MIXED BOUNDARY VALUE PROBLEMS IN QUANTUM MECHANICS

by

Anurag Saksena, B.Sc., M.Sc.

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To Millie, Michelle and Sean

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ABSTRACT

Quantum dynamics of a system of non-relativistic particles confined to a region Ω in R^d with piecewise smooth boundary is investigated. Particles mutually interact through a time dependent scalar field and couple to an arbitrary time varying external electromagnetic field. Based on large mass expansion of quantum propagator a parametrix (or approximate propagator) is constructed for sufficiently smooth potentials. It is shown that for sufficiently smooth initial data, the parametrix generates an approximate evolution operator which satisfies an uniquely solvable inhomogeneous equation of motion in $L^2(\Omega)$. Explicit L^2-error estimates are obtained and the approximate expectation value of a special class of observables is determined.

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CHAPTER 1

INTRODUCTION AND SUMMARY

This thesis is concerned with the problem of quantum evolution of a many body system confined to a region. In mathematical literature such problems are referred to as mixed boundary value problems (or initial-boundary value problems) [CH,Mi]. We have the following definition by [CH]. Consider a fixed domain Ω in the space of variables $x_1, x_2 \ldots x_d$ with piecewise smooth boundary $\partial\Omega$. A mixed problem consists of finding a function $u(x_1, x_2 \ldots x_d, t)$ $\equiv u(x,t)$ in the domain Ω (for $t \geq 0$) which satisfies a given PDE $L[u] = 0$. The function attains prescribed value on $\partial\Omega$ and satisfies given initial conditions for $t = 0$ in Ω.

A typical mixed problem in quantum mechanics can be formulated as below. The dynamical evolution of a quantum system is determined by the Schrodinger equation

$$i\hbar \frac{\partial\psi(x,t)}{\partial t} = H(x,t)\psi(x,t). \tag{1.1}$$

Here x denotes a generic point in $\Omega \subseteq R^d$ that specifies the position of all the particles in the system. The time parameter t lies in the interval $[0,T]$ and the Hamiltonian has the differential structure

$$H(x,t) = \frac{1}{2m}\left[\frac{\hbar}{i}\nabla - a(x,t)\right]^2 + v(x,t). \tag{1.2}$$

Here ∇ is the d-dimensional gradient. The scalar potential v maps $\Omega \times [0,T] \to R$ while the vector potential a is a d-dimensional vector which maps $\Omega \times [0,T] \to R^d$. The function $\psi(x,t)$ satisfies the following initial-boundary conditions:

(1) the Cauchy initial condition

$$\psi(x,0) = \phi \tag{1.3a}$$

and a boundary condition, for example

(2) the Dirichlet boundary condition:

$$\psi(x,t)\Big|_{x\in\partial\Omega} = 0 \qquad \text{for all } t \in [0,T]$$

or

(3) the Periodic boundary condition:

$$\psi(x+\underline{\bar{X}},t) = \psi(x,t) \qquad \text{for all } t \in [0,T] \tag{1.3b}$$

where $\underline{\bar{X}}$ is some periodic displacement; or

(4) the Neuman boundary condition

$$\frac{\partial\psi(x,t)}{\partial n} = 0 \qquad \text{at } x \in \partial\Omega \tag{1.3c}$$

where $\frac{\partial}{\partial n}$ represents the normal derivative.

This by no means exhausts the variety of possible boundary conditions but they are the ones commonly found in physics literature.

From the point of view of quantum dynamics the object of importance is the quantum propagator (evolution kernel) [cf. Definition 3.1], which not only provides the evolution of a quantum state in Hilbert space but gives also the space-time geometrical insight into this process. If $(y,s) \in \Omega \times [0,T]$ is some initial space-time point, then the propagator $K(x,t;y,s)$ for the system (1.2) determines the wave function $\psi(x,t)$ via the relation

$$\psi(x,t) = \int_{\Omega} K(x,t;y,s)\phi(y)dy. \tag{1.4}$$

Quantum propagators have been of much interest in recent years [OPC,POM,AH,CS]. For example, in [OPC] it was shown that for potentials which can be represented as the Fourier transform of complex bounded measures, the method of Dyson's Series [Dy1,Dy2] can be used to construct the quantum propagator. For this class of potentials Albeverio et al [AH] have shown that the exact propagator can be constructed by using Feynman path integration. A comprehensive summary of the method of path integration may be found in [DMN,M]. For potentials which do not belong to this class both of the methods mentioned above fail to provide the rigorous solutions of Schrödinger equation. For example, Dyson's series in [OPC] has no known convergence – either in pointwise or in abstract sense. On the other hand path integration technique provides only the non-rigorous solutions in some special cases [FH].

This motivates us to consider the possibility of developing an approximation scheme to solve the problem of quantum evolution where the potentials are not as restrictive as seen in [OPC,AH]. One well-known method which utilizes the analytic structure of formal propagator in the expansion parameter (e.g., m, $\hbar$ or t) is the method of parametrix [Ga]. The parametric method has been very successful in dealing with the heat or diffusion problems [MP,Ch]. With regard to quantum evolution Maslov comments [MF, page no.185], ".... However, an open question remained: is the approximate solution close to the exact solution? This question is very important indeed, and extremely hard to answer." In this thesis we will show that under suitable conditions on smoothness of potentials and the initial data, the method of parametrix can be successfully adapted to the problem of quantum evolution. The remainder of this chapter gives a summary of the thesis.

Since a general quantum state evolves as a vector in Hilbert space $L^2(\Omega)$, the most natural approximation would be the one which is valid in L^2-topology. We begin by examining the solutions of the equation

$$i\hbar \frac{d\psi(t)}{dt} = H(t)\psi(t) \tag{1.5}$$

in the $L^2(\Omega;C)$ topology. Here $\Omega \subseteq R^d$ and the boundary $\partial\Omega$ is assumed to be piecewise smooth. We shall place sufficient conditions on a and v to show that for a given boundary condition the Hamiltonian operator $H(\cdot,t)$ whose differential form is given by (1.2) is self-adjoint with a time invariant domain in $L^2(\Omega)$. The boundary conditions play the role of determining the domain of the Hamiltonian. Let T_Δ be the closed triangular region

$$T_\Delta = \{(s,t) \in [0,T] \times [0,T]: \ 0 \le s \le t \le T\}.$$

For each $s < T$ we seek a solution of (1.5) that satisfies the initial condition

$$\psi(s,s) = \phi; \qquad \phi \in E_0. \tag{1.6}$$

We shall see that under weak assumptions on scalar and vector potentials, a unique solution of (1.5, 1.6) exists and defines a family of bounded linear operators via the mapping $\phi \to \psi(t,s)$. For each (s,t) we denote this mapping by $U(t,s)$ and we call the collection of these mappings $\{U(t,s)\}_{(t,s)\in T_\Delta}$, the Schrödinger evolution. In Chapter 2 we shall discuss the properties of a Schrödinger evolution. It will be shown that $U(t,s): D(H) \to D(H)$; $U(s,s) = I$ and that the operator $U(t,s)$ is strongly continuously differentiable and satisfies the equation

$$i\hbar \frac{\partial}{\partial t} U(t,s)\phi = H(t)U(t,s)\phi; \quad \phi \in D(H). \tag{1.7}$$

In the special case when the Hamiltonian operator $H(t)$ is time independent, the Schrödinger evolution has the familiar form

$$U(t,s) = \exp[-\frac{i(t-s)}{\hbar} H]. \tag{1.8}$$

The next step in this approach is to construct an appropriate parametrix (or approximate propagator). By the term appropriate parametrix it is implied that we seek a function which satisfies the initial-boundary conditions listed above. Moreover, the function should be such that when interpreted as an integral kernel, it generates a bounded operator in $L^2(\Omega)$.

For the special case when $\Omega = R^d$, no boundary conditions are required and the choice of parametrix is particularly simple [cf. Chapter 3]. It is obtained by simply truncating the large mass asymptotic expansion of $K(x,t;y,s)$ and multiplying it by a smooth cut-off function that is one for small $|x-y|$ and vanishes for large $|x-y|$. A similar candidate parametrix can be obtained by truncating the WKB semi-classical expansion (i.e., $\hbar \to 0$) [ETW]. This was considered in some detail by Maslov et al [MF]. In [MF] it was established that for a fixed rapidly oscillating (in $\hbar$) initial data of compact support an approximate solution of the Schrödinger equation can be obtained which is valid in $L^2(\Omega)$. Furthermore, mixed boundary value problems are not discussed in [MF]. Large mass approximation on the other hand does not require the initial data to be compactly supported or be mass dependent. In particular, the large mass approximation remains valid for arbitrary initial data satisfying some smoothness restrictions. Moreover, as will be seen in Chapters 4 and 5, the results of quantum evolution in R^d can be readily extended to find the L^2-approximate solutions for mixed problems. An additional advantage of choosing mass instead of $\hbar$ as an analytic parameter is the absence of caustics that commonly occur in WKB approximation. This greatly simplifies the analysis.

In the circumstance when $\Omega \subseteq R^d$ and admits tessalation we use the method of images to construct the parametrix. In Chapter 4, we will carry out an explicit calculation of the formal propagator which will show that if the Dirichlet boundary conditions are imposed then expansion coefficients of the formal propagator exhibit anomalous singular behaviour at the boundary, i.e., analytic behaviour not found in the exact propagator. This situation is further clarified in Chapter 5 where it is shown that the contribution of these anomalous coefficients (surface terms) to the wave function is not of the leading order in mass parameter and thus can be dropped from the definition of the parametrix. The parametrix so obtained does not solve the Schrödinger equation but satisfies an inhomogeneous PDE identity.

The third and the final step is to bound the L^2-error in this approximation. We will show that for sufficiently smooth initial data ϕ the PDE identity satisfied by the parametrix determines an inhomogeneous abstract equation of motion

$$i\hbar \frac{d}{dt} U_M(t,s)\phi = H(t,m)U_M(t,s)\phi + m^{-(M+1)} R_M(t,s) \qquad (1.9)$$

where the suffix M determines the order of mass dependence in the parametrix (i.e., m^{-M}). The operator $U_M(t,s)$ will be called the approximate evolution operator. By a standard result in the theory of differential equations in Banach space [Kr], it follows that the equation (1.9) is uniquely solvable and the solution is given by

$$U_M(t,s)\phi = U(t,s)\phi + \int_s^t m^{-(M+1)} U(t,\tau) R_M(t,\tau) d\tau. \qquad (1.10)$$

From here we will show that the approximate solution $U_M(t,s)\phi \equiv \psi_M(t)$ is asymptotically close to the exact solution $U(t,s)\phi \equiv \psi(t)$ in L^2-norm, i.e.,

$$\| \psi_M(t) - \psi(t) \| \sim O(m^{-M-1}). \qquad (1.11)$$

In case of a general mixed problem, this norm difference takes a modified form,

$$\| \psi_M(t) - \psi(t) \| \sim O(m^{-M-\epsilon}) \quad \text{for some } \epsilon > 0. \qquad (1.12)$$

Chapter 2

THE ABSTRACT THEORY OF EVOLUTION

2.0 Introduction

This chapter establishes the existence and describes the properties of Time Evolution operator for a variety of mixed boundary value problems in Quantum Mechanics. Our discussion begins with a brief summary of the general theory of differential equations in Banach Space with unbounded operator coefficients. A detailed account of this theory may be found in the book by Krein [Kr]. Informally we will often refer to this theory of abstract evolution operators on Banach Space as Krein's Theory. This theory is then adapted to the study of Schrödinger evolution operator for a general mixed boundary value problem.

2.1: Evolutions in Banach Space

Let E be a Banach space with norm $\|\cdot\|$. In this space we consider a first order differential equation

$$\frac{d\psi}{dt} = A(t)\psi, \qquad 0 \le t \le T \tag{2.1}$$

where ψ: $[0,T] \to E$ and $\{A(t)\}$ is a family of unbounded operators on E. The $\{A(t)\}$ are assumed to be closed and share a common (stable) dense domain $D(A(t)) = D(A) \subset E$ for all $t \in [0,T]$.

In describing (2.1) rigorously it is helpful to recall some of the standard concepts of differentiability in Banach spaces.

Definition 2.1: *Let* L(t), $t \in [0,T]$ *be a closed, densely defined operator on a* t-*invariant domain* D(L). *Then*

(a) L(t) *is said to be strongly differentiable on* [0,T] *if* $\phi(t) = L(t)\phi$, $\phi \in D(L)$ *has a strong derivative* $\frac{d\phi}{dt}(t)$ *in the norm topology of the Banach Space* E. *We denote this strong derivative of* L(t) by $\dot{L}(t)$ *i.e.*,

$$\dot{L}(t) = \underset{\delta t \to 0}{\text{s-lim}} \frac{L(t+\delta t)\phi - L(t)\phi}{\delta t}, \qquad t \in [0,T]$$

(b) L(t) *is said to be strongly continuously differentiable on the interval* [0,T] *if* $\dot{L}(t)$, *defined above, is continuous throughout the interval* [0,T].

$$||\dot{L}(t+\delta t) - \dot{L}(t)|| \underset{\delta t \to 0}{\to} 0, \qquad t \in [0,T]$$

Definition 2.2: *A solution of* (2.1) *on the segment* [s,T] *for a fixed* $s \in [0,T]$ *is a function* $\psi(t,s)$ *taking values in* D(A) *and having a strong derivative* $\partial_t\psi(t,s)$ *satisfying* (2.1) *at every* $t \in [s,T]$. *By the Cauchy problem on the closed triangle* $T_\Delta \equiv \{(t,s): 0 \le s \le t \le T\}$ *we mean the problem of finding for each fixed* $s \in [0,T]$ *a solution*, $\psi(t,s)$ *of* (2.1) *that satisfies the initial data*

$$\psi(s,s) = \psi_0 \in D(A) \tag{2.2}$$

Definition 2.3: *The Cauchy problem is said to be uniformly correct if the following statements hold:*

(1) *For each* $s \in [0,T]$ *and for any* $\psi_0 \in D(A)$ *there exists a unique solution of* (2.1) *on the segment* $[s,T]$ *satisfying initial data condition* (2.2).

(2) *The function* $\psi(t,s)$ *and its* t *derivative* $\partial_t \psi(t,s)$ *are continuous in the triangle* T_Δ.

(3) *The solution depends continuously on the initial data in the sense that if* $\psi_{0,n} \in D(A)$ *converges to zero as* $n \to \infty$ *the corresponding solutions* $\psi_n(t,s)$ *converges to zero uniformly with respect to* $(t,s) \in T_\Delta$. □

In the circumstance where the Cauchy problem is uniformly correct, the evolution operator $\mathcal{U}(t,s)$ can be defined as the linear map $\psi_0 \to \psi(t,s)$ on $D(A)$ for each $(t,s) \in T_\Delta$, i.e.,

$$\psi(t,s) = \mathcal{U}(t,s)\psi_0. \tag{2.3}$$

From properties (1) and (3) it is evident that $\mathcal{U}(t,s)$ is bounded and since $D(A)$ is dense we can extend $\mathcal{U}(t,s)$, by continuity, to the entire space E. We shall denote the extension by $\mathcal{U}(t,s)$ again.

The uniform correctness of Cauchy problems leads to certain properties for the evolution operator $\{\mathcal{U}(t,s)\}_{(s,t)\in T_\Delta}$, summarized in the following proposition.

PROPOSITION 2.1: *Suppose the Cauchy problem in the triangle* T_Δ *is uniformly correct. Then the evolution operator* $\{\mathcal{U}(t,s)\}_{(s,t)\in T_\Delta}$ *satisfies the following:*

(1) *$U(t,s)$: $D(A) \to D(A)$, $(t,s) \in T_\Delta$.*

(2) *The operator $U(t,s)$ is uniformly bounded in T_Δ.*

(3) *The operator $U(t,s)$ is strongly continuous in T_Δ.*

(4) *The following operator-valued identities hold in T_Δ:*

$$U(t,s) = U(t,\tau)U(\tau,s), \qquad 0 \le s \le \tau \le t \le T \tag{2.4}$$

$$U(s,s) = I \qquad s \in [0,T]. \tag{2.5}$$

(5) *The restriction of the operator $U(t,s)$ to the domain $D(A)$ is strongly differentiable in $t \in [s,T]$. Furthermore, the operator $\partial_t U(t,s)$, defined on $D(A)$, is jointly strongly continuous in $(t,s) \in T_\Delta$ and obeys the relation*

$$\partial_t U(t,s)\psi = A(t)U(t,s)\psi, \qquad \psi \in D(A). \tag{2.6}$$

Proof: See Krein [Kr] (pp.193-195). □

In light of Proposition 2.1 we note that it is sufficient to show that the Cauchy problem (2.1) - (2.2) is uniformly correct for the associated evolution operator $\{U(t,s)\}_{(s,t)\in T_\Delta}$ to exist. The next theorem states the conditions on $A(t)$ that will be sufficient to guarantee the uniform correctness of Cauchy problem. For the details of the associated proof, see Krein [Kr].

THEOREM 2.1: Suppose the operators $A(t)$ ($t \in [0,T]$) are

(1) *densely defined and closed, with t-invariant domain $D(A)$;*

(2) *strongly continuously differentiable on domain $D(A)$; and*

(3) *obey the resolvent estimate*

$$\|R(\lambda;A(t))\| \leq \frac{1}{1+\lambda} \qquad \lambda \geq 0. \tag{2.7}$$

Then

(a) *the Cauchy problem in* T_Δ *is uniformly correct;*

(b) *the restriction of the operator* $U(t,s)$ *to the domain* $D(A)$ *is strongly continuously differentiable in the variable* $s \in [0,T]$ *and satisfies the relation*

$$\partial_s U(t,s)\psi = -U(t,s)A(s)\psi, \qquad (t,s) \in T_\Delta, \ \psi \in D(A); \tag{2.8}$$

and

(c) *the operator* $U(t,s)$ *satisfies the uniform bound*

$$\|U(t,s)\| \leq 1. \tag{2.9}$$

□

We wish to apply this theory to determine the time evolution operator for a general mixed boundary value problem. Let E be the Hilbert space of scalar wave functions ψ, i.e.,

$$H = L^2(\Omega,dx)$$

where Ω denotes the manifold on which ψ is supported and dx represents the volume measure on Ω that is locally equal to the Lebesgue measure in R^d. The domain Ω is assumed to be a simply connected subset of R^d. If Ω has boundaries, $\partial\Omega$, they are assumed to be at least piecewise smooth surfaces.

The Schrödinger equation with its associated Cauchy condition is

$$i\hbar \frac{d\psi}{dt} = H(t)\psi$$

$$\psi(s,s) = \psi_0; \qquad \psi_0 \in D(H). \tag{2.10}$$

Here H(t) is a Hamiltonian family of self-adjoint operators on $\mathcal{H}$ with the common domain D(H). The appearance of t in the Hamiltonian means that the evolution problem is of the non-autonomous type.

THEOREM 2.2: *Let* $A(t)$ *be a family of operators in* $E = \mathcal{H} \equiv L^2(\Omega)$ *given by*

$$A(t) = \frac{1}{i\hbar} H(t) - cI \tag{2.11}$$

where c *is an appropriately chosen constant and let* $A(t)$ *satisfy the hypothesis of Theorem 2.1. Let* $\{\mathcal{U}(t,s)\}_{(s,t)\in T_\Delta}$ *be the associated family of evoluation operators.*

Then the Schrödinger equation (2.10) generates an evolution $\{U(t,s)\}_{(s,t)\in T_\Delta}$*, which satisfies the operator identity:*

$$U(t,s) \equiv e^{c(t-s)}\mathcal{U}(t,s) \qquad (t,s) \in T_\Delta. \tag{2.12}$$

Schrödinger's evolution operator $U(t,s)$ *has the following properties:*

(1) $U(t,s)$: $D(H) \to D(H)$, $(t,s) \in T_\Delta$;

(2) $U(t,s)$ *has the operator norm bound*

$$\|U(t,s)\| \le e^{c(t-s)}; \tag{2.13}$$

(3) $U(t,s)$ *is strongly continuous in* T_Δ;

(4) U(t,s) *satisfies the operator identities*

$$U(t,s) = U(t,\tau)U(\tau,s)$$

$$U(s,s) = 1 \qquad\qquad 0 \le s \le \tau \le t \le T; \qquad (2.14)$$

(5) *on the region* D(H) *the operator* U(t,s) *is strongly differentiable with respect to both* t *and* s *with the strong derivatives*

$$\begin{aligned} \partial_t U(t,s) &= \frac{1}{i\hbar} H(t)U(t,s) \\ \partial_s U(t,s) &= -\frac{1}{i\hbar} U(t,s)H(s). \end{aligned} \qquad (2.15)$$

<u>Proof</u>: From Definition (2.12), Proposition (2.1) and Theorem (2.1), we observe that the properties (1) ~ (4) are trivially satisfied. We verify the validity of (2.15).

