} \delta_\epsilon(x) = \begin{cases} \frac{P_{3j-2}(x)}{(|x|^2 - \epsilon^2)^{3j/2}} \exp\left(\frac{1}{|x|^2 - \epsilon^2}\right) & \text{for } |x| < \epsilon \\ 0 & \text{for } |x| \geq \epsilon, \end{cases}$$
where \( P_{3j-2}(x) \) is a polynomial of degree \( 3j - 2 \) with the property

\[
\lim_{|x| \to \epsilon} P_{3j-2}(x) = (-2\epsilon)^j.
\]

For \( s = 1 \), \( \delta_s \in C_0^\infty(\mathbb{R}) \) and the support of \( \delta_s \) is \( \{ x \in \mathbb{R} : |x| \leq \epsilon \} \). The argument for a general integer \( s > 1 \) is similar. Take some interval \( J \in \mathbb{R}^s \) and for \( n \in \mathbb{N} \), let \( f_n(x) \) be the convolution of \( \delta_{1/n} \) with \( \chi_J \) so that

\[
f_n(x) = \int_{\mathbb{R}^s} \delta_{1/n}(x-y)\chi_J(y) \, dy, \quad x \in \mathbb{R}^s,
\]

The fact that \( \delta_{1/n} \in C_0^\infty(\mathbb{R}^s) \) implies that \( f_n \in C_0^\infty(\mathbb{R}^s) \). Furthermore, if \( x \in \mathbb{R}^s \) is chosen so that the support of \( \delta_{1/n}(x) = [|x| - 1/n, |x| + 1/n] \) does not overlap any portion of the interval \( J \) then \( f_n(x) = 0 \). In a similar fashion, if \( x \in \mathbb{R}^s \) is chosen so that the support of \( \delta_{1/n}(x) \) lies entirely within \( J \) then \( f_n(x) = 1 \). The case where \( J \) is the interval \([-1,1]\) and \( n = 3 \) is depicted in figure B.2. Therefore, for any
value of $x$ that does not lie on the boundary of $\mathcal{J}$, we have $f_n(x) \to \chi_{\mathcal{J}}(x)$. That is, $f_n(x) \to \chi_{\mathcal{J}}(x)$ almost everywhere. By the Lebesgue dominated convergence theorem it follows that

$$\|f_n - \chi_{\mathcal{J}}\|^2 = \int_{\mathbb{R}^d} |f_n(x) - \chi_{\mathcal{J}}(x)|^2 \, dx \to 0$$

or $f_n \to \chi_{\mathcal{J}}$ in the sense of $L^2(\mathbb{R}^d)$. □
Appendix C

Additional Proofs

**Theorem C.1 (General Gronwall inequality)** Let three piecewise continuous non-negative functions, \( h, g \) and \( m \) be defined in the interval \([s,T]\) and satisfy the inequality
\[
m(t) \leq h(t) + \int_{s}^{t} g(r)m(r) \, dr,
\]
except at points of discontinuity of the functions. Then, except at these same points,
\[
m(t) \leq h(t) + \int_{s}^{t} g(r)h(r)e^{\int_{s}^{r} g(u) \, du} \, dr.
\]

**Proof.** It is sufficient to establish the theorem for strictly continuous functions since it would then be true for each piece of the piecewise continuous functions.

The proof is an immediate consequence of the fact that the solution of the linear inhomogeneous equation
\[
\frac{dm}{dt} = g(t)m + h'(t), \quad m(s) = h(s)
\]
has the form
\[
m(t) = h(t) + \int_{s}^{t} g(r) e^{\int_{s}^{r} g(u) \, du} h(r) \, dr.
\]
The result follows from the positivity of the kernel
\[
g(r)e^{\int_{s}^{r} g(u) \, du}. \quad \Box
\]
Theorem C.2 Let $Y$ be a reflexive Banach space. If $J : \mathbb{R} \to Y$ is Lipschitz continuous with respect to $t$, then $J$ is differentiable with respect to $t$ a.e. and