Let $\psi_0 \in D(H) = D(A)$; then

$$\begin{aligned} \partial_t U(t,s)\psi_0 &= \partial_t (e^{c(t-s)}\mathcal{U}(t,s)\psi_0) \\ &= cU(t,s)\psi_0 + e^{c(t-s)}A(t)\mathcal{U}(t,s)\psi_0 \\ &= cU(t,s)\psi_0 + e^{c(t-s)}(\frac{1}{i\hbar} H(t) - cI)\mathcal{U}(t,s)\psi_0 \\ &= \frac{1}{i\hbar} H(t)U(t,s)\psi_0. \end{aligned} \qquad \square$$

A similar derivation establishes the second equation in (2.15).

In the following we shall investigate the question of the existence of a unique self-adjoint Hamiltonian operator by explicit constructive methods. This not only suffices to establish the desired self-adjointness for a given boundary condition but also has the additional merit of providing an explicit statement of the domains of definition. This is often not the case for a self-adjointness analysis based on essentially self-adjoint operators. Self-adjointness is first studied for the Hamiltonians without potentials and in the latter part of the chapter extended to include perturbations.

2.2 The Free Hamiltonian and Self-Adjointness Properties

Throughout this thesis we will be considering a family of evolution problems in non-relativistic quantum mechanics. This section is devoted entirely to the construction of free Hamiltonian (kinetic energy) operator compatible with a given boundary condition. Let us begin by defining the class of coordinate domains of interest. The symbol Ω will always denote an open connected region contained in R^d. $\bar{\Omega}$ will be closure of Ω and $\partial\Omega$ the boundary $\bar{\Omega}/\Omega$. A domain is called bounded if it is contained within a compact set of R^d.

Definition 2.4: *We say* $\Omega \in$ HR, *if* Ω *is a hyperrectangular subset of* R^d, *i.e.*,

$$\Omega = \mathop{X}_{i=1}^{d} (a_i, b_i)$$

where (a_i,b_i) *can be the half-axis* (a_i,∞), *the full-axis* $(-\infty,+\infty)$ *or the interval* (a_i,b_i). *Thus* Ω *can be either a bounded or unbounded hyperrectangular subset of* R^d. □

Definition 2.5: *Let* $\Omega \subseteq R^d$ *be a bounded domain. The boundary* $\partial\Omega$ *is said to be of class* C^m *if for each* $x_0 \in \partial\Omega$ *there exists a ball* $B_0 \subseteq R^d$ *with centre* x_0 *such that* $\partial\Omega \cap B_0$ *can be represented in the form*

$$x_i = h(x_1,\ldots,x_{i-1},x_{i+1},\ldots,x_m)$$

for some i, *with* $h \in C^m(B_0)$. □

Consider the hyperrectangular region together with associated boundary conditions of interest, e.g., periodic, Dirichlet, Neuman and mixed Dirichlet-Neuman. Let Z denote the set of integers; then we have the following definition.

Definition 2.6: *Let* $\Omega \in$ HR *and let* Ω_p *be a* d-*dimensional bounded rectangle* $\{0 \le x_i \le \ell_i,\ i = 1 \sim d\}$ *with end points identified. The* d-*torus*, T_d , *associated with* Ω_p *is* $\{(e^{2\pi i x_1/\ell_1},\ldots,e^{2\pi i x_d/\ell_d}) \in C^d : (x_1,x_2,\ldots,x_d) \in \Omega_p\}$.
If the volume measure in T_d *is chosen to be equal to the* R^d-*Lebesgue measure in* Ω *then there is a self-evident isomorphism between* $L^2(T_d)$ *and* $L^2(\Omega) = L^2(\Omega_p)$ [SW, page 245-246]. *Let* $\Lambda = \{\xi\colon \xi = (\xi_1\ldots\xi_d);\ \xi_i = \frac{\pi}{\ell_i}\zeta_i,\ \zeta_i \in Z\}$ *denote the* d-*dimensional lattice. Suppose* f: $\Lambda \to C^d$ *is a function on the lattice*

and $|f(\xi)|^2 = \sum_{i=1}^{d} |f_i(\xi)|^2$ *is the usual Euclidean norm on* C^d *then* $\ell^p(\Lambda)$, $p \geq 1$ *is defined by*

$$\ell^p(\Lambda) = \{f: \sum_{\xi\in\Lambda} |f(\xi)|^p < \infty\}$$

If $p = 2$ *then* $\ell^2(\Lambda)$ *is a Hilbert space with the inner product given by*

$$(f,g)_{\ell^2(\Lambda)} = \sum_{\xi\in\Lambda} \overline{f(\xi)}\, g(\xi).$$

We define the Fourier transform operator $F: L^2(T_d) \to \ell^2(\Lambda)$ *by* $Ff = \hat{f}$ *where*

$$\hat{f}(\xi) = (\mathrm{vol}\Omega)^{-1} \int_\Omega f(x)\, e^{-ix\cdot\xi}\, dx\,. \tag{2.16}$$

The operator F *has the following useful properties* [SW, Theorem 1.7, Chapter VII].

1°. *The inverse operator* $F^{-1}: \ell^2(\Lambda) \to L^2(T_d)$, $F^{-1}\hat{f} = f$ *is given by*

$$f(x) = \sum_{\xi\in\Lambda} \hat{f}(\xi)\, e^{ix\cdot\xi} \tag{2.17}$$

which is convergent in L^2*-norm.*

2°. F *is a unitary mapping of* $L^2(T_d)$ $(= L^2(\Omega))$ *onto* $\ell^2(\Lambda)$.

3°. *There is a Plancherel formula*

$$||f||^2 = \sum_{\xi\in\Lambda} |\hat{f}(\xi)|^2. \tag{2.18}$$

4°. *For* $f \in C^k(T_d)$: $k > d/2$ *the sum* $\sum_\xi |\hat{f}(\xi)|$ *converges* [SW, Corollary 1.9, page 249]. □

In what follows we shall require a suitable abstract understanding of boundary conditions on the lattice Λ (e.g., Dirichlet, periodic, Neuman, mixed). We define a family of reflection operators $S_i: \Lambda \to \Lambda$ by

$$S_i\xi = (\xi_1,\ldots,-\xi_i,\ldots,\xi_d);\quad \xi \in \Lambda;\ i = 1 \sim d.$$

Under S_i the lattice reflection symmetry assumes the general form $\hat{f}(S_i\xi) = (-1)^{s_i}\hat{f}(\xi)$, $i = 1 \sim d$. In the last expression s_i is the i-th component of an extended symmetry multi-index (ESM) $s = (s_1,\ldots,s_d)$. The components s_i can be either 0, 1 or $\cdot$ corresponding to whether $\hat{f}$ is symmetric (even), antisymmetric (odd) or the case when no symmetry restrictions are imposed, respectively. In particular when $s_i = 0$ for all $i = 1 \sim d$, $\hat{f}(\xi)$ is symmetric and consequently the sum in equation (2.17) gives a form compatible with Neuman boundary conditon, i.e., a product of cosines. On the other hand, if $s_i = 1$, $i = 1 \sim d$ one obtains a form of (2.17) consistent with Dirichlet boundary condition, i.e., a product of sines. Similarly if $s_i = \cdot$, $i = 1 \sim d$, no symmetry restrictions are imposed on $\hat{f}(\xi)$ leaving (2.17) unchanged which is required for periodic boundary conditions. In general, one also has mixed boundary conditions. For example, consider a bounded 4-dimensional hyperrectangle and set $s = (1,0,\cdot,1)$. This means that directions 1 and 4 are subjected to Dirichlet boundary conditions whereas Neuman and Periodic boundary conditions are imposed on directions 2 and 3 respectively. Altogether, with this classification, there are 3^d different boundary conditions that one can associate with a d-dimensional hyperrectangle.

For a given ESM, the corresponding subspace $\ell^2_s(\Lambda) \subseteq \ell^2(\Lambda)$ is defined to be

$$\ell^2_s(\Lambda) \equiv \{\hat{f} \in \ell^2(\Lambda): \hat{f}(S_i\xi) = (-1)^{s_i}\hat{f}(\xi),\ i = 1 \sim d\}.$$

Moreover, each of these subspaces are mutually orthogonal and thus $\ell^2(\Lambda)$ can be decomposed in 2^d subspaces,

$$\ell^2(\Lambda) = \sum_s \oplus\ \ell^2_s(\Lambda).$$

The sum above extends over all s with arguments $s_i = 1$ or 0. In the special case when $s_i = \cdot$ for all $i = 1 \sim d$, the range of Fourier operator F is the entire $\ell^2(\Lambda)$.

We are now ready to construct the free Hamiltonian for $\Omega \in$ HR with a given boundary condition. Define a linear operator $\tilde{H}_{0s}$: $D(\tilde{H}_{0s}) \subset \ell^2_s(\Lambda) \to \ell^2(\Lambda)$

$$\tilde{H}_{0s}\hat{f} = \xi^2\hat{f}(\xi)$$

where the domain of $\tilde{H}_{0s}$ is given by

$$D(\tilde{H}_{0s}) = \{\hat{f} \in \ell^2_s(\Lambda): \xi^2\hat{f}(\xi) \in \ell^2(\Lambda)\}.$$

$\tilde{H}_{0s}$ is self-adjoint because it is the operator of maximal multiplication by a real valued function [AJS, Proposition 2.16]. Setting $D(H_{0s}) = F^{-1}D(\tilde{H}_{0s})$, the free Hamiltonian $H_{0s}: D(H_{0s}) \to L^2(\Omega)$ is

$$H_{0s}f = F^{-1}\tilde{H}_{0s}F\,f\,. \tag{2.19}$$

Since F is unitary and $\tilde{H}_{0s}$ is self-adjoint it follows that H_{0s} is also self-adjoint [P, Lemma 4.3].

Next, we consider the case when $\Omega \in HR$ is unbounded. In particular we assume that $\Omega \equiv R_+^d = \{x = (x_1 \ldots x_d) \in R^d: x_1 > 0\}$.

<u>*Definition 2.7:*</u> *Define a linear operator* $\Pi: L^2(R_+^d) \to L^2(R^d)$ *by*

$$g(x) \equiv (\Pi f)(x) = \frac{1}{\sqrt{2}} f(x_1,\ldots,x_d) \qquad x_1 > 0,\ f \in L^2(R_+^d) \tag{2.20a}$$

$$= \frac{-1}{\sqrt{2}} f(-x_1,\ldots,x_d) \qquad x_1 < 0,\ f \in L^2(R_+^d). \tag{2.20b}$$

The operator Π *has the following easy to prove properties*

1°. *The inverse operator* $\Pi^{-1}: \Pi L^2(R_+^d) \subset L^2(R^d) \to L^2(R_+^d)$ *is given by*

$$f(x) = (\Pi^{-1}g)(x) = \sqrt{2}\, g(x_1,x_2\ldots x_d);\ x_1 > 0,\ g \in L^2(R_+^d)\,. \tag{2.20c}$$

2°. *The adjoint* $\Pi^*: L^2(R^d) \to L^2(R_+^d)$ *exists and is equal to* Π^{-1}, *i.e.,* Π *is an isometry.* □

To construct the free Hamiltonian for domain R_+^d we again define it via multiplication on a suitably symmetrized Fourier space. Let

$$L^2_{\delta_+}(R^d) = \{\hat{f} \in L^2(R^d): \hat{f}(S_1k_1,\ldots,k_d) = -\hat{f}(k_1,\ldots,k_d)\} \tag{2.21a}$$

where $\delta_+ = (1,\cdot,\cdot,\cdot,\ldots,\cdot)$. $L^2_{\delta_+}(R^d)$ is compatible with Dirichlet boundary conditions on the surface $x_1 = 0$. First define $\tilde{H}_{0_+} : D(\tilde{H}_{0_+}) \subset L^2_{\delta_+}(R^d) \to L^2(R^d)$ by

$$\tilde{H}_{0_+}\hat{f} = |k|^2\,\hat{f} \tag{2.21b}$$

with

$$D(\tilde{H}_{0_+}) = \{\hat{f} \in L^2_{\delta_+}(R^d): |k|^2\,\hat{f} \in L^2(R^d)\}. \tag{2.21c}$$

Since $\tilde{H}_{0_+}$ is an operator of maximal multiplication by a real valued function it is self-adjoint [AJS, Proposition 2.16]. The free Hamiltonian $H_{0_+} : D(H_{0_+}) \subset L^2(R^d_+) \to L^2(R^d_+)$ is given by

$$H_{0_+}f = Y^{-1}\tilde{H}_{0_+}Y f \tag{2.22a}$$

where

$$Y = F\Pi \qquad \text{and} \qquad D(H_{0_+}) = Y^{-1}\,D(\tilde{H}_{0_+}). \tag{2.22b}$$

Note that Y is the product of two unitary operators and is thus unitary. This combined with the fact that $\tilde{H}_{0_+}$ is self-adjoint, we obtain the result that H_{0_+} given by (2.22a,b) is also self-adjoint [P, Lemma 4.3]. In the above discussion we have shown that

* *LEMMA 2.1*: *Let $\Omega \in$ HR [Definition 2.4], then every free Hamiltonian $H_0 \in \{H_{0s}, H_{0_+}\}: D(H_0) \to L^2(R^d)$ is self-adjoint. The subscript s identifies a given boundary condition.* □

REMARK 2.1: The boundary conditions are realized in coordinate space via the following mechanism.

(1) Let $\Omega \in$ HR be bounded; then for $d \leq 3$, $D(\tilde{H}_{0s}) \subset \ell^1(\Lambda)$. To see this we note that for $\hat{f} \in D(\tilde{H}_{0s})$

$$\sum_{\xi\in\Lambda} |\hat{f}(\xi)| = \sum_{\xi\in\Lambda} \frac{1}{(1+\xi^2)} |\hat{f}(\xi)|(1+\xi^2)$$

$$\leq \left(\sum_{\xi\in\Lambda} \frac{1}{(1+\xi^2)}\right)^{\frac{1}{2}} \left(\sum_{\xi\in\Lambda} (1+\xi^2)^2 \; |\hat{f}(\xi)|^2\right)^{\frac{1}{2}}$$

$$< \infty .$$

Thus the sum in equation (2.17) is uniformly convergent. This is all we need to satisfy the boundary conditions in coordinate space. Considering Dirichlet case, the uniform convergence of (2.17) implies

$$\lim_{x\to\partial\Omega} f(x) = \sum_{\xi\in\Lambda} \hat{f}(\xi) \lim_{x\to\partial\Omega} \prod_{i=1}^{d} 2\sin(x_i\xi_i) = 0 .$$

For $d > 3$, the same argument can be applied for the functions $f \in D(H_{0s})$ such that $\hat{f} \in D(\tilde{H}_{0s}) \cap \ell^1(\Lambda)$.

(2) In the case when Ω is Euclidean half-space we defined an operator Π which maps $L^2(R^3_+)$ to a subspace of odd functions.

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* See Supplement, page 144, for Dirichlet Hamiltonian.

These functions are not necessarily continuous and may have a jump at $x_1 = 0$. However, every $f \in D(H_{0_+})$ means that f is (equivalent to) bounded uniformly continuous function [K, page 301]. Continuity plus x_1-oddness means that the Dirichlet boundary condition is fulfilled for every point on the boundary ∂R_+^d, i.e., $f(0,x_2 \ldots x_d) = 0$. In the case when $d > 3$, the same argument works provided that $\hat{f} \in D(\tilde{H}_{0_+}) \cap L^1(R^d,k)$.

(3) The argument presented for the self-adjointness of H_{0_+} can be further extended to include hyperrectangular subsets of R^d where a given number of sides of a hyperrectangle are half-intervals while others are $(-\infty,+\infty)$. The symmetry restrictions are determined by noting that $\delta_i = \cdot$ for each direction i having $(a_i,b_i) = (-\infty,+\infty)$ while in the directions where $(a_j,b_j) = (0,\infty)$, the component δ_j of ESM is equal to 1. □

2.3 The Exact Hamiltonian

In this section we determine assumptions on scalar and vector potentials needed for the exact (fully interacting) Hamiltonian to satisfy the hypotheses of Theorem 2.2.

Let $H_v = L^2(\Omega;C^d)$, $\Omega \subset R^d$ denote the Hilbert space of vector valued functions. The norm in H_v will be denoted by $||\cdot||_v$. We say that the vector and scalar fields are of class A if they satisfy the following hypotheses.

Assumption 1: (vector field hypothesis): *The vector field* $a: \bar{\Omega} \times [0,T] \to R^d$ *is a* d-*dimensional vector whose components* $a_i: \bar{\Omega} \to R$ *satisfy the following assumptions:*

(i) *Boundedness and* x-*continuity:*

$$a_i(\cdot,t) \in L^\infty(\bar{\Omega}) \cap C^1(\bar{\Omega}) \quad \text{and} \quad \nabla\cdot a(\cdot,t) \in L^\infty(\bar{\Omega}); \; t \in [0,T].$$

(ii) *Continuous* t-*differentiability:* $a_i(\cdot,t)$ $[i = 1 \sim d]$ *and* $\nabla\cdot a(\cdot,t)$ *are continuously differentiable with respect to* $t \in [0,T]$ *in* L^∞-*norm. That is, there exist functions* $\dot{a}_i(\cdot,t) \in L^\infty(\bar{\Omega})$ *and* $\nabla\cdot\dot{a}(\cdot,t)$ *such that*

$$\left\|\frac{1}{\delta t}[a_i(\cdot,t+\delta t) - a_i(\cdot,t)] - \dot{a}_i(\cdot,t)\right\|_\infty \to 0$$

$$\text{as } \delta t \to 0, \; t \in [0,T]$$

$$\|\dot{a}_i(\cdot,t) - \dot{a}_i(\cdot,\tau)\|_\infty \to 0 \qquad \text{as } \tau \to t$$

and

$$\left\|\frac{1}{\delta t}[\nabla\cdot a(\cdot,t+\delta t) - \nabla\cdot a(\cdot,t)] - (\nabla,\dot{a})(\cdot,t)\right\|_\infty \to 0$$

$$\text{as } \delta t \to 0, \; t \in [0,T]$$

$$\|\nabla\cdot\dot{a}(\cdot,t) - \nabla\cdot\dot{a}(\cdot,\tau)\|_\infty \to 0 \qquad \text{as } \tau \to t. \qquad \square$$

Assumption 2: (scalar field hypothesis): *The scalar field* $v: \bar{\Omega} \times [0,T] \to R$ *is assumed to have the following properties:*

(i) x-*boundedness and continuity:*

$$v(\cdot,t) \in L^\infty(\bar{\Omega}) \cap C^1(\bar{\Omega}).$$

(ii) t-differentiability: $v(\cdot,t)$ *is continuously differentiable with respect to* $t \in [0,T]$ *in* L^{∞}*-norm. That is, there exists a function* $\dot{v}(\cdot,t) \in L^{\infty}(\bar{\Omega})$ *such that*

$$\left\|\frac{1}{\delta t}\left[v(\cdot,t+\delta t) - v(\cdot,t)\right] - \dot{v}(\cdot,t)\right\|_{\infty} \to 0 \qquad \textit{as } \delta t \to 0$$

and

$$\|\dot{v}(\cdot,t) - \dot{v}(\cdot,\tau)\|_{\infty} \to 0 \qquad \textit{as } \tau \to t. \qquad \square$$

Next goal is to show that for potentials of class A, the fully interacting Hamiltonian is self-adjoint with a time invariant domain. We first consider the case when $\Omega \in HR$ [c.f. Definition 2.4]. We are interested in a family of Hamiltonians $\{H_{s}, H_{+}\}$ which are the perturbed counterparts to the free Hamiltonians $\{H_{0s}, H_{0_+}\}$. Each Hamiltonian $H \in \{H_{s}, H_{+}\}$ shares a common differential form

$$H(x,t) = \frac{1}{2m}\left(\frac{\hbar}{i}\nabla_x - a(x,t)\right)^2 + v(x,t). \tag{2.23}$$

In showing the self-adjointness we shall use the method of relative boundedness. In doing so we require the definition of momentum operator $P: \mathcal{H} \to \mathcal{H}_v$. We define the momentum operator by specifying the effect of each of its components P_j:

$$P_j = \hbar F^{-1} \tilde{P}_j F f \qquad j = 1 \sim d \tag{2.24a}$$

with

$$(\tilde{P}_j \hat{f})(\xi) = \xi_j \hat{f}(\xi) \tag{2.24b}$$

and

$$D(\tilde{P}_j) = \{\hat{f} \in \ell^2(\Lambda): \quad \xi_j\hat{f} \in \ell^2(\Lambda)\}. \tag{2.24c}$$

The domain of P is given by $D(P) = F^{-1}D(\tilde{P})$. In case when $\Omega = R_+^d$, equations (2.24a,b) are valid while (2.24c) should be replaced by

$$D(\tilde{P}_j) = \{\hat{f} \in L_{s_+}(R^d): \xi_j\hat{f} \in L^2(R^d)\}. \tag{2.24d}$$

□

We now define a family of perturbing operators $W(t): D(P) \to L^2(R^d)$ by the equation

$$W(t) = \frac{1}{m}\, a(t)\cdot P + \frac{i\hbar}{2m}\,(\nabla\cdot a)(\cdot,t) + \frac{1}{2m}\, a^2(t) + v(t). \tag{2.25}$$

Here $a(t): H \to H_v$ is a d-dimensional vector whose components $a_i(t)$ are the operator mappings $H \to H_v$ defined by maximal multiplication by a real valued function $a_i(\cdot,t): \bar{\Omega} \to R$, satisfying Assumption 1. Likewise $v(t)$ is defined by multiplication by a real valued function $v(\cdot,t): \bar{\Omega} \to R$ satisfying Assumption 2.