$$J' \in L^1((0,t_{\text{max}});Y).$$

Proof. Define

$$f(t) := \langle \varphi, J(t) \rangle \quad \forall \varphi \in Y^*$$

which ensures [20] that $^1 f \in L^1_{\text{loc}}$. For each $t$, the map $\varphi \to \langle \varphi, J(t) \rangle'$ which takes elements of $Y$ into $\mathbb{R}$ is a bounded linear operator on $Y^*$. The linearity follows from the linearity of $\langle \cdot, \cdot \rangle$ and the boundedness follows from the estimate

$$\left| \frac{d}{dt} \langle \varphi, J(t) \rangle \right| = \left| \lim_{\delta \to 0} \left\langle \varphi, \frac{J(t + \delta) - J(t)}{\delta} \right\rangle \right| \leq \|\varphi\|_{Y^*}C.$$

The constant is the Lipschitz bound of $J$. From the definition of $Y^{**}$, this implies that there exists some $\phi : \mathbb{R} \to Y^{**}$ with the property that

$$\langle \phi(t), \varphi \rangle = \frac{d}{dt} \langle \varphi, J(t) \rangle$$

a.e. $t$. Since $Y$ is reflexive, $\phi \in Y = Y^{**}$. $\square$

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$^1 L^1_{\text{loc}} = \{ f : f\varphi \in L^1 \ \forall \varphi \in C^0_{\text{loc}} \}$. 

C: Additional Proofs 166
Appendix D

A Dirac Notation Primer

D.1 Dirac Formulation

The three most popular formulations of quantum theory are Schrödinger's wave mechanics, Heisenberg's matrix mechanics, and Dirac's abstract vector space method. While these descriptions are all equivalent, Dirac's method is more compact and more general than the first two. We will restrict ourselves to a one-particle system; the generalization to a many-particle system is straightforward. Throughout the material described in this appendix, \( m \) denotes the (positive) mass of a particle and \( \hbar \) is an empirical real valued constant.

In the Schrödinger formalism, the state of a system at time \( t \) is described by a wave function, \( \psi(x,t) : \mathbb{R}^3 \times \mathbb{R} \rightarrow \mathbb{C} \) and its complex conjugate \( \psi^*(x,t) \) while the dynamical variables are given by differential operators (position) \( x \), (momentum) \(-i\hbar \nabla_x\), or any function of the position and momentum \( A(x, -i\hbar \nabla_x) \) which act on the wave function. A typical example is the energy operator\(^1\)

\[
H = -\frac{\hbar^2}{2m} \Delta + V(x)
\]

where \( V(x) \) is some real valued potential energy. One constructs the wave function

---

\(^{1}\) This appendix makes systematic use of capitals for operators and lower case for ordinary numbers.
\( \psi(x, t) \) by solving the time dependent Schrödinger equation

\[
H\psi = i\hbar \frac{\partial}{\partial t} \psi.
\]

The observed values of any operator \( \hat{A} \) are the eigenvalues \( a_j \) of

\[
\hat{A}\phi_j(x) = a_j \phi_j(x)
\]

where the \( \phi_j \) are the corresponding eigenfunctions that satisfy the orthonormality condition

\[
\int_{\mathbb{R}^3} \overline{\phi}_j(x) \phi_k(x) \, dx = \delta_{jk}.
\]

The Kronecker delta is denoted by \( \delta_{jk} \), i.e. \( \delta_{jj} = 1 \) for all \( j \) and \( \delta_{jk} = 0 \) for all \( j \neq k \). The probability of observing the eigenvalue \( a_j \) is \( |A_j(t)|^2 \) where \( A_j(t) \) is the projection of the wave function onto the corresponding \( j^{th} \) eigenfunction. That is,

\[
\psi(x, t) = \sum_j A_j(t) \phi_j(x), \quad A_j(t) = \int_{\mathbb{R}^3} \overline{\phi}_j(x) \psi(x, t) \, dx.
\]