<u>*LEMMA 2.2:*</u> *Assume that* a,v $\in$ A.

* *(a) Let Ω be a bounded hyperrectangle and let s be appropriate for either Dirichlet or periodic boundary condition, i.e., $s = (1,1,\ldots,1)$ or $s = (\cdot,\cdot,\ldots,\cdot)$, respectively. Then the perturbed Hamiltonians*

$$H_s(t)f = H_{0s}f + W(t)f, \qquad f \in D(H_{0s}) \tag{2.26a}$$

* See Supplement, page 144, for Dirichlet Hamiltonian.

are self-adjoint for each $t \in [0,T]$ *and have a time invariant domain*

$$D(H_s(t)) = D(H_{0s}). \tag{2.26b}$$

(b) *Let* Ω *be the half-space* R_+^d *and let* H_{0_+} *be the unperturbed Hamiltonian defined by the Dirichlet boundary condition (cf. equation 2.22a) on* ∂R_+^d. *Then the perturbed Hamiltonians*

$$H_+ f = H_{0_+} f + W(t) f, \qquad f \in D(H_{0_+}) \tag{2.27a}$$

are self-adjoint for each $t \in [0,T]$ *and have time invariant domain*

$$D(H_+(t)) = D(H_{0_+}). \tag{2.27b}$$

<u>Proof</u>: (a) By Assumptions 1 and 2 we note that the operators $\nabla \cdot a$, a^2 and V are all bounded which implies that they are Kato small relative to $H_0(m)$ [RS, vol.II, page 162]. It remains to show that $\frac{1}{m} a(\cdot,t) \cdot P$ is Kato small relative to the free Hamiltonian H_0. Since a is bounded it is clear that $D(\frac{1}{m} a(\cdot,t) \cdot P) \supseteq D(H_{0s})$. Now for $f \in D(H_0)$

$$\begin{aligned} \|a_j P_j f\|^2 &\le \|a_j\|_\infty^2 \; \|P_j f\|^2 \\ &\le \sum_{k=1}^{d} \|a_k\|_\infty^2 \; \sum_{k=1}^{d} \|P_k \hat{f}\|^2 \\ &= \sum_{k=1}^{d} \|a_k\|_\infty^2 \sum_{\xi \in \Lambda} |\xi \hat{f}(\xi)|^2 . \end{aligned}$$

In the last expression we have used the Plancherel formula for Fourier series. Recall that for a given $\alpha < 1$ there exists a $\beta > 0$ such that

$$|\xi|^2 \leq \alpha \ |\xi|^4 + \beta.$$

Using this inequality and Plancherel formula we obtain

$$||a\cdot Pf||^2 \leq ||a||_\infty^2 [\alpha \ ||H_{0\delta} f||^2 + \beta \ ||f||^2]$$

or

$$||a\cdot Pf|| \leq \alpha' \ ||H_{0\delta} f|| + \beta' \ ||f||.$$

Since α' can be made arbitrarily small, we have thus shown that $a\cdot P$ is Kato small relative to $H_{0\delta}$. An application of Kato-Rellich theorem [AJS] shows that $H_\delta(t)$ is self-adjoint. An identical argument works for the case when $\Omega = R_+^d$ and $\delta = \delta_+$ thereby proving part (b) of the lemma. □

<u>REMARK 2.2</u>: Lemma (2.2) establishes the self-adjointness of $H(t)$ when $\delta = (1,1,1...1)$. This proof is also valid when periodic boundary conditions are imposed. However, in Neuman case when $\delta = (0,0,...,0)$ the Hamiltonian operator with $a(t) \neq 0$ is not self-adjoint. We demonstrate this point by showing that the operator $\frac{1}{2m}(i\hbar\nabla - a(\cdot,t))^2$ is not symmetric when Neuman conditions are imposed. It suffices to consider one dimensional case. Let $f,g \in C^2[a,b]$ and for convenience set $\hbar = m = 1$ and suppress the t-dependence in $a(\cdot,t)$, then partial differential equation form of the Hamiltonian is

$$L = (i \frac{d}{dx} - a(x))^2 = -\frac{d^2}{dx^2} + i \frac{da(x)}{dx} + 2ia(x) \frac{d}{dx} + a^2(x).$$

A simple integration by parts yields

$$(f,Lg) = (Lf,g) + 2i\, a(x)\, g(x)\, \overline{f(x)} \Big|_a^b + [g(x) \frac{\overline{df(x)}}{dx} - \overline{f}(x) \frac{dg(x)}{dx}]_a^b.$$

The term in [...] vanishes if $\frac{df}{dx} = \frac{dg}{dx} = 0$ for $x = a$ and $x = b$. However, the second term above is generally not zero. Thus from the last expression we may conclude that L is not symmetric when $s = (0,\ldots,0)$. Due to this fact the Neuman problem is not of substantial physical interest in quantum evolution theory when electromagnetic fields are present. For this reason we exclude the Neuman case from the class of boundary value problems studied in the remainder of the thesis. □

Next we turn our attention to the discussion of bounded regions $\Omega \subseteq R^d$ with smooth boundaries. Only the Dirichlet condition is considered. For the potentials of class A it will be shown that it is possible to define a self-adjoint Hamiltonian with an explicit statement of its domain. We will also establish that this domain is time invariant.

<u>*Definition 2.8:*</u> *Let Ω be an open connected subset in R^d and let $u,v \in L^1(\Omega)$. We say that $D^\alpha u = v$ in the weak sense (and call v the α-th weak derivative of u) if, for every $\phi \in C_0^\infty(\Omega)$*

$$\int_\Omega u\, D^\alpha \phi\, dx = (-1)^{|\alpha|} \int_\Omega v\phi\, dx .$$ □

At this stage, it is useful to summarize several of the major results found in the study of eliptic boundary value problems. All of these results are to be found in the book by Friedman on Partial Differential Equations [F].

Definition 2.9: *A linear differential operator is an expression of the form*

$$B(x,D) = \sum_{|\alpha| \leq m} a_\alpha(x)\, D^\alpha \tag{2.28}$$

where the (complex) coefficients $a_\alpha(x)$ *are defined in some open set* Ω. *If the operator* $\sum_{|\alpha|=m} a_\alpha(x) D^\alpha$ *is not identically zero, then it is called the principal part of the operator defined in (2.28), and* m *is called the order of the operator in (2.28). The coefficients* a_α *with* $|\alpha| = m$ *are then called the principal coefficients. For operators of even order set* $m = 2p$, $p > 0$. *If*

$$(-1)^p \operatorname{Re}\left\{ \sum_{|\alpha|=2p} a_\alpha(x)\, \xi^\alpha \right\} \geq C_0 \;|\xi|^{2p}$$

for all $\xi \in R^d$ *and* $x \in \Omega$, *where* $C_0 > 0$ *is independent of* $x \in \Omega$ *and if the principal coefficients are bounded in* Ω, *then the operator (2.28) is said to be the uniformly strongly elliptic in* Ω. □

We now introduce the Sobolev spaces $\hat{C}^{j,p}(\Omega)$, $H^{j,p}(\Omega)$ and $H_0^{j,p}(\Omega)$.

$$\hat{C}^{j,p}(\Omega) = \left\{u \in C^{j}(\Omega):\ |u|^{\Omega}_{j,p} \equiv \left\{\sum_{|\alpha|\le j} \int_{\Omega} |D^{\alpha}u(x)|^{p}dx\right\}^{\frac{1}{p}} < \infty\right\}. \tag{2.29}$$

$H^{j,p}(\Omega)$ is the completion of $\hat{C}^{j,p}(\Omega)$ with respect to the norm $|\cdot|^{\Omega}_{j,p}$. Likewise $H^{j,p}_{0}(\Omega)$ is the completion of $C^{j}_{0}(\Omega)$ with respect to the norm $|\cdot|^{\Omega}_{j,p}$. A special case of interest is when $p = 2$. In this case we shall use the following abbreviated notation, i.e.,

$$H^{j}(\Omega) \equiv H^{j,2}(\Omega) \quad ; \quad H^{j}_{0}(\Omega) \equiv H^{j,2}_{0}(\Omega)$$

and

$$\|\ \|^{\Omega}_{j} \equiv |\cdot|^{\Omega}_{j,2} .$$

$H^{j}(\Omega)$ is a Hilbert space with scalar product $(\#,\#)_{j}$. In the special case when $j = 0$, $H^{0}(\Omega) = L^{2}(\Omega)$.

Armed with this notation we recall the following important results whose proof is found in Friedman's book [F, Lemma 18.2].

<u>LEMMA 2.3</u>: *Let Ω be a bounded domain with $\partial\Omega \in C^{2m}$ and assume that B: D_B $(\equiv H^{2m}(\Omega) \cap H^{m}_{0}(\Omega)) \to L^{2}(\Omega)$ is uniformly strongly elliptic in Ω with $a_{\alpha} \in C^{0}(\bar{\Omega})$. Then for all λ with $-\pi/2 + \epsilon \le \arg\lambda \le \pi/2 - \epsilon$, $|\lambda| \ge \Lambda_0$ ($\epsilon > 0$, arbitrarily small; Λ_0 sufficiently large), the operator $B+\lambda I$ maps D_B onto $L^{2}(\Omega)$.* □

<u>LEMMA 2.4</u>: *Let Ω be a bounded domain with $\partial\Omega \in C^{2}$ and assume that the potentials $a, v \in A$. Denote by $H_{\Omega}(t)$: $H^{2}(\Omega) \cap H^{1}_{0}(\Omega) \to L^{2}(\Omega)$, the operator generated by the strongly*

uniformly elliptic linear partial differential expression (2.23) in Ω. Then, the Hamiltonian $H_\Omega(t)$ (compatible with Dirichlet boundary condition) is self-adjoint.

Proof: By integration by parts it can be shown that the PDE form of $H_\Omega(t)$ [equation 2.23] is symmetric. Lemma 2.3, for $\tau = \pm i$ shows that the range $R(H_\Omega \pm i) = L^2(\Omega)$. Under these circumstances it follows [AJS , Proposition 2.14] that $H_\Omega(t)$ is self-adjoint.

REMARK 2.3:

(1) To see how $H^2(\Omega) \cap H_0^1(\Omega)$ suffices to 'coerce' the boundary values of $f \in D(H_\Omega(t))$ thereby showing that H_Ω is consistent with Dirichlet boundary conditions we recall the following result from PDE literature [F, Lemmas 13.2, 13.3].

LEMMA 2.5: *(a) Assume* $\partial\Omega \in C^k$. *If* $u \in H_0^k(\Omega) \cap C^{k-1}(\bar{\Omega})$ *then* $\frac{\partial^j u}{\partial v^j} = 0$ *on* $\partial\Omega$ *for* $0 \le j \le k-1$.

(b) Assume $\partial\Omega \in C^k$. *If* $u \in C^k(\bar{\Omega})$ *and if* $\frac{\partial^j u}{\partial v^j} = 0$ *on* $\partial\Omega$ *for* $0 \le j \le k-1$, *then* $u \in H_0^k(\Omega)$. □

In the special case when $k = 2$ and $j = 0$ we observe from Lemma (2.5) that $D(H_\Omega(t))$ is consistent with Dirichlet boundary conditions.

(2) If $d \le 3$, the results of Lemmas (2.2) and (2.4) can be further enhanced to include boundaries having finitely many

piecewise smooth surfaces satisfying an external cone condition [R, section 6.4]. Richtmeyer [R, Section 11.7] has shown that an operator $\hat{A}_0$, defined as minus the Laplacian acting on sufficiently smooth functions f(x) that vanish on boundary:

$$D(\hat{A}_0) = \{f \in C(\bar{\Omega}) : \Delta f \in C(\Omega) \text{ and } f = 0 \text{ on } \partial\Omega\} \tag{2.30a}$$

$$\hat{A}_0 f = -\Delta f \; , \quad f \in D(\hat{A}_0) \tag{2.30b}$$

is essentially self-adjoint in $L^2(\Omega)$. Thus $\hat{A}_0$ has a unique self-adjoint extension, say H_0, in $L^2(\Omega)$. We call H_0 to be the free Hamiltonian for the problem at hand. Once H_0 is defined we can once again invoke Kato-Rellich theorem to show that for $a,v \in A$ the perturbed Hamiltonian H(t) is self-adjoint with time invariant domain $E_0 \equiv D(H_0)$. It is reasonable to expect that the same results hold in higher dimensions. Note that the bounded hyperrectangular regions and domains with C^2-boundaries discussed in Lemmas (2.2) and (2.4) are special examples of the region considered in this remark. □

The next task is to show that the operator A(t) defined by (2.11) satisfies the hypotheses of Theorem 2.1, needed to generate an evolution. We begin by showing that a given Hamiltonian $H(t) \in \{H_\Delta, H_+, H_\Omega\}$ is strongly continuously differentiable with respect to t. Let $a,v \in A$ and define the family of operators $\dot{H}(t)$ by the equation

$$\dot{H}(t) = -\frac{1}{m}\dot{a}(t)\cdot P + \frac{i\hbar}{2m}(\nabla\cdot\dot{a})(\cdot,t) + \frac{1}{m}a(t)\cdot\dot{a}(t) + \dot{v}(t) . \tag{2.31}$$

By our assumptions on scalar and vector potentials it is easy to see that $\dot{H}(t)$ is well defined on $D(H_0)$. We assert that $H(t,m)$ is the strongly continuous t-derivative of $H(t)$.

<u>LEMMA 2.6</u>: *Let* $a, v \in A$, *then any* $H(t) \in \{H_s, H_+, H_\Omega\}$ *is strongly continuously differentiable on* $D(H_0)$. *Moreover the value of the strong derivative of* $H(t)$ *is given by the formula*

$$\frac{d}{dt} H(t)\psi = \dot{H}(t)\psi \quad , \qquad \psi \in D(H_0). \tag{2.32}$$

<u>Proof</u>: Let $\delta t \neq 0$, $\psi \in D(H_0)$ and consider the following in the limit $\delta t \to 0$:

$$\begin{aligned}
&\left\|\frac{1}{\delta t}[H(t+\delta t) - H(t)]\psi(\cdot) - \dot{H}(t)\psi\right\| \\
&\quad \le \frac{1}{m}\left\|\frac{a(\cdot,t+\delta t)-a(\cdot,t)}{\delta t} - \dot{a}(\cdot,t)\right\|_\infty \|P\psi\|_V \\
&\qquad + \frac{\hbar}{2m}\left\|\frac{(\nabla\cdot a)(\cdot,t+\delta t)-(\nabla\cdot a)(\cdot,t)}{\delta t} - (\nabla\cdot\dot{a})(\cdot,t)\right\|_\infty \|\psi\| \\
&\qquad + \frac{1}{2m}\left\|\frac{a(\cdot,t+\delta t)^2-a(\cdot,t)^2}{\delta t} - 2\dot{a}(\cdot,t)\cdot a(\cdot,t)\right\|_\infty \|\psi\| \\
&\qquad + \left\|\left[\frac{v(\cdot,t+\delta t)-v(\cdot,t)}{\delta t} - \dot{v}(\cdot,t)\right]\right\|_\infty \|\psi\|
\end{aligned}$$

By the hypotheses on potentials $a(t)$ and $v(t)$ we note that the right hand side in the above inequality vanishes in the limit $\delta t \to 0$. This establishes equation (2.32). The strong continuity of $\dot{H}(t)$ on $D(H_0)$ follows from the assumptions on potentials and from an argument similar to the one presented above. □

The last step in our study of Hamiltonian properties is to show that the resolvent of A(t) defined by (2.11) satisfies the resolvent estimate (2.7) for a suitably chosen constant c.

We first derive a simple relation between the resolvents of $H(t) \in \{H_\delta, H_+, H_\Omega\}$ and the corresponding A(t).

$$R(\lambda, A(t)) \equiv [A(t) - \lambda]^{-1} = [\frac{1}{i\hbar} H(t) - c - \lambda]^{-1}$$

$$= i\hbar[H(t) - ih(c+\lambda)]^{-1}$$

$$= i\hbar \cdot R(i\hbar(c+\lambda), H(t)) . \qquad (2.33)$$

Since H(t) is self-adjoint its spectrum is contained by the real line. If $d(Z,\sigma(H))$ denote the distance between a complex number Z and $\sigma(H)$ then

$$||R(i\omega, H(t))|| = \frac{1}{d(i\omega,\sigma(H))} \leq \frac{1}{\omega} \leq \frac{1}{\omega-\alpha} ; \quad \omega > \alpha . \qquad (2.34)$$

From (2.33) and (2.34) it follows that

$$||R(\lambda, A(t))|| = h\, ||R(i\hbar(c+\lambda), H(t))||$$

$$\leq \frac{\hbar}{\hbar(c+\lambda)-\alpha} = \frac{1}{(c+\lambda) - \alpha/\hbar}$$

We choose the constant $c = 1 + \alpha/\hbar$, thereby obtaining the required result

$$||R(\lambda, A(t))|| \leq \frac{1}{1+|\lambda|} . \qquad (2.35)$$

Conclusion

In the preceding discussion we have shown that for $a, v \in A$, the operator $A(t)$ satisfies the hypotheses of Theorem (2.2) with constant $c = 1 + \alpha/\hbar$. This establishes the existence of Schrödinger evolution operator for all boundary value problems described in this chapter.

CHAPTER 3

THE APPROXIMATE QUANTUM EVOLUTION

3.0 Introduction

In this chapter we propose a large mass approximation scheme to solve the problem of quantum evolution for a many body system. The coordinate manifold Ω is assumed to be a d-dimensional Euclidean space R^d. Extensions of this method to include various hyperrectangular subsets of R^d as the coordinate manifolds will be discussed in later chapters. Our discussion begins with the mathematical definition of the problem [Section 3.1]. In order to provide an adequate background we devote Section 3.2 to summarizing some of the recent results concerning the existence of the quantum propagator and the associated large mass asymptotic expansion. For the class of real analytic potentials that can be represented as the Fourier transform of time-dependent complex valued measures it is known that a constructive representation of the propagator K is possible [OPC] and that the propagator admits a large mass asymptotic expansion [POM] which is valid on compact subsets of $R^d \times R^d$. In our summary we note that for potentials which are not in this class of real analytic potentials the Dyson's series method used in [OPC, POM] will no longer construct the rigorous pointwise propagator nor provide the analytic foundation for asymptotic approximation to the propagator. This motivates us to consider the idea of

Parametrix (approximate) solutions of Schrödinger's PDE. Guided by the [POM] results we select an appropriate parametrix solution valid for a system with finitely differentiable scalar and electromagnetic vector fields. The Section 3.2 concludes with the derivation of a non-homogeneous PDE satisfied by the parametrix kernel. The task of Section 3.3 is to show that the inhomogeneous identity satisfied by the parametrix determines an abstract inhomogeneous equation of motion in $L^2(R^d)$. In Section 3.4 we show that there is a unique solution to this abstract equation which defines the approximate evolution operator $U_M(t,s)$ generated by the parametrix of Section 3.2. Next we compute the difference between the exact and approximate abstract evolutions in the L^2-norm and show that it vanishes as mass $m \to \infty$. This establishes that we have constructed an asymptotic expansion to the quantum dynamics that is valid in L^2-topology. Finally, in Section 3.5 we use the results obtained in previous sections to compute the expectation value of all $H(t)$-bounded observables in the approximate quantum state $\psi_M = U_M\phi$ and show that it is asymptotically close to the expectation value in exact quantum state. In the foregoing analysis we shall require a number of auxillary estimates which are placed in the Appendix 3.1 following the main text of this chapter.