Heisenberg’s formalism replaces \( \psi, \psi^* \) by the column and row vectors

\[
\begin{pmatrix}
\psi_1 \\
\psi_2 \\
\vdots \\
\psi_k \\
\vdots 
\end{pmatrix},
\begin{pmatrix}
\overline{\psi}_1 \\
\overline{\psi}_2 \\
\vdots \\
\overline{\psi}_k \\
\vdots 
\end{pmatrix}, (\overline{\psi}_1, \overline{\psi}_2, \ldots, \overline{\psi}_k, \ldots)
\]

respectively which are considered as sequences in the Hilbert space \( L^2(\mathbb{R}^3) \). One obtains this representation for \( \psi, \psi^* \) by expanding \( \psi \) over some complete set of functions \( \{\phi_k\}_{k \in \mathbb{N}} \). Specifically,

\[
\psi_j = \int_{\mathbb{R}^3} \overline{\phi}_j(x) \psi(x, t) \, dx.
\]
Typically, the \( \{ \phi_k \}_{k \in \mathbb{N}} \) are the eigenfunctions of some Schrödinger operator. In a similar fashion, dynamical variables are represented by square matrices

\[
\begin{pmatrix}
A_{11} & A_{12} & \cdots \\
A_{21} & A_{22} & \\
& \ddots & \ddots \\
& & & A_{jk} \\
& \vdots & & \ddots \\
\end{pmatrix}
\]

with

\[
A_{jk} = \int_{\mathbb{R}^3} \phi_j^*(x) A(x, -i\hbar \nabla_x) \phi_k(x) \, dx.
\]  

(D.6)

The column vectors satisfy

\[
\begin{pmatrix}
H_{11} & H_{12} & \cdots \\
H_{21} & H_{22} & \\
& \ddots & \ddots \\
& & & H_{jk} \\
& \vdots & & \ddots \\
\end{pmatrix}
\begin{pmatrix}
\psi_1 \\
\psi_2 \\
\vdots
\end{pmatrix} = i\hbar \frac{\partial}{\partial t}
\begin{pmatrix}
\psi_1 \\
\psi_2 \\
\vdots
\end{pmatrix}
\]

analogous to (D.1), and the eigenvalue equation (D.2) is expressed as

\[
\begin{pmatrix}
A_{11} & A_{12} & \cdots \\
A_{21} & A_{22} & \\
& \ddots & \ddots \\
& & & A_{jk} \\
& \vdots & & \ddots \\
\end{pmatrix}
\begin{pmatrix}
\phi_1^j \\
\phi_2^j \\
\vdots
\end{pmatrix} = a_j \begin{pmatrix}
\phi_1^j \\
\phi_2^j \\
\vdots
\end{pmatrix}
\]

with the orthonormality condition (D.3)

\[
(\phi_1^{j*}, \phi_2^{j*}, \ldots) \begin{pmatrix}
\phi_1^j \\
\phi_2^j \\
\vdots
\end{pmatrix} = \delta_{jk}.
\]

In this formalism, the probability of observing the eigenvalue \( a_j \) is still given by \( |A_j(t)|^2 \) where

\[
\begin{pmatrix}
\psi_1 \\
\psi_2 \\
\vdots
\end{pmatrix} = \sum_j A_j(t) \begin{pmatrix}
\phi_1^j \\
\phi_2^j \\
\vdots
\end{pmatrix}, \quad A_j(t) = (\phi_1^{j*}, \phi_2^{j*}, \ldots) \begin{pmatrix}
\psi_1 \\
\psi_2 \\
\vdots
\end{pmatrix}.
\]

\( A_j(t) \) is the projection of the wave function \( \psi \) onto the \( j \)-th eigenvector as in (D.4).
For the Dirac formalism, the starting point is a separable Hilbert space $\mathcal{H}$ with inner product $\langle \cdot, \cdot \rangle$. Let the family $\{e_\alpha : \alpha \in \mathcal{A}\}$ of elements from $\mathcal{H}$ be an orthonormal basis of $\mathcal{H}$ so that

$$\langle e_\alpha, e_\beta \rangle = \delta_{\alpha \beta} \quad \text{for} \quad \alpha, \beta \in \mathcal{A}. \quad (D.7)$$

This system has the following expansion properties which can be found in any of the standard references [66].