3.1 Mathematical Definition of the Problem

We begin with a statement providing the general definition of the pointwise form of the quantum propagator.

Definition 3.1: *A two-parameter family (in* T_Δ, $t \neq s$*) of functions* $K(\cdot,t;\cdot,s): R^d \times R^d \to C$ *that are measurable and* $L^1(R^d \times R^d)$ *is called the propagator for evolution* $\{U(t,s);\ t,s \in T_\Delta\}$ *if for all bounded* $L^2(R^d)$ *functions of compact support* f, g

$$(f,U(t,s)g) = \int_{R^d \times R^d} \bar{f}(x)K(x,t;y,s)g(y)\,dxdy. \tag{3.1}$$

□

In some circumstances, the propagator can be obtained as the fundamental solution of the partial differential equation realization of Schrödinger's equation of motion,

$$i\hbar \frac{\partial}{\partial t} K(x,t;y,s) = H(x,-i\hbar\nabla_x,t,m)K(x,t;y,s) \tag{3.2}$$

for all $(t,s;x,y) \in T_\Delta \times \Omega \times \Omega$ where $\Omega \in HR$. The fundamental solution satisfies the following two restrictions:

(a) the initial condition;

$$\lim_{t\to s^+} K(x,t;y,s) = \delta(x-y) \tag{3.3a}$$

and if $\Omega \neq R^d$ a boundary condition on $\partial\Omega$. For example,

(b) the Dirichlet boundary condition

$$K(x,t;y,s)\Big|_{x\in\partial\Omega} = K(x,t;y,s)\Big|_{y\in\partial\Omega} = 0. \tag{3.3b}$$

It is the presence of the two conditions (3.3a) and (3.3b) that characterizes a mixed boundary value problem.

Let $H(t,m)$ be any of the self-adjoint operators $\{H_\delta, H_+, H_\Omega\}$ of Lemma 2.2. Acting on smooth functions, all these operators have a common local differential form:

$$H(x,-i\hbar\nabla_x,t;m) = \frac{1}{2m}\left(\frac{\hbar}{i}\nabla_x - a(x,t)\right)^2 + v(x,t). \qquad (3.4)$$

The function a above represents a time-dependent vector field mapping $R^d \times [0,T] \to R^d$ while v is a time dependent scalar potential from $R^d \times [0,T] \to R$.

In the remainder of this chapter we shall focus our attention on a special problem, namely the case where $\Omega = R^d$. Note that this particular problem is not a mixed boundary value problem.

3.2 The Parametrix or Approximate Propagator

To provide an adequate background for the study of approximate quantum evolution, we devote this entire section (3.2) to summarizing the details of two recent papers [OPC,POM] followed by comments regarding the construction of approximate propagators.

The analysis of [OPC POM] requires analytic fields. This class of potentials is much narrower than those found in Assumption I of Chapter 2. Specifically the vector and scalar fields used in [POM] satisfy the following hypothesis.

Vector Field Hypothesis: The vector field a: $R^d \times [0,T] \to R^d$ *is assumed to be the fourier image of a vector measure with* *finite total variation,*

$$a(x,t) = \int_{R^d} e^{i\alpha\cdot x} d\gamma(t). \tag{3.5}$$

Here α *is the variable of integration (not displayed in the measure).* $\gamma(t)$ *is a compactly supported,* C^d*-valued measure on* R^d *obeying a reflection property* [OPC]. *For each* $t \in [0,T]$ $\operatorname{supp}\gamma \subset S_{k/2}$ *where* $S_{k/2}$ *is the sphere of radius* $k/2$ *in* R^d. *The reflection property insures that* a *is real while the compact support of* γ *implies that* $a(x,t)$ *is real analytic function of* x.

<u>*Scalar Field Hypothesis*</u>: *The scalar field* $v\colon R^d \times [0,T] \to R$ *is assumed to be the fourier image of a scalar measure with finite total variation*

$$v(x,t) = \int_{R^d} e^{i\alpha\cdot x} d\nu(t) \tag{3.6}$$

where $\nu(t)$ *is a compactly supported, scalar valued complex measure with a reflection property which ensures the real valuedness of* v [OPC]. *Furthermore,* $\operatorname{supp}\nu(t) \subset S_k$, *for* $t \in [0,T]$. *Thus for each* $t \in [0,T]$, $v(x,t)$ *has bounded derivatives of any order in* x. □

Let $H(t,m)$ be one of the self-adjoint operators of Lemma 2.2; then the abstract Schrödinger evolution problem in $T_\Delta \equiv \{(t,s) \in R^2;\ 0 \le s \le t \le T\}$ consists of solving

$$i\hbar \frac{d}{dt} \psi(t) = H(t,m)\psi(t), \quad \psi(t) \in D(H(t,m)) = D(H_0(m)) \tag{3.7}$$

with

$$\psi(s) = \phi; \quad \phi \in D(H_0(m)). \tag{3.8}$$

Here $H_0(m)$ is understood to be the free self-adjoint operator of Lemma 2.1, i.e., $H_0 \in \{H_{0\delta}, H_{0_+}, H_\Omega\}$ that results from $H(t,m)$ if the vector potential $a(x,t)$ and the scalar potential $v(x,t)$ are absent.

The first goal is to determine a bounded operator family $U(t,s)$: $\mathcal{H} \to \mathcal{H}$ such that

$$\psi(t) = U(t,s)\phi, \qquad t,s \in T_\Delta. \tag{3.9}$$

Let $H(t)$ be interpreted as the perturbation of the self-adjoint free Hamiltonian H_0. Then using (3.9) the abstract integral equation equivalent to (3.7) and (3.8) can be formally written as

$$U(t,s) = U_0(t,s) - \frac{i}{\hbar} \int_s^t d\tau \; U_0(t,\tau)V(\tau)U(\tau,s) \tag{3.10}$$

with

$$U(s,s) = 1 \tag{3.11}$$

where U_0 is the free evolution operator $\exp[i\hbar^{-1}H_0(t-s)]$.

A standard approach (in the physics literature) of investigating $U(t,s)$ is to iterate (3.10) to obtain the familiar Dyson's expansion

$$U(t,s)\phi = U_0(t,s)\phi$$
$$+ \sum_{n=1}^{\infty} (-\tfrac{i}{\hbar})^n \int_< dt_n \ldots dt_1 U_0(t,t_n) V(t_n) U_0(t_n,t_{n-1}) \ldots$$
$$\ldots V(t_1) U_0(t_1,s)\phi \qquad (3.12)$$

where the integral subscript $<$ denotes the time-ordered domain $t \geq t_n \geq \ldots \geq t_1 \geq s$ and ϕ is some initial data wave function in $L^2(\Omega)$. In general (K, Chapter IX) the unboundedness of the operators $V(t_i)$ usually means that this iteration method does not yield a rigorous result for $U(t,s)\phi$. Specifically the integrand contains the point $t_n = t_{n-1} = \ldots = t_1 = s$ with the associated operator integrand $V(s)^n$. As $n \to \infty$ the domain of this operator can shrink to zero.

Nevertheless, for the evolution problem in coordinate domain $\Omega = R^d$ and with analytic potentials (3.5) and (3.6), it has been shown [OPC] that for a specific class of Cauchy initial data (i.e., $\hat{\phi} \in C_0^\infty(R^d)$) the series (3.12) provides a solution of the evolution problem (3.7) and (3.8). Furthermore, it is also established that, for masses with positive imaginary part the right hand side of (3.12) generates a bounded integral operator with a Carleman kernel [HS] given by

$$K(Q) = \sum_{n=0}^{\infty} d_n(Q) \qquad (3.13)$$

where $Q = (x,t;y,s)$ and $d_n(Q)$ is the kernel associated with the n^{th} term on the right hand side of equation (3.12). Finally by using the method of mass continuation to the real mass axis the following result was determined.

<u>*PROPOSITION 3.1:*</u> *Let* $\Omega = R^d$ *and suppose* a *and* v *satisfy hypothesis* (3.5) *and* (3.6). *Assume that* $\phi \in L_0^2(R^d)$, $m > 0$ *and* $0 < \frac{2ek(t-s)}{|m|}\gamma_T < 1$. *If* $U(t,s)$ *is the Schrödinger evolution operator generated by the Hamiltonian family* $\{H(t,m);\ t \in [0,T]\}$ *and if* $K(\cdot,t;\cdot,s): R^d \times R^d \to C$ *is the continuous function given by* (3.13), *then for a.a.* $x \in R^d$, $t \neq s$

$$[U(t,s)\phi](x) = \int K(t,x;s,y;m)\phi(y)dy; \quad m \in R^+. \tag{3.14}$$

Furthermore, one can explicitly verify that $K(Q)$ *is the fundamental solution (in a pointwise sense) of the classical PDE* (3.2).

<u>Proof</u>: [OPC, Theorem 3, POM Proposition 2]. □

In conclusion, the above results demonstrate that for vector and scalar fields of the form (3.5) and (3.6) it is possible to show that the Dyson series is convergent. Moreover, by using the method of mass continuity explicit construction of the propagator $K(Q)$ is possible.

To discuss various parametrices of interest we need to know the analytic structure in mass of the quantum propagator $K(Q)$. This problem was investigated in a recent paper [POM]. It was shown that the propagator K of (3.14) admits a factorization

$$K(Q) = K_0(Q)F(Q;m^{-1}) \tag{3.15}$$

where K_0 is the propagator for the evolution problem associated with the free Hamiltonian $H_0(m)$ acting in $L^2(R^d)$. This free propagator carries all the essential singularity of the exact propagator K in the variable $m^{-1} = 0$. It is given by the following well known expression

$$K_0(\Omega) = \left[\frac{m}{2\pi i\hbar(t-s)}\right]^{d/2} \exp\left[\frac{im}{2\hbar(t-s)} (x-y)^2\right]. \tag{3.16}$$

In the subsequent considerations it was established that the function F can also be factorized as a product of two functions. Upon setting $u = m^{-1}$, one has

$$F(Q;u) = \exp[(i\hbar)^{-1}J(Q)]T(Q;u) \tag{3.17}$$

where

$$J(Q) = (t-s)\int_0^1 v(w(\xi))d\xi - \int_0^1 (x-y)\cdot a(w(\xi))d\xi. \tag{3.18}$$

In the last expression w is the linear path in $R^d \times [0,T]$ connecting the initial space time point (y,s) to the final point (x,t)

$$w(\xi) = w(\xi;Q) = (y+\xi(x-y),\ s+\xi(t-s)), \qquad \xi \in [0,1]. \tag{3.19}$$

Observe that J is a mass-independent function and the function T(Q;u) in (3.17) admits a small u asymptotic expansion. The following result summarizes these details.

PROPOSITION 3.2: Let us assume that

(a) *the potentials* a *and* v *are given by* (3.5) *and* (3.6);

(b) $u_0 < (2ekT\gamma_T)^{-1}$;

(c) $u \in C(u_0) = \{Z \in C: |Z| < u_0;\ \mathrm{Im}\ Z \leq 0\}$;

then, for all integers $M \geq 1$ *the function* $T\colon T_\Delta \times R^d \times R^d \times C(u_0) \to C$ *has the small* u *asymptotic expansion in* $C(u)$

$$T(Q;u) = \sum_{j=0}^{M-1} u^j T_j(Q) + u^M E_M(Q;u) \tag{3.20}$$

where

$$|E_M| \leq c_1 \exp(c_2|x-y|) \tag{3.21}$$

with c_1 *and* c_2 *being independent of* M. *The functions* $T_j\colon T_\Delta \times R^d \times R^d \to C$ *possess continuous partial derivatives to an arbitrary order in* (x,y). *Furthermore, for all* $Q \in T_\Delta \times R^d \times R^d$, $T_0(Q) = 1$ *and the higher order coefficient functions* $\{T_j(Q)\}_1^{M-1}$ *are uniquely determined by the transport recurrence relation*

$$T_j(Q) = (t-s) \int_0^1 g_{j-1}(\omega(\xi;Q);y,s)\,d\xi \tag{3.22}$$

where

$$g_{j-1}(Q) = \frac{1}{2}\{(ih)\cdot\Delta_1 - 2\bar{f}\cdot\nabla_1 + [-\nabla_1\cdot\bar{f} + (ih)^{-1}\bar{f}^2]\}T_{j-1}(Q) \tag{3.23a}$$

where $\bar{f}(Q)$ *is a vector function of the external forces and electromagnetic fields and* $\nabla_1(\Delta_1)$ *denotes the gradient (Laplacian) with respect to first vector argument of a function. In particular the* i^{th} *component of* $\bar{f}$ *is*

$$\bar{f}_i(Q) = (t-s) \int_0^1 d\xi\ \xi\left\{f_i(\omega(\xi)) + \sum_{j=1}^{d} \frac{(x-y)_j}{(t-s)}\left[\frac{\partial}{\partial x^i} a_j(\omega(\xi)) - \frac{\partial}{\partial x^j} a_i(\omega(\xi))\right]\right\}; \tag{3.23b}$$

$$f_i(Q) = -\frac{\partial}{\partial x_i} v(x,t) - \frac{\partial}{\partial t} a_i(x,t). \tag{3.23c}$$

The {}-bracket portion of the integrand in (3.23b) corresponds to the Lorentz force in d-dimensions.

Proof: See [POM]. □

A careful survey of the method used above reveals that the specific analytic form of potentials a and v given by (3.5) and (3.6) is crucial in showing the convergence of Dyson's series. For potentials which do not belong to this class, finite partial sums of Dyson's series can be shown to exist but it is no longer possible to prove in either the L^2-norm or the pointwise norm (for kernels) that the Dyson's series converges. Nevertheless, the formal truncated m^{-1} asymptotic expansion for $K(\Omega)$ [cf. (3.20)] will remain useful if the potential supports enough continuous derivatives to calculate $T_i(\Omega)$ via (3.22). In general the existence of the exact propagator and its analytic properties are not available for non-analytic potentials. This motivates us to consider the idea of parametrix (approximate) solution to the PDE Problem (3.2), (3.3a) and (3.3b). For example, one evident choice is to truncate the m^{-1} asymptotic expansion of K and consider it to be the candidate parametrix. This type of parametrix solution does not provide a solution of the Schrödinger PDE but rather it can be shown to satisfy an inhomogeneous Schrödinger Equation. The inhomogeneous term is typically a smooth function of all of its arguments and is completely determined by the definition of the approximate propagator. The second stage of this approach is to show that a suitably modified version of this parametrix defines a bounded strongly t-differentiable operator, i.e., an approximate evolution operator. Then if it can be shown that the approximate wave function approaches the exact wave-function, in an appropriate norm (i.e., L^2-norm), one can claim to have a bonafide asymptotic expansion of the evolution problem.

For the approximate propagator we seek a function which shares most of the properties of the exact propagator $K(Q)$. An obvious choice for such a function is

$$W_M(Q) = K_0(Q) \exp(-\frac{i}{\hbar} J(Q)) \sum_{i=0}^{M} \frac{1}{m^i} T_i(Q). \tag{3.24}$$

For the real analytic potentials, the coefficient functions $T_i(Q)$ are given by the recurrence relation (3.22). It is also known [POM] that T_i's exhibit a polynomial growth in $|x-y|$. On the other hand W_M has an oscillatory multiplicative factor $\exp[\frac{im}{2\hbar(t-s)} (x-y)^2]$ which for large (x-y) oscillates vigorously and could be expected to offset the aforementioned growth in T_i's. This suggests that after integration with a smooth test function, the wave function receives small contribution from $W_M(Q)$ for large (x-y). For this reason we define a parametrix obtained by multiplying W_M in (3.24) by a smooth cut-off function that is one in the neighbourhood of the diagonal $x = y$ and is zero for sufficiently large $|x-y|$. The resulting parametrix will be denoted by $K_M(Q)$.

We are now ready to make precise definition of the parametrix solution of Schrödinger's PDE (3.2). We begin by stating the assumptions on scalar and vector potentials explicitly. This class of potentials will be substantially wider than found in (3.5) and (3.6). Next follows a useful result regarding the pointwise bounds for the corresponding coefficient functions $T_i(Q)$. With this result in hand, we will then define the parametrix $K_M(Q)$. Finally, a derivation of the PDE identity satisfied by K_M will conclude this section.

Assumption 3: For integer $M > 0$ we say that vector potential a and scalar potential v belong to class A(M) if a and v satisfy

(i) Assumptions 1 and 2 of Chapter 2;

(ii) $a_i(\cdot,t) \in C^M(R^d)$; $\frac{\partial}{\partial t} a_i(\cdot,t) \in C^M(R^d)$; $i = 1 \sim d$;

and $v(\cdot,t) \in C^M(R^d)$; $\frac{\partial}{\partial t} v(\cdot,t) \in C^M(R^d)$

where $M < \infty$ and $t \in [0,T]$;

(iii) There is a k such that for all $t \in [0,T]$; $|\gamma| \leq M$, the following (x,t)-uniform bounds hold:

$$|\nabla^\gamma a_i(\cdot,t)| \leq c_1(\gamma) \equiv k^{|\gamma|}\tilde{c}_1 < \infty$$

$$|\nabla^\gamma (\tfrac{\partial}{\partial t})^\alpha a_i(\cdot,t)| \leq c_3(\gamma) \equiv k^{|\gamma|}\tilde{c}_3 < \infty; \quad \alpha = 1,2$$

and

$$|\nabla^\gamma v(\cdot,t)| \leq c_2(\gamma) \equiv k^{|\gamma|}\tilde{c}_2 < \infty$$

$$|\nabla^\gamma \tfrac{\partial}{\partial t} v(\cdot,t)| \leq c_4(\gamma) \equiv k^{|\gamma|}\tilde{c}_4 < \infty. \qquad \square$$

For potentials in class A(M) the function W_M in (3.24) is defined and the corresponding coefficient functions T_i are determined via the recurrence relation quoted in (3.22). For the pointwise bounds on T_i's we have the following result.

LEMMA 3.1: *Let* $n \geq 1$ *and suppose* a *and* v *are in class* A(2M+n); *then for* $i = 1 \sim M$ *and* $|\beta| \leq n$

$$|\nabla_1^\beta T_i(Q)| \leq \left(\frac{d\Delta t}{2h}\right)^i k^{|\beta|} Z[2^{|\beta|} Z + \lambda_i \hbar k]^{2i-1} \tag{3.25}$$

where $\Delta t \equiv (t-s)$, $Z \equiv Z(|x-y|,\Delta t) = 2\tilde{c}_1\sqrt{d}\,(k|x-y|+n) + \Delta t(k\tilde{c}_2+\tilde{c}_3)$ *and* $\lambda_i = 2^{2i-3} + \frac{1}{2}\lambda_{i-1}$; $\lambda_1 = 1$.

Proof: See Appendix 3.1. □

Next, we define a smooth cut-off function.

Definition 3.2: *(Regularized Heaviside function)* [*Bre*].

Let $\chi_D\colon R^d \to R^+$ *be a characteristic function defined by*

$$\chi_D(x) = 1 \quad \text{if } |x| < D;\quad D > 0$$
$$= 0 \quad \textit{otherwise.}$$

Introduce a function $\rho_\ell \in C^\infty(R^d)$; $\ell < D$

$$\rho_\ell(x) = 0 \qquad \textit{if } |x| > \ell$$
$$= k_\ell \exp\left(-\frac{\ell^2}{\ell^2-|x|^2}\right) \qquad \textit{otherwise}$$

where $k_\ell = \frac{k}{\ell^d}$ *and the normalization constant*

$$k^{-1} = \int_{|x|\leq 1} \exp[-(1-|x|^2)^{-1}]dx.$$

The regularized Heaviside function is given by

$$(\chi_D * \rho_\ell)(x) = \int_{R^d} \chi_D(y)\rho_\ell(x-y)\,dy$$

$$= \int_{R^d} \chi_D(x-y)\rho_\ell(y)\,dy. \tag{3.26}$$

The regularized Heaviside function $(\chi_D * \rho_\ell)$ *defined above has the following obvious properties:*

1°. $\chi_D * \rho_\ell \in C^\infty(R^d)$

2°. $$\chi_D * \rho_\ell(x) = 1 \quad \textit{if} \quad |x| < D-\ell$$
$$= 0 \quad |x| > D+\ell$$

3°. *For any multi index* $\gamma > 0$

$$\nabla_x^\gamma \chi_D * \rho_\ell(x) \neq 0 \quad \textit{only if} \quad D-\ell \le |x| \le D+\ell.$$

Moreover,

$$\| \nabla_x^\gamma(\chi_D * \rho_\ell) \|_{L^1(R^d)} = C(\gamma, D, \ell) < \infty.$$

4°. *For any integer* $n > 0$ *define* $\chi_n^+ : R^d \to R^+$ *by*

$$\chi_n^+(x) = \sup_{|\gamma| \le n} |\nabla_x^\gamma(\chi_D * \rho_\ell)(x)|.$$

Then

$$\chi_n^+ \in L^1(R^d) \cap L^\infty(R^d).$$ □

Now, define the parametrix $K_M(Q)$ for the PDE (3.2) by setting

$$K_M(Q) = (\chi_D * \rho_\ell)(x-y)W_M(Q) \tag{3.27}$$

where $W_M(Q)$ is given by (3.24). In this case the coordinate manifold is $\Omega = R^d$ and thus no supplemental boundary conditions are present.

The next step in our analysis is to state and prove some of the properties of the approximate propagator. To begin with, we recall the following useful multi-dimensional stationary phase asymptotic formula [Fed].

LEMMA 3.2: *Let* $h: R^d \times R^+ \to C$ *be a function satisfying:*
(i) There exists a compact set $Y \subset R^d$*, whose interior contains* $\operatorname{supp} h(\cdot,\lambda)$ *for all* $\lambda \in R^+$ *and*
(ii) For every d*-component multi index* γ *of length* $|\gamma| \leq d$*, the partial derivatives* $\nabla^\gamma h: R^d \times R^+ \to C$ *exist and are continuous.*

For $0 \neq \lambda \in R^+$*, define the integral*

$$I(\lambda) \equiv \left(\frac{1}{\pi i \lambda}\right)^{d/2} \int_{R^d} \exp[iy^2/\lambda]h(y,\lambda)\,dy. \tag{3.28}$$

Then

$$\lim_{\lambda \to 0} I(\lambda) = h(0,0). \tag{3.29}$$

Proof: See [POM, Lemma 4; Fed]. □

<u>*LEMMA 3.3:*</u> *Let* $a(\cdot,t)$ *and* $v(\cdot,t)$ *be in class* $A(2M+2)$ *and assume that* $\phi \in D_0 = D(H(t))$. *Define*

$$\psi(x,t) = \int K_M(Q)\phi(y)\,dy.$$

Then,

$$\psi(\cdot,t) \in C^2(R_x^d) \;;\; t \in (s,T]$$

$$\psi(x,\cdot) \in C^1(s,T) \;;\; \textit{for each } x \in R^d.$$

Furthermore,

(a) $$\nabla_x^\gamma \psi(x,t) = \int \nabla_x^\gamma K_M(Q)\phi(y)\,dy \;; \qquad |\gamma| \le 2 \tag{3.30}$$

$$\frac{\partial}{\partial t}\psi(x,t) = \int \frac{\partial}{\partial t} K_M(Q)\phi(y)\,dy. \tag{3.31}$$

(b) *For* $\phi \in C_0^d(R^d) \cap D_0$

$$\lim_{t\to s^+} \int K_M(Q)\phi(y)\,dy = \phi(x); \qquad (x,t) \in R^d \times [0,T]. \tag{3.32}$$

<u>Proof</u>: (a) Proof of this lemma uses a theorem in analysis justifying the interchange of partial derivatives and integration. Note that

(i) For a.a. $y \in R^d$; $K_M(Q)\phi(y) \in C^2(R_x^d)$.

(ii) For every $x \in R^d$, $\nabla_x^\gamma K_M(x,t;\cdot,s)$ is a function of compact support and furthermore

$$\nabla_x^\gamma K_M(x,t;\cdot,s)\phi(\cdot) \in L^1(R_y^d); \qquad |\gamma| \le 2.$$

(iii) For every compact set $X \subset R^d$ and γ with $|\gamma| = 2$

$$|\nabla_x^\gamma K_M(x,t;\cdot,s)\phi(\cdot)| \leq C(\gamma,X;D,\ell); \quad (x,y) \in X \times R^d.$$

Under conditions (i) ~ (iii) a standard theorem in analysis based primarily on dominated convergence theorem [Car] yields that

$$\psi(\cdot,t) \in C^2(R_x^d)$$

and for $|\gamma| \leq 2$

$$\nabla_x^\gamma \psi(x,t) = \nabla_x^\gamma \int K_M(Q)\phi(y)\,dy = \int \nabla_x^\gamma K_M(Q)\phi(y)\,dy.$$

This proves the validity of (3.30).

Since $K_M(Q)$ has continuous first order partial derivates with respect to t and s, one can revise the above arguments to prove equation (3.31).

(b) Let $\phi \in C_0^d(R^d)$, then for $x \in R^d$

$$\psi(x,t) = \int_{R^d} dy\left(\frac{m}{2\pi i\hbar\Delta t}\right)^{d/2} (\chi_D * \rho_\ell)(x-y)$$
$$\times \exp\left[\frac{im}{2\hbar\Delta t}(x-y)^2 - \frac{i}{\hbar}J(Q)\right]\sum_{i=0}^{M} m^{-i}T_i(Q)\phi(y).$$

Let $y \to y+x$ and set $\lambda = 2\hbar\frac{\Delta t}{m}$, then

$$\psi(x,t) = \left(\frac{1}{\pi i\lambda}\right)^{d/2} \int_{R^d} dy\, h(y,\lambda)\, e^{-iy^2/\lambda}$$

where

$$h(y,\lambda) = (\chi_D * \rho_\ell)(y)\exp[-\frac{i}{\hbar}J(x,s+\frac{m\lambda}{2\hbar};y+x,s)]$$
$$\times \sum_{i=0}^{M} m^{-i}T_i(x,s+\frac{m\lambda}{2\hbar};y+x,s)\phi(y+x).$$

Since $\phi \in C_0^d(R^d)$ we observe that $h(\cdot,\lambda) \in C_0^d(R^d)$. An application of Lemma 3.2 leads to the following result:

$$\lim_{t\to s^+} \psi(x,t) = \lim_{\lambda\to 0} \psi(\lambda) = h(0,0).$$

But

$$h(0,0) = (\chi_D * \rho_\ell)(0)\exp[-\frac{i}{\hbar}J(x,s;x,s)] \sum_{n=0}^{M} m^{-n}T_n(x,s;x,s)\phi(x)$$

$$= \phi(x).$$

This proves (3.32). □

Our parametrix $K_M(Q)$ has been constructed such that if interpreted as an integral kernel of an operator on $L^2(R^d)$, it will define a family of operators that share many of the abstract properties of the evolution family $\{U(t,s): (t,s) \in T_\Delta\}$.

Notation: We denote by $\mathcal{B}(\mathcal{H})$ the Banach space of all bounded operators on the Hilbert space $\mathcal{H}$.

PROPOSITION 3.3: For $M \geq 0$ *assume that* a *and* v *are in class* A(2M+2). *Then*

(*i*) *The parametrix kernel* $K_M(Q)$ *generates a family of uniformly bounded operators* $\{U_M(t,s) \in \mathcal{B}(L^2(R^d)): (t,s) \in T_\Delta,\ t \neq s\}$ *via the relation*

$$[U_M(t,s)\phi](x) = \int_{R^d} K_M(Q)\phi(y)dy; \quad \phi \in L^2(R^d); \; x \in R^d.$$

(ii) *For* $\{(t,s) \in T_\Delta : t > s\}$, $U_M(t,s): D_0 \to D_0$.

(iii) *The restriction of* $U_M(t,s)$ *to the domain* D_0 *is strongly continuously differentiable in* $t \in [s,T]$.

(iv) *Let* $\nabla^\gamma\phi \in L^2(R^d)$; $|\gamma| \leq \max(M + [\frac{d}{2}] + 1, d)$ *and assume that* a *and* v *belong to the potential class* $A(\max(3M + \frac{d}{2} + 1, 2M + d)$; *then*

$$\operatorname*{s-lim}_{t\to s} U_M(t,s)\phi = \phi.$$

<u>Proof</u>:

(i) For $\phi \in L^2(R^d)$

$$|[U_M(t,s)\phi](x)| \leq \int_{R^d} |K_M(Q)| \, |\phi(y)|dy.$$

From (3.24) and Lemma 3.1 we notice that $K_M(Q)$ admits the convolution bound

$$|K_M(Q)| \leq h_{t,s}(x-y) \quad \text{where} \quad h_{t,s} \in L^1(R^d); \quad t > s.$$

Thus, using Young's inequality, we get

$$||U_M(t,s)\phi|| \leq ||h_{t,s}||_1 ||\phi|| < \infty.$$

This implies that $U_M \in B(H)$.

(ii) From Lemma 3.3 we have for $\phi \in D_0$; $t > s$

$$\Delta_x\psi(x,t) = \int_{R^d} \Delta_x K_M(Q)\phi(y)dy \tag{a}$$

$$\Delta_x K_M(Q) = \Delta_x[W_M(Q)(\chi_D * \rho_\ell)(x-y))]$$

$$= W_M(Q)\Delta_x[(\chi_D*\rho_\ell)(x-y)] + 2(\nabla_x W_M(Q))\cdot(\nabla_x(\chi_D*\rho_\ell)(x-y))$$

$$+ (\chi_D*\rho_\ell)(x-y)\Delta_x W_M(Q).$$

Now using property 4° of $(\chi_D*\rho_\ell)$ we get

$$|\Delta_x K_M(Q)| \le \chi_2^+(x-y)[|W_M(Q)| + 2|\nabla_x W_M(Q)| + |\Delta_x W_M(Q)|].$$

From Lemma (A3) we thus have that there is a finite constant C

$$|\Delta_x K_M(Q)| \le C\ \chi_2^+(x-y)\ m^{d/2+2}\ (\Delta t)^{-d/2-2}$$

$$\equiv f_{t,s}(x-y). \tag{b}$$

Clearly, $f_{t,s} \in L^1(R^d)$.

Using the last estimate in (a) we obtain via Young's inequality

$$||\Delta\psi|| \le ||f_{t,s}||_1 ||\phi|| < \infty.$$

This shows that $\psi \in D_0$ which in turn implies that $U_M\colon D_0 \to D_0$.

(iii) See Lemma (A2) [Appendix 3.1].

(iv) We defer the proof of this property until we have shown that

$$||[U(t,s) - U_M(t,s)]\phi|| = 0((\Delta t)^M).$$

This will be done in Section 3.4. □

The next natural task is then to determine the inhomogeneous partial differential equation satisfied by $K_M(Q)$.

Let L be the partial differential operator

$$L = i\hbar \frac{\partial}{\partial t} - H(x,t) \tag{3.34}$$

where

$$H(x,t) = -\frac{\hbar^2}{2m}\Delta_x + \frac{i\hbar}{m} a(x,t)\cdot\nabla_x + \frac{1}{2m} a^2(x,t) + \frac{i\hbar}{2m}\nabla_x\cdot a(x,t) + v(x,t). \tag{3.35}$$

After a little algebra we arrive at the following expressions:

$$i\hbar \frac{\partial}{\partial t} W_M(Q) = i\hbar K_0(Q)\exp(-\frac{i}{\hbar}J(Q)) \times [-\frac{d}{2(\Delta t)} - \frac{i}{\hbar}\frac{\partial J(Q)}{\partial t} - \frac{im|x-y|^2}{2\hbar(\Delta t)^2} + \frac{\partial}{\partial t}] \sum_{i=0}^{M} m^{-i} T_i(Q)$$

$$\nabla_x W_M(Q) = K_0(Q)\exp(-\frac{i}{\hbar}J(Q)) \times [\frac{im(x-y)}{\hbar\,\Delta t} - \frac{i}{\hbar}\nabla_x J(Q) + \nabla_x] \sum_{i=0}^{M} m^{-i} T_i(Q)$$

$$-\frac{\hbar^2}{2m}\Delta_x W_M(Q) = K_0(Q)\exp(-\frac{i}{\hbar}J(Q)) \times [-\frac{i\hbar}{\Delta t}\frac{d}{2} + \frac{i\hbar}{2m}\Delta_x J(Q) - \frac{\hbar^2}{2m}(\frac{im(x-y)}{h\,\Delta t} - \frac{i}{\hbar}\nabla_x J(Q))^2 - \frac{\hbar^2}{m}(\frac{im(x-y)}{\hbar\,\Delta t} - \frac{i}{\hbar}\nabla_x J(Q))\cdot\nabla_x - \frac{\hbar^2}{2m}\Delta_x] \sum_{i=0}^{M} m^{-i} T_i(Q).$$

Thus, from (3.34) and using the above expressions we obtain

$$LK_M(Q) = \chi_D*\rho_\ell(x-y)LW_M(Q)$$

$$+[\frac{\hbar^2}{2m}\Delta_x(\chi_D*\rho_\ell)(x-y)+\frac{i\hbar}{m}a(x,t)\cdot\nabla_x(\chi_D*\rho_\ell)(x-y)$$

$$+\frac{\hbar^2}{m}\nabla_x(\chi_D*\rho_\ell)(x-y)\cdot\nabla_x]W_M(Q). \tag{3.36}$$

Rearranging (3.36) in powers of m^{-1} we get

$$LW_M(Q) = K_0(Q)\exp(-\frac{i}{\hbar}J(Q))\left\{\sum_{i=0}^{M}\frac{1}{m^i}[L_1T_i(Q)+L_2T_{i-1}(Q)]\right.$$

$$\left.+\frac{1}{m^{M+1}}L_2T_M(Q)\right\} \tag{3.37}$$

where

$$L_1 \equiv i\hbar(\frac{\partial}{\partial t}+\frac{x-y}{\Delta t}\cdot\nabla_x)+[\frac{\partial J(Q)}{\partial t}+(\nabla_xJ(Q)+a(x,t))\cdot\frac{x-y}{\Delta t}-v(x,t)] \tag{3.38}$$

$$L_2 \equiv \frac{\hbar^2}{2m}\Delta_x - i\hbar(\nabla_xJ(Q)+a(Q))\cdot\nabla_x$$

$$-\frac{1}{2m}[(\nabla_xJ(Q)+a(x,t))+i\hbar\nabla_x]\cdot(\nabla_xJ(Q)+a(x,t)). \tag{3.39}$$

The $T_i(Q)$'s are defined by (3.22)-(3.23) and, in particular, they are solutions of recurrence relation

$$L_1T_i(Q) + L_2T_{i-1}(Q) = 0 \; ; \qquad i \geq 1, \; T_0 = 1. \tag{3.40}$$

The phase function $J(Q)$ is defined by (3.18). It is a simple exercise to show that J satisfies the following PDE.

$$\frac{\partial J(Q)}{\partial t} + \frac{x-y}{\Delta t}\cdot\nabla_x J(Q) - (-a(x,t)\cdot\frac{x-y}{\Delta t} + v(x,t)) = 0. \tag{3.41}$$

Then, equation (3.37) becomes

$$LW_M(Q) = K_0(Q)\exp\left\{-\frac{i}{\hbar}J(Q)\right\}\frac{1}{m^{M+1}}L_2T_M(Q). \tag{3.42}$$

Now including the derivative terms of the cut-off function found in equation (3.36) we finally have the inhomogeneous partial differential equation satisfied by K_M, i.e.,

$$[i\hbar\frac{\partial}{\partial t} - H(x,-i\hbar\nabla,t,m)]K_M(Q) = m^{-(M+1)}R_M^0(Q) + \sum_{i=1}^{3}R_M^i(Q) \tag{3.43}$$

where

$$R_M^0(Q) = K_0(Q)\exp(-\frac{i}{\hbar}J(Q))[-i\hbar g_M(Q)](\chi_D*\rho_\ell)(x-y) \tag{3.44}$$

$$R_M^1(Q) = \frac{\hbar^2}{2m}[\Delta_x(\chi_D*\rho_\ell)(x-y)]W_M(Q) \tag{3.45}$$

$$R_M^2(Q) = \frac{\hbar^2}{m}[\nabla_x(\chi_D*\rho_\ell)(x-y)\cdot\nabla_x]W_M(Q) \tag{3.46}$$

$$R_M^3(Q) = \frac{i\hbar}{m}[a(x,t)\cdot\nabla_x(\chi_D*\rho_\ell)(x-y)]W_M(Q). \tag{3.47}$$

Note that $\{R_M^i(Q)\}_{i=1}^3$ are not of the order m^{-M-1} in the pointwise sense. Nevertheless, it can be shown that after integration with a smooth test function each $R_M^i(Q)$ determines a bounded operator with an L^2-norm of the order of m^{-M-1}. A common feature of $\{R_M^i(Q)\}_{i=1}^3$, worth mentioning, is that these functions are zero if $|x-y| < D-\ell$. This proves very helpful in subsequent integration by parts application associated with the kernels R_M^i.

The results of Proposition 3.3 lead to the following provisional conclusion. If a and v are in potential class A(2M+2), then the parametrix $K_M(Q)$ given by (3.27) seems a reasonable candidate for defining approximate evolution in L^2-norm.

3.3 Abstract Equation of Motion

In this section we show that the pointwise inhomogeneous equation (3.43) determines an inhomogeneous equation of motion in Hilbert space, $L^2(R^d)$.

Let ϕ be some sufficiently smooth L^2-function; then multiplying (3.43) on the right by ϕ and integrating, we obtain

$$\int LK_M(Q)\phi(y)dy = m^{-(M+1)}\int R_M^0(Q;m)\phi(y)dy + \sum_{i=1}^{3}\int R_M^i(Q;m)\phi(y)dy. \tag{3.48}$$

In the following analysis we shall show that the right hand side of equation (3.48) generates a bounded operator in $L^2(R^d)$ and in the left hand side, the order of operation of L and integration can be interchanged. This will lead to the following equation of motion in $L^2(R^d)$:

$$[i\hbar \frac{d}{dt} - H(t,m)]U_M(t,s) = m^{-(M+1)}R_M(t,s) \tag{3.49}$$

where $\frac{d}{dt}$ is understood as the strong derivative in $L^2(R^d)$.

Let us first consider the left hand side of equation 3.48. By using the result of Lemma 3.3 we have

$$\int H(x,-i\hbar\nabla,t,m)K_M(Q)\phi(y)dy = H(x,-i\hbar\nabla,t)\psi_M(x,t)$$

where

$$\psi_M(x,t) = \int K_M(Q)\phi(y)dy.$$

From Proposition 3.3 and Lemma 3.3 we know that $\psi_M(\cdot,t) \in D_0 \cap C^2(R_x^d)$. On functions of this class, the action of $H(t,m)$ is the same as that of the classical differential operator, i.e.,

$$[H(t,m)\psi_M(\cdot,t)](x) = H(x,-i\hbar\nabla,t)\psi_M(x,t) \quad \text{for a.a. } x. \tag{3.50}$$

Next we show that the similar result is valid for the strong t-derivative, $\frac{d}{dt}\psi_M(\cdot,t)$.

At this stage we recall Proposition 3.3(iii) where we had shown that $\psi_M(t)$ is strongly continuously t-differentiable, i.e.,

$$\left\| \frac{\psi_M(t+\delta) - \psi(t)}{\delta} - \frac{d}{dt}\psi_M(t) \right\| \underset{\delta \to 0}{\to} 0$$

From this convergent sequence we may extract a subsequence which converges pointwise almost everywhere in R^d [Ru, Theorem 3.12]. Since $\psi_M(x,\cdot) \in C^1(s,T)$ [Lemma 3.3], this pointwise limit is just the classical partial derivative $\frac{\partial\psi_M}{\partial t}$, i.e.,

$$[\frac{d}{dt}\psi_M(\cdot,t)](x) = \frac{\partial\psi_M}{\partial t}(x,t); \quad \text{a.a. } x. \tag{3.51}$$

Thus from (3.50) and (3.51) we obtain the required result for the left hand side of equation (3.48), i.e.,

$$\int[i\hbar \frac{\partial}{\partial t} - H(\cdot,-i\hbar\nabla,t,m)]K_M(\cdot,t;y,s)\phi(y)dy$$

$$= [i\hbar \frac{d}{dt} - H(t,m)]U_M(t,s)\phi. \tag{3.52}$$

Next, we analyze the right hand side of equation (3.48). In doing so we shall use the method of integration by parts in d-dimensions. One general requirement for this method to work is that the test function ϕ be sufficiently smooth, i.e., $\nabla^\gamma\phi \in L^2(R^d)$, $|\gamma| \leq n < \infty$. It is useful to introduce the following notation for the norm of derivatives of ϕ

$$\sup_{|\gamma|\leq n} ||\nabla^\gamma\phi||_2 \leq |||\phi|||_n$$

Associated with the norm $|||\phi|||_n$ is a complete Sobolev space [R] H_n given by

$$H_n = \{\phi \in L^2(R^d): |||\phi|||_n < \infty\}$$

It is to be noted here that the completeness property of H_n is not used in the following analysis.