$$f = \sum_{\alpha \in \mathcal{A}} \langle e_\alpha, f \rangle e_\alpha \quad \forall f \in \mathcal{H}. \quad (D.8)$$

$$\langle g, f \rangle = \sum_{\alpha \in \mathcal{A}} \langle g, e_\alpha \rangle \langle e_\alpha, f \rangle \quad \forall f, g \in \mathcal{H}. \quad (D.9)$$

The functions, $f \in \mathcal{H}$, are also normalized such that

$$\|f\|^2 = \sum_{\alpha \in \mathcal{A}} |\langle e_\alpha, f \rangle|^2 = 1. \quad (D.10)$$

The states of a system are described by vectors $|\psi(t)\rangle \in \mathcal{H}$ and their transpose conjugates $\langle \psi(t)|$ denoted as $\langle \psi(t)\rangle$. The symbol $|\psi(t)\rangle$ is called a ket vector and its conjugate transpose is known as a bra vector.

With this representation, the operator product of $|A\rangle$ and $|B\rangle$ is denoted as $C = |A\rangle \langle B|$. This is indeed a linear operator since

$$C|R\rangle = |A\rangle \langle B|R\rangle = |A\rangle \langle B, R\rangle$$

is a vector. By convention, a bra vector to the left of a ket vector generates an inner product. In other words, $\langle A|B \rangle = \langle A, B \rangle$. It is not a coincidence that another name for the Dirac formalism is bra–ket notation. The unity operator is denoted by

$$\sum_j |\phi_j\rangle \langle \phi_j| = 1 \quad \text{or} \quad \int |\phi\rangle \langle \phi| \, d\phi = 1 \quad (D.11)$$

---

2 The inner product $\langle f, g \rangle$ is assumed to be linear in $g$ (Reed Simon) notation [55].
D.1: Dirac Formulation

in the sense of Hilbert space and depending on whether or not the eigenstates over which we expand are discrete or continuous. Expression (D.11) is just a restatement of property (D.9).

Dynamical variables are described by linear operators over \( \mathcal{H} \). That is, \( x, p \) or any function \( A(x,p) \). In particular we have the energy operator

\[
H = \frac{p^2}{2m} + V(x).
\]

The state vector satisfies

\[
H|\psi\rangle = i\hbar \frac{\partial |\psi\rangle}{\partial t},
\]

and the observed values of any operator \( A \) are the eigenvalues \( a_j \) of

\[
A|\phi_j\rangle = a_j|\phi_j\rangle
\]

where the \( |\phi_j\rangle \) satisfy the orthonormality condition

\[
\langle \phi_j, \phi_k \rangle = \delta_{jk}.
\]

For example, the position operator \( X \) satisfies the eigenvalue equation

\[
X|x_j\rangle = x_j|x_j\rangle, \quad \langle x_j, x_k \rangle = \delta(x_j - x_k)
\]

where \( x_j \) is a continuous eigenvalue.

The probability of observing the eigenvalue \( a_j \) is \( |A_j(t)|^2 \) where \( A_j(t) \) is the projection of the wave function onto the corresponding \( j^{th} \) eigenfunction. That is,

\[
|\psi(t)\rangle = \sum_j A_j(t)|\phi_j\rangle, \quad A_j(t) = \langle \phi_j, \psi(t) \rangle
\]

from the expansion property (D.8).

One can see that the Heisenberg formulation is just the Dirac formulation with \( \mathcal{H} = L^2(\mathbb{R}^3) \) expressed in terms of a particular basis. To obtain the Schrödinger
formulation one picks the basis vectors to be the position eigenvectors given in
\((D.15)\) and expresses all other vectors and operators in terms of their projections
along the \(|x_j\rangle\). In this case, it can be shown that the Schrödinger wave function is
just the components of the Dirac state vector, \(|\psi(t)\rangle\), expressed in the position basis

\[
\psi(x,t) = \langle x, \psi(t) \rangle, \quad \psi^*(x,t) = \langle \psi(t), x \rangle.
\]