We require a convenient symbol for the open interior of the triangular time domain T_Δ. To this end set

$$T_\Delta^0 = \{(t,s) \in T_\Delta: \quad T > t > s > 0\}$$

<u>LEMMA 3.4</u>: *Let δ be an arbitrary* d-*component multi-index and assume that $\phi \in H_{n+|\delta|+1}$. Further suppose that* a *and* v *belong to the potential class* A(2M+n+|δ|+1); *then*

$$\|\nabla^{\delta} R_M^1(t,s)\phi\|$$

$$\leq \text{const. } m^{d/2-n-1} (\Delta t)^{n-d/2} \|\chi^+_{n+|\delta|+2}\|_1 |||\phi|||_{n+|\delta|}$$

$$\|\nabla^{\delta} R_M^2(t,s)\phi\|$$

$$\leq \text{const. } m^{d/2-n-1} (\Delta t)^{n-d/2} \|\chi^+_{n+|\delta|+2}\|_1 |||\phi|||_{n+|\delta|+1}$$

$$\|\nabla^{\delta} R_M^3(t,s)\phi\|$$

$$\leq \text{const. } m^{d/2-n-1} (\Delta t)^{n-d/2} \|\chi^+_{n+|\delta|+1}\|_1 |||\phi|||_{n+|\delta|}.$$

The constant in the above estimates depends only on the parameters D, ℓ *and the coefficients* $\tilde{c}_i$ *[see Assumption* 3].

Moreover, the operators $R_M^i(t,s): H_{n+1} \to L^2(R^d)$ *generated by the kernels* $R_M^i(Q)$ *are strongly continuously* t-*differentiable for* $(t,s) \in T_\Delta^0$.

<u>Proof</u>: In view of equations (3.45)-(3.47) we note that each $R_M^i(Q)$ can be factorized as

$$R_M^i(Q) = K_0(Q)\tilde{R}_M^i(Q)$$

where $\tilde{R}_M^i(Q)$ is $(n+|\delta|+1)$-times continuously differentiable in x and y and it is compactly supported in (x-y). We present the detailed proof for the case when $|\delta| = 0$ and then extend it to include the general case.

For i = 1,

$$[R_M^1(t,s)\phi](x) = \int_{R^d} \frac{m^{d/2}}{(2\pi i\hbar\Delta t)^{d/2}} \exp[\frac{im}{2\hbar\Delta t}(x-y)^2]\tilde{R}_M^1(Q)\phi(y)dy \tag{3.54a}$$

where

$$\tilde{R}_M^1(Q) = \frac{\hbar^2}{2m}[\Delta_x(\chi_D * \rho_\ell)(x-y)]\exp(-\frac{i}{\hbar}J(Q))\sum_{i=0}^{M} m^{-i}T_i(Q). \tag{3.54b}$$

Recall that

$$\vec{\nabla}\cdot(\eta\vec{\xi}) = \eta\vec{\nabla}\cdot\vec{\xi} + (\vec{\nabla}\eta)\cdot\vec{\xi} \tag{3.55a}$$

Take

$$\eta = \exp[(2\hbar\Delta t)^{-1}im(x-y)^2] \quad \text{and} \quad \vec{\xi} = \tilde{R}_M^1(Q)\phi(y)\vec{\alpha}$$

where

$$\vec{\alpha}(x,y) = \frac{\nabla_y(x-y)^2}{|\nabla_y(x-y)^2|^2}. \tag{3.55b}$$

Note that $\vec{\alpha}(x,y)$ is bounded on the support of $\Delta_x(\chi_D * \rho_\ell)(x-y)$. Specifically

$$|\vec{\alpha}(x,y)| \le \frac{1}{D-\ell}.$$

Similar bounds hold for the partial derivatives of $\vec{\alpha}(x,y)$. From (3.55a) it follows that

$$e^{\frac{im}{2\hbar\Delta t}(x-y)^2}\tilde{R}_M^1(Q)\phi(y) = -i(\frac{2\hbar\Delta t}{m})\nabla\cdot\left(e^{\frac{im}{2\hbar\Delta t}(x-y)^2}\tilde{R}_M^1(Q)\phi(y)\vec{\alpha}\right)$$

$$+ i(\frac{2\hbar\Delta t}{m})e^{\frac{im}{2\hbar\Delta t}(x-y)^2}\nabla\cdot(\tilde{R}_M^1(Q)\phi(y)\vec{\alpha}).$$

Substituting this in the relation defining $[R_M^1(t,s)\phi]x$, we get

$$[R_M^1(t,s)\phi](x) = \frac{1}{(\pi i)^{d/2}}\left(\frac{m}{2\hbar\Delta t}\right)^{d/2-1}\left\{-i\int_{R^d}\nabla_y\cdot\left[e^{\frac{im}{2\hbar\Delta t}(x-y)^2}\tilde{R}_M^1(Q)\phi(y)\vec{\alpha}\right]dy\right.$$

$$\left.+\int_{R^d} e^{\frac{im}{2\hbar\Delta t}(x-y)^2}\, i\nabla_y\cdot(\tilde{R}_M^1(Q)\phi(y)\vec{\alpha})\,dy\right\}.$$

Applying divergence theorem to the first term on the right and using the fact that $\tilde{R}_M^1(Q)$ is zero for sufficiently large $|y|$, we observe that the first term vanishes. Using this argument we repeat the above process n-times to obtain

$$[R_M^1(t,s)\phi](x)$$

$$= \frac{1}{(\pi i)^{d/2}}\left(\frac{m}{2\hbar\Delta t}\right)^{d/2-n}\int_{R^d} dy\,\exp\left[\frac{im}{2\hbar\Delta t}(x-y)^2\right]D_y^n[\tilde{R}_M^1(Q)\phi(y)] \tag{3.56}$$

where

$$D_y[\tilde{R}_M^1(Q)\phi(y)] \equiv i\nabla_y\cdot(\tilde{R}_M^1(Q)\phi(y)\vec{\alpha}).$$

From (3.56)

$$|[R_M^1(t,s)\phi](x)| \le \left(\frac{m}{2\hbar\Delta t}\right)^{d/2-n}\frac{1}{\pi^{d/2}}\int |D_y^n(\tilde{R}_M^1(Q)\phi(y))|\,dy. \tag{3.57}$$

For n = 1

$$D_y(\tilde{R}_M^1(Q)\phi(y)) = i[(\nabla_y\cdot\vec{\alpha})\tilde{R}_M^1(Q) + \vec{\alpha}\cdot\nabla_y\tilde{R}_M^1(Q)]\phi(y)$$

$$+ i\tilde{R}_M^1(Q)\vec{\alpha}\cdot\nabla_y\phi(y). \tag{3.58}$$

From (3.54b) it follows that

$$\nabla^{\beta}\tilde{R}_M^1(Q) = \frac{\hbar^2}{2m}\sum_{\alpha=0}^{\beta}\binom{\beta}{\alpha}\nabla^{\beta-\alpha+2}(\chi_D*\rho_\ell)(x-y)$$

$$\times\sum_{\delta=0}^{\alpha}\binom{\alpha}{\delta}\left(\nabla^{\delta}e^{-\frac{i}{\hbar}J(Q)}\right)\nabla^{\alpha-\delta}\left(\sum_{i=0}^{M} m^{-i}T_i(Q)\right).$$

Now using the property 4° of $(\chi_D*\rho_\ell)(x-y)$, the Lemma 3.1 and the inequalities $0 < D-\ell \leq |x-y| \leq D+\ell$, we obtain after a manipulation similar to the one displayed in Lemma A3,

$$|\nabla^{\beta}\tilde{R}_M^1(Q)| \leq \text{const. } m^{-1}(\Delta t)^0\chi^+_{\beta+2}(x-y). \tag{3.59}$$

The constant in the last estimate is independent of m and Δt. Using (3.59) in (3.58) we get

$$|D_y(\tilde{R}_M^1(Q)\phi(y))|$$

$$\leq \frac{h^2}{2m}[(|\nabla_y\cdot\alpha|\,|\tilde{R}_M^1(Q)| + |\vec{\alpha}|\;|\nabla_y\tilde{R}_M^1(Q)|)|\phi(y)|$$

$$+ |\vec{\alpha}|\;|\tilde{R}_M^1(Q)|\;|\nabla_y\phi(y)|]$$

$$\leq \text{const. } m^{-1}(\Delta t)^0\chi_3^+(x-y)\sup_{|\gamma|\leq 1}|\nabla^{\gamma}\phi(y)|.$$

Using similar technique one obtains

$$|D_y^n(\tilde{R}_M^1(Q)\phi(y))| \leq \text{const. } m^{-1}(\Delta t)^0\chi^+_{n+2}(x-y)\sup_{|\gamma|\leq n}|\nabla^{\gamma}\phi(y)|. \tag{3.60}$$

From (3.57), (3.60) and Young's inequality we obtain

$$||R_M^1(t,s)\phi|| \leq \text{const. } m^{d/2-n-1}(\Delta t)^{n-d/2}||\chi^+_{n+2}||_1\;|||\phi|||_n. \tag{3.61}$$

Note that the estimation of $R_M^2(t,s)$ requires bounds for $\nabla_x W_M(Q)$ which according to Lemma A3 is of the order $(\frac{m}{\Delta t})^{d/2+1}$. To get the required m^{-1}-ordering we must integrate by parts n+1 times. On the other hand, estimation for $R_M^3(t,s)$ proceeds just the same way as shown for $R_M^1(t,s)$. With this observation one simply repeats the above analysis to obtain the required estimates for $R_M^2(t,s)$ and $R_M^3(t,s)$.

For $|\delta| > 0$, we have from (3.54a)

$$[\nabla_x^\delta R_M^i(t,s)\phi](x)$$

$$= \left(\frac{m}{2\pi i\hbar\Delta t}\right)^{d/2} \int_{R^d} \sum_{j=0}^{\delta} \binom{\delta}{j} \left[\nabla_x^j \exp\left(\frac{im(x-y)^2}{2\hbar\Delta t}\right)\right][\nabla_x^{\delta-j} R_M^i(Q)]\phi(y)\,dy.$$

For i = 1 and 3 the above integral is of the order $(\frac{m}{t})^{d/2+|\delta|}$ and for i = 2 it is of the order $(\frac{m}{t})^{d/2+|\delta|+1}$. A computation identical to the one displayed above establishes the result for any $|\delta| > 0$. Finally, by mimicking the proof of Lemma A2, one easily establishes the strong t-differentiability of $R_M^i(t,s)$. □

Next step in our analysis is to compute the L^2-norm of the operator $R_M^0(t,s)$ generated by the kernel $R_M^0(Q)$ [equation (3.44)]. Note that $R_M^0(Q)$ has a multiplicative factor of m^{-M-1}. Thus in order that the aggregate error term be of the correct m^{-1}-order, we must show that $||R_M^0(t,s)\phi|| \sim O(m^0(\Delta t)^{n-d/2})$.

In doing so we shall again employ the technique of integration by parts but this time we shall use an antiderivative of the function $e^{i\lambda x^2}$ commonly used in the study of stationary phase expansions [Er].

<u>LEMMA 3.5</u>: *Let δ be an arbitrary* d-*component multi-index and assume that $\phi \in H_{d+|\delta|}$. Further suppose that* a *and* v *belong to the potential class* $A(2M+d+|\delta|)$, *then*

$$\|\nabla^{\delta} R_M^0(t,s)\phi\| \le \text{const. } m^0(\Delta t)^M \|\chi^+_{d+|\delta|}\|_1 \, |||\phi|||_{d+|\delta|}$$

where the constant depends only on D, ℓ *and the constants* $\tilde{c}_i$ *appearing in the Assumption 3.*

Moreover $R_M^0(t,s): H_d \to L^2(R^d)$ *is strongly continuously* t-*differentiable for* $(t,s) \in T_\Delta^0$.

<u>Proof</u>: For convenience we establish this lemma in 1-dimension and then extend it to d-dimensions. Set

$$\eta(x,t) = \int_R K_0(Q)B(Q)\phi(y)dy \tag{3.62}$$

where

$$B(Q) = (\chi_D * \rho_\ell)(x-y)\exp(-\tfrac{i}{\hbar}J(Q))[-i\hbar\, g_M(Q)]. \tag{3.63}$$

The function B: $R^d \times R^d \times T_\Delta \to C$, has the following useful properties.

(i) For fixed $(t,s) \in T_\Delta^0$: $B(\cdot,t;\cdot,s) \in C^{d+|\delta|}(R^d \times R^d)$.

(ii) Let γ be a multi-index, then

$$\nabla_y^\gamma B(Q) = 0 \quad \text{if} \quad |x-y| \geq D+\ell; \ |\gamma| \leq d+|\delta|. \tag{3.64}$$

(iii) From Lemma 3.1, equation (3.18), (3.23a) and the property 4^0 of $\chi_D * \rho_\ell$, we have

$$\| \nabla_y^\gamma B(\cdot,t;\cdot,s) \|_\infty$$

$$\leq C(D,\ell,|\gamma|,\tilde{c}_i) m^0 (\Delta t)^M \chi^+_{d+|\delta|}(x-y); \quad |\gamma| \leq d+|\delta| \tag{3.65}$$

where $\tilde{c}_i$ are the same constants appearing in the Assumption 3.

Define the function $Y(x;\lambda)$

$$Y(x;\lambda) = - \int_x^{x+\infty e^{i\pi/4}} \exp(i\lambda\tau^2)\, d\tau; \quad \lambda > 0, \ \tau \in C. \tag{3.66}$$

The function $Y(x;\lambda)$ is known to have the following important properties [Er,W].

(a) $$\frac{d}{dx} Y(x;\lambda) = \exp(i\lambda x^2) \tag{3.67}$$

(b) $$Y(0;\lambda) = -\frac{1}{2}\left(\frac{\pi i}{\lambda}\right)^{\frac{1}{2}}; \qquad \lambda > 0 \tag{3.68}$$

(c) For all $x \geq 0$, $$|Y(x;\lambda)| \leq \frac{1}{2}\left(\frac{\pi}{\lambda}\right)^{\frac{1}{2}}. \tag{3.69}$$

<u>Case 1</u>: $|\delta| = 0$

Substituting $\lambda = \frac{m}{2\hbar\Delta t}$ in (3.62) we get

$$\eta(x,\lambda) = \left(\frac{\lambda}{\pi i}\right)^{\frac{1}{2}} \int_{-\infty}^{+\infty} \exp(i\lambda(x-y)^2) B(Q)\phi(y)\,dy \tag{3.70}$$

$$= \left(\frac{\lambda}{\pi i}\right)^{\frac{1}{2}} \left[\int_{-\infty}^{x} \left(-\frac{d}{dy} Y(x-y;\lambda)\right) B(Q)\phi(y)\,dy \right.$$

$$\left. + \int_{x}^{\infty} \left(\frac{d}{dy} Y(y-x;\lambda)\right) B(Q)\phi(y)\,dy \right].$$

Integrating by parts once and using the fact that $B(Q)$ vanishes for sufficiently large $|y|$, we obtain

$$\eta(x,\lambda) = \frac{\lambda^{\frac{1}{2}}}{(\pi i)^{\frac{1}{2}}} \left[-2Y(0;\lambda) B(x,t;x,s)\phi(x) \right.$$

$$+ \int_{x}^{\infty} Y(y-x;\lambda) \frac{d}{dy} (B(Q)\phi(y))\,dy$$

$$\left. - \int_{-\infty}^{x} Y(x-y;\lambda) \frac{d}{dy} (B(Q)\phi(y))\,dy \right]. \tag{3.71}$$

Using equations (3.68)-(3.69), the property (iii) of $B(Q)$ and the Young's inequality we get

$$||\eta(\cdot,m)|| \le C(D,\ell,\tilde{c}_i) m^0 (\Delta t)^M [\, ||\chi_0^+||_\infty \; ||\phi|| + ||\chi_1^+||_1 \; |||\phi|||_1]$$

$$\le C(D,\ell,\tilde{c}_i) m^0 (\Delta t)^M ||\chi_1^+||_1 \; |||\phi|||_1 < \infty.$$

Generalization to d-dimensions

For $x \in R^d$, rewrite $\eta(x,\lambda)$ as

$$\eta(x,\lambda) = \int_R dy_1 \left(\frac{\lambda}{\pi i}\right)^{\frac{1}{2}} e^{i\lambda(x_1-y_1)^2} \int_R dy_2 \left(\frac{\lambda}{\pi i}\right)^{\frac{1}{2}} e^{i\lambda(x_2-y_2)^2} \cdots$$

$$\cdots \int_R dy_{d-j} \left(\frac{\lambda}{\pi i}\right)^{\frac{1}{2}} e^{-i\lambda(x_{d-j}-y_{d-j})^2}$$

$$\times \cdots \times \int_R dy_d \left(\frac{\lambda}{\pi i}\right)^{\frac{1}{2}} e^{i\lambda(x_d-y_d)^2} B(Q)\phi(y)dy. \tag{3.72}$$

Let

$$h_{d-j}(x_1 \cdots x_{d-(j+1)}, y_1 \cdots y_{d-(j+1)}; t,s)$$

$$= \int_R dy_{d-j} \left(\frac{\lambda}{\pi i}\right)^{\frac{1}{2}} e^{i\lambda(x_{d-j}-y_{d-j})^2} \times \cdots$$

$$\times \int_R dy_d \left(\frac{\lambda}{\pi i}\right)^{\frac{1}{2}} e^{i\lambda(x_d-y_d)^2} B(Q)\phi(y) . \tag{3.73}$$

Note that for a fixed x, the function h_{d-j} has compact support $N^{d-(j+1)} \subset R^{d-(j+1)}$. In view of the properties of $B(Q)\phi(y)$, one can show by induction that it has all derivatives

$$\nabla^{\gamma_1 \cdots \gamma_{d-(j+1)}}_{y_1 \cdots y_{d-(j+1)}} h_{d-j}(y_1 \cdots y_{d-(j+1)}; t,s)$$

$$\text{with } |\gamma_i| \le 1; \; i = 1 \sim d-(j+1)$$

which are continuous functions in $N^{d-(j+1)}$. With this property we can apply the identity (3.71) successively to obtain the desired result.

Case 2: $|\delta| \neq 0$

$$\nabla_x^{\delta}\eta(x,\lambda) = \int_{R^d} \sum_{j=0}^{\delta} \binom{\delta}{j} [\nabla_x^j K_0(Q)][\nabla_x^{\delta-j} B(Q)]\phi(y)\,dy. \tag{3.74}$$

The above d-dimensional integral can be rewritten as a product of d one dimensional integrals. Since each member of this product is of the order $(\frac{m}{\Delta t})^{\frac{1}{2}+|\delta|}$ we must integrate by parts more than once. The calculations leading to the final result are tedious but straightforward and thus details are confined to Lemma A4 in the Appendix 3.1. To establish t-differentiability of $R_M^0(t,s)$ we appeal to Lemma A2. □

From Lemmas 3.4 and 3.5 we can claim to have shown that for $n \geq M+d/2$, the pointwise PDE identity (3.48) determines an inhomogeneous abstract equation of motion in $L^2(R^d)$ [equation (3.49)].

Next we look for the solution of equation (3.49) and compute the difference between the exact and approximate solutions of Schrödinger's equation in L^2-norm and show that the difference vanishes in the limit $m \to \infty$.

3.4 The Error Analysis

To begin with, recall the following result concerning the solutions of inhomogeneous differential equations in $H = L^2(R^d)$ [Kr, Theorem 3.1, 3.3].

Consider the equation

$$\frac{d\psi}{dt} = A(t)\psi + f(t) \tag{3.75}$$

where $f(t) \in L^2(R^d)$ is a continuous function on $[0,T]$.

PROPOSITION 3.4: *If the Cauchy problem for the homogeneous equation*

$$\frac{d\psi}{dt} = A(t)\psi; \qquad t \in [0,T],\ \psi(s) = \phi \in D(A)$$

is uniformly correct and if the

(i) operator $A(t)$ *is strongly continuously differentiable on* $D(A)$, *and*

(ii) $f(t)$ *has a continuous derivative,*

then equation (3.75) has a unique solution given by

$$\psi(t,s) = U(t,s)\phi + \int_s^t U(\tau,s)f(\tau)d\tau. \tag{3.76}$$

□

We can now state and prove our main result of this chapter. Notice from Lemma 3.4 and 3.5 that the degree of smoothness of initial data ϕ and the potentials depend on M and d. In the following theorem we shall require a convenient symbol to display the role played by M and d in stating the assumptions on the initial data and the potentials. To this end, set

$$N \equiv N(M,d) = \max(M+[\tfrac{d}{2}]+1,d)$$

and

$$N^* \equiv N^*(M,d) \equiv 2M+N = \max(3M+[\tfrac{d}{2}]+1,\ 2M+d).$$

In the above definitions $[\frac{d}{2}]$ denotes the smallest integer greater than or equal to $\frac{d}{2}$.

<u>THEOREM 3.1</u>: *Let the initial data* $\phi \in H_N$ *and assume that* a *and* v *belong to the potential class* A(N*); *then,*

$$\|U_M(t,s)\phi - U(t,s)\phi\|$$

$$\leq C(D,\ell,\tilde{c}_i)m^{-M-1}(\Delta t)^{M+1}\|\chi^{+}_{N+1}\|_1 |||\phi|||_N. \tag{3.77}$$

<u>Proof</u>: Let

$$A(t) = \frac{1}{i\hbar} H(t) - cI \tag{3.78}$$

where c is a constant [equation (2.29)] and H(t) is the Hamiltonian operator with a t-invariant domain D_0.

We have shown earlier that A(t) given in (3.78) is strongly continuously differentiable [Lemma 2.5] and that the corresponding Cauchy problem is uniformly correct. Moreover, from Lemmas 3.4 and 3.5 we notice that the operator $R_M(t,s)$: $H_N \to L^2(R^d)$ is strongly continuously t-differentiable for $(t,s) \in T^0_\Delta$. Thus for $\phi \in H_N \subset D_0$, the equation (3.49) satisfies all the hypotheses of Proposition 3.4. Therefore, the solution of equation (3.49) can be written as

$$U_M(t,s)\phi = U(t,s)\phi + \int_s^t U(t,\tau)R_M(t,\tau)\phi\, d\tau . \tag{3.79}$$

It follows from (3.79) that

$$\|U_M(t,s)\phi - U(t,s)\phi\| \le \int_s^t \|U(t,\tau)\| \, \|R_M(t,\tau)\phi\| \, d\tau$$

$$\le \int_s^t e^{c(t-\tau)} \|R_M(t,\tau)\phi\| \, d\tau. \qquad (3.80)$$

Now from Lemmas 3.4 and 3.5 we finally obtain

$$\|U_M(t,s)\phi - U(t,s)\phi\| \le C(D,\ell_i,\tilde{c}_i)m^{-M-1}(\Delta t)^{M+1}\|\chi^+_{N+1}\|_1 |||\phi|||_N.$$

□

From the estimate (3.79) we observe that

$$\operatorname*{s-lim}_{t\to s} U_M(t,s)\phi = U(s,s)\phi = \phi.$$

This proves Proposition 3.3(iv). Since $U_M(t,s)$ is generated by the parametrix $K_M(Q)$ which is well defined only if $(t,s) \in T^0_\Delta$, the initial data condition is satisfied only in the sense of a strong limit.

REMARK 3.1: Note that the functions N and N* take on different values depending on the relative magnitude of M and d. In particular there are two different cases:

(1) If $M < d - [\frac{d}{2}] - 1$, then $N = d$ and $N^* = 2M+d$, whereas

(2) If $M > d - [\frac{d}{2}] - 1$, then $N = M + [\frac{d}{2}] + 1$ and $N^* = 3M + [\frac{d}{2}] + 1$.

3.5 Expectation Value of Observables

Consider the general problem of computing the expectation value of an observable. If $\{B(t) \in \mathcal{B}(\mathcal{H}) : t \in [0,T]\}$ is a family of uniformly bounded self-adjoint operators on $[0,T]$, i.e.,

$$\sup_{t\in[0,T]} \|B(t)\| = B^+ < \infty ,$$

then the M^{th}-order approximate evolving state, $\psi_M(t)$, of Theorem 3.1 trivially provides an M^{th}-order approximation for the time dependent expectation value. We denote the expectation value of an observable A in a state ψ by $\langle A\rangle_\psi \equiv (\psi,A\psi)$ where the latter symbol represents the inner product in H. Setting $\psi(t) = U(t,s)\phi$ and in view of the uniform boundedness of $B(t)$ one has

$$\begin{aligned} &\left|\langle B(t)\rangle_{\psi(t)} - \langle B(t)\rangle_{\psi_M(t)}\right| \\ &\quad \le B^+(\|\psi(t)\| + \|\psi_M(t)\|)(\|\psi(t) - \psi_M(t)\|) \\ &\quad = 0(m^{-M-1}(\Delta t)^{M+1}). \end{aligned} \tag{3.81}$$

However, the most interesting observables in quantum mechanics are unbounded operators, such as position, momentum, energy, etc. The goal of the next proposition is to show for a certain class of unbounded observables that estimates similar to (3.81) remain valid.

PROPOSITION 3.5: Suppose the initial data $\phi \in H_{N+2}$ *and that* a *and* v *belong to the potential class* A(N*+2). *Let* $\{B(t)\colon t \in [0,T]\}$ *be a family of uniformly* H(t)*-bounded observables on the interval* $[0,T]$, *i.e., for all* $f \in D(H(t)) = D_0$;

$t \in [0,T]$ *there exist finite constants* A_0, $B_0 < \infty$ *independent of* f *and* t, *such that*

$$\|B(t)f\| \leq A_0\|f\| + B_0\|H(t)f\|; \qquad t \in [0,T]. \tag{3.82}$$

Then,

$$\left|\langle B(t)\rangle_{\psi(t)} - \langle B(t)\rangle_{\psi_M(t)}\right| = 0(m^{-M-1}(\Delta t)^{M+1}). \tag{3.83}$$

Proof: It suffices to show that

$$\|B[U(t,s)\phi - \psi_M(t)]\| = 0(m^{-M-1}(\Delta t)^{M+1}). \tag{3.84}$$

Recall from equation (3.78) that

$$U(t,s)\phi - \psi_M(t) = -\int_s^t U(t,\tau)R_M(t,\tau)\phi\, d\tau.$$

Now since B is a closed operator, we have

$$B[U(t,s)\phi - \psi_M(t)] = -\int_s^t B\; U(t,\tau)R_M(t,\tau)\phi\, d\tau\, .$$

It follows that

$$\|B[U(t,s)\phi - \psi_M(t)]\| \leq \int_s^t \|B\; U(t,\tau)R_M(t,\tau)\phi\|\, d\tau$$

$$\leq \int_s^t \left\{A_0\|U(t,\tau)R_M(t,\tau)\phi\| + B_0\|H(t)U(t,\tau)R_M(t,\tau)\phi\|\right\} d\tau\, . \tag{3.85}$$

This last inequality follows from Lemmas 3.4 and 3.5 which imply that $R_M(t,s) \in D_0$. Recall from Chapter 2 that

$$A(t) = -\frac{i}{\hbar}H(t,m) - cI; \qquad c = \text{constant} = 1 + \frac{\alpha}{\hbar} \tag{2.11}$$

$$U(t,s) = e^{c(t-s)}\,\mathcal{U}(t,s); \quad (t,s) \in T_\Delta. \tag{2.12}$$

Thus

$$\|H(t)U(t,\tau)R_M(t,\tau)\phi\|$$

$$= \|(-\frac{\hbar}{i}A(t) + c\frac{\hbar}{i})\, e^{c(t-\tau)}\,\mathcal{U}(t,\tau)R_M(t,\tau)\phi\|$$

$$\leq c\hbar e^{c(t-\tau)}\,\|\mathcal{U}(t,\tau)R_M(t,\tau)\phi\| + \hbar\,\|A(t)e^{c(t-\tau)}\,\mathcal{U}(t,\tau)R_M(t,\tau)\phi\|\,. \tag{3.86}$$

At this stage we recall a result from the theory of differential equations in Banach space [Kr. page no. 195] which states that

$$A(t)\,\mathcal{U}(t,s) = V(t,s)A(s) \tag{3.87}$$

where

$$V(t,s) = A(t)\,\mathcal{U}(t,s)A^{-1}(s) \tag{3.88}$$

and

$$\sup_{(t,s)\in T_\Delta} \|V(t,s)\| = C(V) < \infty. \tag{3.89}$$

Using (3.87) in equation (3.86) we obtain

$$\|H(t)U(t,\tau)R_M(t,\tau)\phi\|$$

$$\leq \hbar e^{c(t-s)}\{c\|R_M(t,\tau)\phi\| + \|V(t,\tau)A(\tau)R_M(t,\tau)\phi\|\}$$

$$\leq \hbar e^{c(t-s)}\{c\|R_M(t,\tau)\phi\| + C(V)\|A(\tau)R_M(t,\tau)\phi\|\}$$

$$\le \hbar e^{c(t-s)}\{c\|R_M(t,\tau)\phi\| + cC(V)\|R_M(t,\tau)\phi\|$$

$$+ \hbar^{-1}C(V)\|H(\tau;m)R_M(t,\tau)\phi\|\}. \tag{3.90}$$

Thus from (3.85) and (3.90) we obtain

$$\|B[U(t,s)\phi - \psi_M(t)]\|$$

$$\le \int_s^t \tilde{A}_0\|R_M(t,\tau)\phi\| + \tilde{B}_0\|H(\tau;m)R_M(t,\tau)\phi\|\}d\tau \tag{3.91}$$

with

$$\tilde{A}_0 = A_0 + B_0\hbar e^{c(t-s)}c(1 + C(V))$$

$$\tilde{B}_0 = B_0\, e^{c(t-s)}C(V).$$

Once again an application of Lemmas 3.4 and 3.5 shows that the norm $\|H(\tau,m)R_M(t,\tau)\phi\|$ is uniformly bounded for $\tau \in [t,s]$ and that

$$\|H(\tau,m)R_M(t,\tau)\phi\| = 0(m^{-(M+1)}(t-\tau)^M).$$

Using these estimates in (3.91) we notice that the integrand in (3.91) is of the order $0(m^{-(M+1)}(t-\tau)^M)$. This in turn implies that the right hand side of (3.91) makes sense as a strong Riemann integral, thereby proving (3.84). □

APPENDIX 3.1

Proof of Lemma 3.1

Preliminaries: Rewrite equation (3.22)-(3.23) as

$$T_n(Q) = \Delta t \int_0^1 d\xi \left\{ [\frac{1}{2i\hbar} G^2 - \frac{1}{2} \nabla_1 \cdot G] T_{n-1} - G \cdot \nabla_1 T_{n-1} + \frac{i\hbar}{2} \Delta_1 T_{n-1} \right\} (\omega(\xi); y, s) \qquad (A1)$$

where

$$\omega(\xi) = (y + \xi(x-y),\ s + \xi(t-s))$$

$$G_i(Q) = \Delta t \int_0^1 d\xi\, \xi \left[f_i + \frac{(x-y)_j}{\Delta t} F_{ij} \right] (\omega(\xi)) \qquad (A2)$$

where

$$f_i = -\nabla^i v - \frac{\partial}{\partial t} a_i \ ; \qquad F_{ij} = \nabla^i a_j - \nabla^j a_i . \qquad (A3)$$

Notation: $\delta_i = (0,0\ldots1,0\ldots0)$ with 1 in i^{th} slot.

We first determine the bounds on function G defined in (A3).

LEMMA A1: Let a *and* v *be in potential class* A(2M+n) *and define* $Z = Z(|x-y|, \Delta t)$ *to be*

$$Z = 2\tilde{c}_1 \sqrt{d}\, (k|x-y| + n) + \Delta t (k\tilde{c}_2 + \tilde{c}_3)$$

where the constants k *and* $\tilde{c}_i$ *are the same as given in Assumption 3.*

Then, G *and its partial derivative satisfy, for* $|\beta| \le 2M+n-1$

$$|\nabla_1^\beta G_i| \le k^{|\beta|} Z$$

$$|\nabla_1^\beta G^2| \le (2k)^{|\beta|} d\, Z^2$$

$$|\nabla_1^\beta \nabla_1 \cdot G| \le d\, k^{|\beta|+1} Z\,.$$

Proof: From the bounds on a and v we have

$$\begin{aligned} |\nabla^\beta f_i| &\le |\nabla^\beta(\nabla^i v)| + |\nabla^\beta \partial_t a_i| \\ &= |\nabla^{\beta+\delta_i} v| + |\nabla^\beta \partial_t a_i| \\ &\le k^{|\beta|}(k\tilde{c}_2 + \tilde{c}_3)\,. \end{aligned} \qquad \text{(a)}$$

Similarly

$$\begin{aligned} |\nabla^\beta F_{ij}| &\le |\nabla^{\beta+\delta_i} a_j| + |\nabla^{\beta+\delta_j} a_i| \\ &\le 2k^{|\beta|+1}\tilde{c}_1\,. \end{aligned} \qquad \text{(b)}$$

In the above estimations we have used the fact that $|\delta_i| = 1$. From equation (A2) we notice that we require bounds on the derivatives of $(x-y)_j F_{ij}(\omega(\xi))$.

$$\nabla_x^\beta\{(x-y)_j F_{ij}(\omega(\xi))\}$$

$$= \sum_{j=1}^{d} \sum_{\alpha\le\beta} \binom{\beta}{\alpha} (\nabla_x^\alpha (x-y)_j)\, \nabla_x^{\beta-\alpha} F_{ij}(\omega(\xi))$$

$$= \sum_{j=1}^{d} \sum_{\alpha \le \beta} \binom{\beta}{\alpha} (\nabla_x^{\alpha}(x-y)_j)\, \xi^{|\beta-\alpha|} \nabla^{\beta-\alpha} F_{ij}(\omega(\xi))$$

$$= \sum_{j=1}^{d} (x-y)_j \xi^{|\beta|} \nabla^{\beta} F_{ij}(\omega(\xi)) + \sum_{j=1}^{d} \sum_{\substack{\alpha \le \beta \\ |\alpha|=1}} \binom{\beta}{\alpha} (\nabla_x^{\alpha} x_j)\, \xi^{|\beta-\alpha|} \nabla^{\beta-\alpha} F_{ij}(\omega(\xi)). \tag{c}$$

Note that

$$\binom{\beta}{\alpha} = \prod_{\ell=1}^{d} \binom{\beta_\ell}{\alpha_\ell} = \prod_{\ell=1}^{d} \frac{\beta_\ell!}{\alpha_\ell!(\beta_\ell-\alpha_\ell)!} .$$

But since $|\alpha| = 1$, let $\alpha = \delta_k$; then

$$\text{for } \ell \ne k,\ \binom{\beta_\ell}{\alpha_\ell} = \binom{\beta_\ell}{0} = 1, \text{ and for } \ell = k,\ \binom{\beta_k}{\alpha_k} = \binom{\beta_k}{1} = \beta_k.$$

Thus in the second term of (c) restriction $\alpha \le \beta$ can be lifted to yield

$$\sum_{\substack{|\alpha|=1 \\ \alpha \le \beta}} \iff \sum_{\ell=1}^{d} \quad \text{with} \quad \alpha = \delta_\ell$$

$$\nabla_x^{\beta}\{(x-y)_j F_{ij}(\omega(\xi))\} = \xi^{|\beta|} \sum_{j=1}^{d} (x-y)_j \nabla^{\beta} F_{ij}(\omega(\xi))$$

$$+ \sum_{j=1}^{d} \sum_{\ell=1}^{d} \beta_\ell\, \xi^{|\beta|-1} \frac{\partial x_j}{\partial x_\ell} \nabla^{\beta-\delta_\ell} F_{ij}(\omega(\xi))$$

$$\Rightarrow |\nabla_x^{\beta}\{(x-y)_j F_{ij}(\omega(\xi))|$$

$$\le |x-y| \left| \sum_{j=1}^{d} (\nabla^{\beta} F_{ij})^2 \right|^{\frac{1}{2}} + |\beta| \left(\sum_{j=1}^{d} \theta(\beta_j > 0) [\nabla^{\beta-\delta_j} F_{ij}]^2 \right)^{\frac{1}{2}}$$

$$\le 2\sqrt{d}\, k^{|\beta|} \tilde{c}_1 (|x-y|k + |\beta|). \tag{d}$$

In the last estimate we have used the inequality (b). Similarly,

$$|\nabla_x^\beta f_i(\omega(\xi))| \le k^{|\beta|}(k\tilde{c}_2 + \tilde{c}_3). \tag{e}$$

Thus from equation (A2) and the estimates (d) and (e)

$$\begin{aligned} |\nabla_1^\beta G_i(Q)| &\le \Delta t\, k^{|\beta|}(k\tilde{c}_2 + \tilde{c}_3) + 2\sqrt{d}\, k^{|\beta|}\, \tilde{c}_1(|x-y|k + |\beta|) \\ &\le k^{|\beta|} Z, \qquad\qquad i = 1 \sim d. \end{aligned} \tag{f}$$

Now

$$\begin{aligned} |\nabla_1^\beta G^2| &= \left| \sum_{i=1}^{d} \sum_{\alpha\le\beta} \binom{\beta}{\alpha} \nabla_1^\alpha G_i \nabla_1^{\beta-\alpha} G_i \right| \\ &\le \sum_{i=1}^{d} \sum_{\alpha\le\beta} \binom{\beta}{\alpha} k^{|\alpha|} k^{|\beta-\alpha|} Z^2 \\ &= (2k)^{|\beta|} d Z^2. \end{aligned} \tag{g}$$

Finally,

$$|\nabla^\beta \nabla_1 \cdot G| = \left| \sum_{i=1}^{d} \nabla^{\beta+\delta_i} G_i \right| \le d k^{|\beta|+1} Z. \tag{h}$$

$\square$

Using the results of this lemma we can easily find the estimates for T_n's. Let us now list bounds for T_0, T_1 and T_2 which will be useful in proving the general case.

$$T_0: \quad T_0 = 1 \Rightarrow \nabla_1^\beta T_0 = \delta_{|\beta|,0} \tag{i}$$

$$T_1: \quad \nabla_1^\beta T_1(Q) = \nabla_x^\beta(\Delta t) \int_0^1 d\xi \left[\frac{G^2}{2i\hbar} - \frac{1}{2}\nabla_1 \cdot G\right](\omega(\xi); y, s).$$

$$|\nabla_1^\beta T_1(Q)| \le \Delta t \left| \int_0^1 d\xi\, \xi^{|\beta|} \left(\frac{\nabla_1 G^2}{2i\hbar} - \frac{1}{2}\nabla_1^\beta \nabla_1 \cdot G\right)\right|$$

$$\le \Delta t \left[\frac{(2k)^{|\beta|} d Z^2}{2\hbar} + \frac{1}{2} d\, k^{|\beta|+1} Z\right]$$

$$= \left(\frac{d\Delta t}{2\hbar}\right)[(2k)^{|\beta|} Z^2 + k^{|\beta|+1} Z \hbar].$$

Thus

$$|\nabla_1^\beta T_1(Q)| \le \left(\frac{d\Delta t}{2\hbar}\right) Z k^{|\beta|}(2^{|\beta|} Z + \hbar k) . \tag{j}$$

$$T_2: \quad \nabla_1 T_2(Q) = \Delta t \int_0^1 d\xi\, \xi^{|\beta|} \left\{ \sum_{\alpha \le \beta} \binom{\beta}{\alpha} \left[\nabla_1^\alpha \left(\frac{G^2}{2i\hbar} - \frac{1}{2}\nabla \cdot G\right) \nabla_1^{\beta-\alpha} T_1 + \right.\right.$$

$$\left.\left. - \sum_{j=1}^{d} \nabla_1^\alpha G_j \nabla_1^{\beta-\alpha+\delta_j} T_1\right] + \frac{i\hbar}{2} \nabla_1^\beta \Delta_1 T_1 \right\}(\omega(\xi); y, s) .$$

Using the bounds in Lemma A1 and the estimate (j) for the derivatives of T_1, we obtain after a little algebra

$$|\nabla_1^\beta T_2(Q)| \le \left(\frac{d\Delta t}{2\hbar}\right)^2 Z k^{|\beta|} (2^{|\beta|} Z + \tfrac{5}{2}\hbar k)^3. \tag{k}$$

With these results in hand we are now ready to prove Lemma 3.1.