The Schrödinger operators are given by

\[
\langle x'|A(x,p)|x\rangle := \langle x', A(x,p)x \rangle = A(x, -i\hbar \nabla_x)\delta(x' - x)
\]

which allows one to convert from one formalism to the other. For example, the Dirac
eigenvalue equation \((D.13)\) may be transcribed into the Schrödinger version \((D.2)\)
by projecting expression \((D.13)\) onto \(\langle x'|\) and inserting the unit operator

\[
\int_{\mathbb{R}^3} |x'(x'|dx' = 1.
\]
as follows:

\[
a_j(x, \phi_j) = \langle x, A\phi_j \rangle = \langle x|A|\phi_j \rangle
\]

\[
= \int \langle x, Ax'\rangle\langle x', \phi_j \rangle dx'
\]

\[
= \int A(x', -i\hbar \nabla_{x'})\delta(x' - x)\langle x', \phi_j \rangle dx'
\]

so that we obtain \(A(x, -i\hbar \nabla_x)\phi_j(x) = a_j\phi_j(x)\) as required.

Finding the Heisenberg representation is accomplished by expressing the Dirac
matrices in a particular basis, say \(\{\phi_k\}\). One obtains

\[
\psi_j = \langle \phi_j, \psi \rangle = \int_{\mathbb{R}^3} \langle \phi_j, x'\rangle\langle x', \psi \rangle dx'
\]

\[
= \int_{\mathbb{R}^3} \phi_j^*(x')\psi(x') dx'
\]
which is equation (D.5) and

\[ A_{jk} = \langle \phi_j, A(x,p)\phi_k \rangle = \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \langle \phi_j(x'), \langle x', A(x,p)x'' \rangle \phi_k(x') \rangle \, dx' \, dx'' \]
\[ = \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \phi_j^*(x') A(x'', -i\hbar \nabla_{x''}) \delta(x' - x'') \phi_k(x') \, dx' \, dx'' \]
\[ = \int_{\mathbb{R}^3} \phi_j^*(x') A(x', -i\hbar \nabla_{x'}) \phi_k(x'), \, dx' \]

which is equation (D.6).

### D.2 Position and Momentum Operators

Many operators of interest in quantum mechanics can be constructed from the position and momentum operators. The position operator \( X \) satisfies the eigenvalue equation

\[ X|x'\rangle = x'|x'\rangle, \quad \langle x', x \rangle = \delta(x' - x). \]

This implies that the matrix elements of \( X \) are given by

\[ \langle x', Xx \rangle = x\delta(x' - x). \]

This is a continuous matrix with nonzero entries only on the diagonal \( x' = x \).

Multiplication of the matrix \( X \) with the column state vector \( |\psi\rangle \) gives

\[ X|\psi\rangle = \int_{\mathbb{R}^3} X|x'\rangle \langle x', \psi \rangle \, dx' = x \int_{\mathbb{R}^3} x' \psi(x') \delta(x - x') \, dx' = x|\psi\rangle. \]

If \( |p\rangle \) represents an eigenstate of the momentum operator \( P \) then

\[ P|p'\rangle = p'|p'\rangle. \]

The matrix of \( P \) in the coordinate representation is

\[ \langle x, Px' \rangle = -i\hbar \nabla_x \delta(x - x') \]
from equation (D.17). This relation admits an explicit form for the transfer matrix $(x, p)$.

\[
\begin{align*}
    p(x, p) &= \langle x, Pp \rangle = \int_{\mathbb{R}^3} \langle x, Px' \rangle (x', p) \, dx' \\
    &= -i\hbar \int_{\mathbb{R}^3} \nabla_x \delta(x - x') (x', p) \, dx' \\
    &= -i\hbar \nabla_x (x, p).
\end{align*}
\]

The solution of this differential equation is given by

\[
\langle x, p \rangle = \left( \frac{\hbar}{2\pi} \right)^{3/2} e^{ipx/\hbar} \tag{D.18}
\]

where the constant is chosen so that

\[
\int_{\mathbb{R}^3} \langle x, p \rangle (p, x') \, dp = \delta(x - x')
\]

and using the fact that the Dirac delta function on $\mathbb{R}^n$ can be represented as

\[
\delta(x - x') = \frac{1}{(2\pi)^n} \int_{\mathbb{R}^n} e^{ik \cdot (x - x')} \, dk.
\]