<u>Proof of Lemma 3.1</u>: (By induction)

Set i = 1 and 2 in (3.25) to get

$$|\nabla_1^\beta T_1| \le \left(\frac{d\Delta t}{2\hbar}\right) k^{|\beta|} Z(2^{|\beta|} Z + \hbar k)$$

and

$$|\nabla_1^\beta T_2| \le \left(\frac{d\Delta t}{2\hbar}\right)^2 Z k^{|\beta|}(2^{|\beta|} Z + \tfrac{5}{2}\hbar k)^3 .$$

Thus (3.25) yields correct estimates for T_1 and T_2. Assume that this estimate holds for i-1,i-2,...,1 and recall that

$$\nabla_1^\beta T_i = \Delta t \int_0^1 d\xi\, \xi^{|\beta|} \Big\{ \sum_{\alpha\ \beta} \binom{\beta}{\alpha} \Big[\nabla_1^\alpha \Big(\frac{G^2}{2i\hbar} - \frac{1}{2}\nabla\cdot G\Big) \nabla_1^{\beta-\alpha} T_{i-1}$$

$$- \sum_{j=1}^{d} \nabla_1^\alpha G_j \nabla_1^{\beta-\alpha+\delta_j} T_{i-1} \Big] + \frac{i\hbar}{2} \nabla_1^\beta \Delta_1 T_{i-1} \Big\} (\omega(\xi);y,s)$$

$$\equiv I_1 + I_2 + I_3, \text{ say.} \qquad (\ell)$$

Using (3.25) for T_{i-1} and Lemma A1 we find

$$I_1 \le (\Delta t) \sum_{\alpha\le\beta} \binom{\beta}{\alpha} \Bigg[\Big(\frac{(2k)^{|\alpha|} dZ^2}{2\hbar} + \frac{d\hbar\, k^{|\alpha|+1} Z}{2h} \Big) \Big(\frac{d\Delta t}{2\hbar}\Big)^{i-1} k^{|\beta|-|\alpha|} Z \times$$

$$\times (2^{|\beta|-|\alpha|} Z + \lambda_{i-1}\hbar k)^{2i-3} \Bigg]$$

$$\le \Big(\frac{d\Delta t}{2\hbar}\Big)^i \sum_{\alpha\le\beta} \binom{\beta}{\alpha} (2^{|\beta|} Z^2 + \hbar k Z) k^{|\beta|} Z (2^{|\beta|} Z + \lambda_{i-1} k\hbar)^{2i-3}$$

$$\le \Big(\frac{d\Delta t}{2\hbar}\Big)^i k^{|\beta|} Z^2\, 2^{|\beta|} (2^{|\beta|} Z + \lambda_{i-1}\hbar k)^{2i-2}. \qquad (m)$$

In the last estimate we have used the fact that $2^{|\alpha|} \le 2^{|\beta|}$ and $\lambda_{i-1} \ge 1$.

Similarly,

$$I_2 \le \Big(\frac{\Delta t}{2\hbar}\Big) \sum_{\alpha\le\beta} \binom{\beta}{\alpha} dZ \Big(\frac{d\Delta t}{2\hbar}\Big)^{i-1} Z\, k^{|\beta|+1} (2\hbar) (2^{|\beta|-|\alpha|+1} Z + \lambda_{i-1} k\hbar)^{2i-3}$$

$$\le \Big(\frac{d\Delta t}{2\hbar}\Big)^i k^{|\beta|} Z^2 (2\hbar k)\, 2^{|\beta|} (2^{|\beta|+1} Z + \lambda_{i-1}\hbar k)^{2i-3} \qquad (n)$$

and

$$I_3 \le \left(\frac{d\Delta t}{2\hbar}\right)^i k^{|\beta|} Z (\hbar k)^2 (2^{|\beta|} Z + \lambda_{i-1}\hbar k)^{2i-3}. \tag{o}$$

Thus,

$$I_1 + I_2 + I_3 \le \left(\frac{d\Delta t}{2\hbar}\right)^i k^{|\beta|} Z \cdot F \tag{p}$$

where

$$F = (2^{|\beta|} Z + \lambda_{i-1}\hbar k)^{2i-3} \Bigg\{ Z\, 2^{|\beta|} (Z\, 2^{|\beta|} + \lambda_{i-1}\hbar k) + Z(2\hbar k) 2^{|\beta|} \left[\frac{2^{|\beta|+1} Z + \lambda_{i-1}\hbar k}{2^{|\beta|} Z + \lambda_{i-1}\hbar k}\right]^{2i-3} + \hbar^2 k^2 \Bigg\}. \tag{q}$$

Note that for all $a \ge 0$, $b \ge 0$

$$\left(\frac{2a+b}{a+b}\right)^{2i-3} = \left(\frac{a+b}{a+b} + \frac{a}{a+b}\right)^{2i-3} \le 2^{2i-3}.$$

It follows that,

$$\begin{aligned} F &\le (2^{|\beta|} Z + \lambda_{i-1}\hbar k)^{2i-3} \Big\{ (Z2^{|\beta|})^2 + (Z2^{|\beta|}) \lambda_{i-1}\hbar k + \hbar^2 k^2 \\ &\qquad + (Z2^{|\beta|})(2\hbar k) 2^{2i-3} \Big\} \\ &\le (2^{|\beta|} Z + \lambda_{i-1}\hbar k)^{2i-3} \left\{ 2^{|\beta|} Z + \left(2^{2i-3} + \frac{\lambda_{i-1}}{2}\right)\hbar k \right\}^2 \\ &\le (2^{|\beta|} Z + \lambda_i \hbar k)^{2i-1} \qquad \text{if} \quad \lambda_i \le 2^{2i-1} \end{aligned} \tag{r}$$

where $\lambda_i \equiv 2^{2i-3} + \dfrac{\lambda_{i-1}}{2}$.

Finally from (r) and (p) we get the required result.

Corollary A1: *Let* a *and* v *be as in Lemma A1, then*

$$\left|\nabla_1^{\beta}\,\frac{\partial T_i}{\partial t}\,(Q)\right| \le \frac{1}{t}\,\left(\frac{d\Delta t}{2\hbar}\right)^{i} k^{|\beta|}\, Z\,[2^{|\beta|} Z + \lambda_i \hbar k]^{2i-1}$$

$$+ \left(\frac{d\Delta t}{2\hbar}\right)^{i} k^{|\beta|}\, Z^*[2^{|\beta|} Z^* + \lambda_i \hbar k]^{2i-1}$$

where

$$Z^* = \left[\frac{Z}{\Delta t} + 2\sqrt{d}\left(\tilde{c}_3 + \frac{\tilde{c}_1}{\Delta t}\right)(|x-y|k+M) + \Delta t(k\tilde{c}_4 + \tilde{c}_3)\right]$$

$$\lambda_i = 2^{2i-3} + \frac{\lambda_{i-1}}{2}\;; \qquad \lambda_1 = 1.$$

Proof: Noting that the conditions on derivatives of a and v were chosen so as to make T_n's differentiable functions of time one arrives at the following preliminary bounds:

$$\left|\nabla^{\beta}\,\frac{\partial G_i}{\partial t}\right| \le k^{|\beta|} Z^*\,, \qquad\qquad i = 1 \sim d$$

$$\left|\nabla^{\beta}\,\frac{\partial G^2}{\partial t}\right| \le d(2k)^{|\beta|} Z^{*2} \qquad \text{etc.}$$

Using these bounds one arrives at the required result by following identical process of estimation as displayed above for the proof of Lemma 3.1. It is worth noting that Z^* is a linear function of $|x-y|$. □

LEMMA A2: *Let* a *and* v *be as in Proposition 3.1; then the restriction of* $U_M(t,s)$ *to* D_0 *is strongly continuously differentiable in* $t \in [s,T]$.

Proof: Let $(t,s) \in T_\Delta$ and define

$$\frac{U_M(t+\delta,s) - U_M(t,s)}{\delta} \equiv U_\delta(t,s) \tag{1}$$

where, for $\phi \in L^2(R^d)$,

$$[U_\delta(t,s)\phi](x) = \int_{R^d} \left[\frac{1}{\delta}\int_t^{t+\delta} dt' \frac{\partial}{\partial t'} K_M(x,t';y,s)\right]\phi(y)dy, \tag{2}$$

and define

$$[\dot{U}(t,s)\phi](x) = \int_{R^d} \frac{\partial K_M}{\partial t}(x,t;y,s)\phi(y)dy. \tag{3}$$

From Lemma 3.1 and the Corollary A1, we observe that

$$\left|\frac{1}{\delta}\int_t^{t+\delta} dt' \frac{\partial}{\partial t'} K_M(x,t';y,s)\right| \le h_{t,s}(x-y) \tag{4}$$

where

$$h_{t,s} \in L^1(R^d); \qquad t > s$$

and

$$\left|\frac{\partial K_M}{\partial t}(x,t;y,s)\right| \le \tilde{h}_{t,s}(x-y) \tag{5}$$

where

$$\tilde{h}_{t,s} \in L^1(R^d); \qquad t > s.$$

Now from estimate (4) and Young's inequality we obtain the result that $U_\delta(t,s)$ determines a family of uniformly bounded operators for $\delta \in [0,1]$. Similarly, estimate (5) leads to the result that $\dot{U}$ is a bounded operator.

Since C_0^∞ is dense in L^2, we can select a sequence of C_0^∞ functions $\{\phi_i\}_{i=1}^\infty$ such that

$$\|\phi-\phi_i\| \le \frac{1}{i} .$$

Now for a given ϕ_i,

$$\|[U_\delta(t,s) - \dot{U}(t,s)]\phi_i\|^2$$

$$= \int dx \left| \int \left[\frac{K_M(x,t+\delta;y,s)-K_M(Q)}{\delta} - \frac{\partial K_M(Q)}{\partial t}\right]\phi_i(y)\,dy\right|^2 .$$

Since ϕ_i is compactly supported the above integral is non-zero only in a compact subset of $R^d \times R^d$, say $X_i \times Y_i$. Thus for each i,

$$\|[U_\delta(t,s) - \dot{U}(t,s)]\phi_i\|^2$$

$$\le \mathrm{vol}(X_i)[\mathrm{vol}(Y_i)]^2 \, \|\phi_i\|_\infty^2$$

$$\times \left\|\frac{K_M(\cdot,t+\delta t;\cdot,s)-K_M(\cdot,t;\cdot,s)}{\delta t} - \frac{\partial K_M(\cdot,t;\cdot,s)}{\partial t}\right\|_{L^\infty(X_i \times Y_i)} \underset{\delta \to 0}{\to} 0. \tag{6}$$

The last result follows because

$$\left\|\frac{K_M(\cdot,t+\delta;\cdot,s)-K_M(\cdot,t; \ ,s)}{\delta t} - \frac{\partial K_M(\cdot,t;\cdot,s)}{\partial t}\right\|_{L^\infty(X_i \times Y_i)} \underset{\delta \to 0}{\to} 0.$$

In other words, for each $i > 0$ there exists a $\delta_i > 0$ such that

$$\|[U_\delta(t,s) - \dot{U}(t,s)]\phi_i\| \le \frac{1}{i}, \qquad 0 < \delta < \delta_i. \tag{7}$$

Now from (6) and (7) we have

$$\|[U_\delta(t,s) - \dot{U}(t,s)]\phi\|$$

$$\le \|[U_\delta(t,s) - \dot{U}(t,s)](\phi-\phi_i)\| + \|[U_\delta(t,s) - \dot{U}(t,s)]\phi_i\|$$

$$\le (\|h_{t,s}\|_1 + \|\tilde{h}_{t,s}\|_1)\|\phi-\phi_i\| + \frac{1}{i} \to 0$$

$$\le \frac{1}{i}[1 + \|h_{t,s}\|_1 + \|\tilde{h}_{t,s}\|_1] \to 0 \quad \text{as} \quad i \to \infty. \tag{8}$$

Thus we have shown that for all $\phi \in L^2(R^d)$, $(t,s) \in T_\Delta^0$ that $U(t,s)\phi$ has a strong t-derivative with the value $\dot{U}(t,s)\phi$. Next we show that the strong derivative $\dot{U}(t,s)$ is strongly continuous.

From (3)

$$\|[\dot{U}(t+\delta,s) - \dot{U}(t,s)]\phi_i\|^2$$

$$= \int_{R^d} dx \left| \int_{R^d} dy \left[\frac{\partial K_M(x,t+\delta;y,s)}{\partial t} - \frac{\partial K_M(\Omega)}{\partial t}\right]\phi_i(y)\right|^2$$

Since $\phi_i \in C_0^\infty(R^d)$ and $\frac{\partial K_M}{\partial t}$ is a function of compact support in $|x-y|$, the above integral is non-zero only on a compact subset of $R^d \times R^d$. An application of Lemma 3.1 and Corollary A1 leads to the result that

$$\left\|\frac{\partial K_M(\cdot,t+\delta;\cdot,s)}{\partial t} - \frac{\partial K_M(\cdot,t;\cdot,s)}{\partial t}\right\|_{L^\infty(X_i \times Y_i)} \underset{\delta \to 0}{\to} 0.$$

Thus a modified version of the analysis presented above establishes the required result.

In the foregoing we have shown that $U_M(t,s)$ is strongly continuously t-differentiable in the open triangular domain T_Δ^0.

<u>LEMMA A3</u>: *Let* a *and* v *belong to the potential class* A(2M+2); *then the following* x, y *uniform bounds hold,*

$$|\nabla_x W_M(Q)| \le \text{const. } m^{d/2+1} (\Delta t)^{-d/2-1}$$

$$|\Delta_x W_M(Q)| \le \text{const. } m^{d/2+2} (\Delta t)^{-d/2-2} .$$

<u>Proof</u>: (a) From (3.24) we have

$$\nabla_x W_M(Q) = K_0(Q)\exp(-\frac{iJ(Q)}{\hbar})[\frac{im}{\hbar\Delta t}(x-y) - \frac{i}{\hbar}\nabla_x J(Q) + \nabla_x] \times \sum_{i=0}^{M} m^{-i} T_i(Q)$$

It follows that

$$|\nabla_x W_M(Q)| \le (\frac{m}{2\hbar\Delta t})^{d/2} \left\{ [\frac{m}{\hbar} |\frac{x-y}{\Delta t}| + \frac{1}{\hbar} |\nabla_x J(Q)|] \left| \sum_{i=0}^{M} m^{-i} T_i(Q) \right| + \sum_{i=0}^{M} m^{-i} |\nabla_x T_i(Q)| \right\}.$$

From (3.18) and the inequality $|x-y| < D+\ell$, we note that

$$|\nabla_x J(Q)| \le \text{const. } m^0 (\Delta t)^0 .$$

Also from Lemma 3.1

$$|\nabla_x T_i(Q)| \le \text{const. } (\frac{d\Delta t}{2})^i .$$

Using these bounds we obtain

$$|\nabla_x W_M(Q)| \le \text{const. } m^{d/2+1} (\Delta t)^{-d/2-1} .$$

The constant in the above inequality does not depend on m or on (Δt).

(b)

$$\Delta_x W_M(Q) = K_0(Q)\exp(-\frac{i}{\hbar}J(Q))[\frac{imd}{\hbar} - \frac{i}{\hbar}\Delta_x J(Q)$$

$$+ (\frac{im(x-y)}{\hbar\Delta t} - \frac{i}{\hbar}\nabla_x J(Q))^2 + 2(\frac{im(x-y)}{\hbar\Delta t} - \frac{i}{\hbar}\nabla_x J)\cdot\nabla_x + \Delta_x] \sum_{i=0}^{M} m^{-i} T_i(Q) .$$

Following the same type of argument we obtain

$$|\Delta_x W(Q)| \le \text{const. } m^{d/2+2} (\Delta t)^{-d/2-2} .$$

The constant in the above inequality is independent of m and Δt. □

LEMMA A4: *Let* $\phi \in H_{d+|\delta|}$ *and assume that* a *and* v *belong to the potential class* $A(2M+d+|\delta|)$; *then, for* $|\delta| > 0$

$$\|\nabla^\delta R_M^0(t,s)\phi\| \le \text{const. } m^0 (\Delta t)^M \|\overset{+}{\chi}_{d+|\delta|}\| \; |||\phi|||_{d+|\delta|} .$$

Proof: Let $\delta = 1$ and $d = 1$; then from (3.70)

$$\frac{d\eta(x,\lambda)}{dx} = (\frac{\lambda}{\pi i})^{\frac{1}{2}} \int_{-\infty}^{+\infty} dy \frac{d}{dx}(e^{i\lambda(x-y)^2} B(Q))\phi(y)$$

$$= (\frac{\lambda}{\pi i})^{\frac{1}{2}} \left\{ \int_{-\infty}^{+\infty} dy\, e^{i\lambda(x-y)^2} \frac{dB(Q)}{dx} \phi(y) \right.$$

$$\left. + \int_{-\infty}^{+\infty} dy \frac{d}{dx} e^{i\lambda(x-y)^2} B(Q)\phi(y) \right\}$$

$$= \eta_1' + \eta_2' . \tag{A4.1}$$

Note that

$$\frac{d}{dx} e^{i\lambda(x-y)^2} = - \frac{d}{dy} e^{i\lambda(x-y)^2}.$$

Thus

$$\eta_2'(x,\lambda) = -\left(\frac{\lambda}{\pi i}\right)^{\frac{1}{2}} \int_{-\infty}^{+\infty} dy \left(\frac{d}{dy} e^{i\lambda(x-y)^2}\right) B(Q)\,\phi(y)$$

$$= \left(\frac{\lambda}{\pi i}\right)^{\frac{1}{2}} \left\{ -e^{i\lambda(x-y)^2} B(Q)\,\phi(y) \Big|_{-\infty}^{+\infty} \right.$$

$$\left. + \int_{-\infty}^{+\infty} dy\, e^{i\lambda(x-y)^2} \frac{d}{dy} (B(Q)\,\phi(y)) \right\}.$$

Since $B(Q) = 0$ for sufficiently large $|y|$, the surface term in $\{\cdot\}$ vanishes and thus

$$\eta_2'(x,\lambda) = \left(\frac{\lambda}{\pi i}\right)^{\frac{1}{2}} \int_{-\infty}^{+\infty} dy\, e^{i\lambda(x-y)^2} \frac{d}{dy} (B(Q)\,\phi(y)). \tag{A4.2}$$

From equations (A4.1) and (A4.2) we observe that $\frac{d\eta}{dx}(x,\lambda)$ is similar to the integral given in (3.70). Initial state ϕ and potentials were chosen so that analysis of Lemma 3.5 can be repeated for integrals of the type given above.

For $\delta = 2$, $\frac{d^2\eta}{dx^2}$ can be rewritten in the above form by observing that

$$\frac{d^2}{dx^2} e^{i\lambda(x-y)^2} = \frac{d^2}{dy^2} e^{i\lambda(x-y)^2}.$$

Similar technique works for any $|\delta| > 0$. Generalization to d-dimensions is done in an analogous way as shown in the proof of Lemma 3.5. □

CHAPTER 4

THE FORMAL PROPAGATOR FOR A MIXED PROBLEM

4.0 Introduction

In this chapter we identify and discuss the special features of mixed boundary value problems in quantum mechanics. We select the problem of evolution in half-space as a model to display the necessary computations in the simplest possible fashion.

In the following analysis we will use the method of images to find the formal quantum propagator $K_M^+(Q)$ for the problem of evolution in half-space, R_+^3. The application of the method of images to this problem requries the definition of an appropriate extended Hamiltonian $H^e(t,m)$. In section (4.1) the extended Hamiltonian will be defined and remarks will be made concerning its useful properties. Section (4.2) calculates the coefficient function $T_1^e(Q^r)$ in the $m \to \infty$ expansion of the extended propagator $K_M^e(Q^r)$. For convenience all the calculations in sections (4.1) and (4.2) are performed in three dimensions. Section (4.3) elaborates on the results obtained in previous sections. The chapter concludes with a few remarks concerning the generalization to arbitrary dimensions.

4.1 The Extended Hamiltonian

The problem of quantum evolution in three-dimensional half-space $R_\pm^3 \equiv \{x \in R^3\colon x_1 \gtrless 0\}$ consists of solving the pointwise PDE (3.2) subjected to the initial-boundary conditions (3.3a,b). The differential form of the Hamiltonian corresponding to the perturbed $H_{0_+}(m)$ [cf. Lemma 2.1] in half-space R^3_+ is

$$H_+(x,-i\hbar\nabla_x,t;m) = \frac{1}{2m}\left(\frac{\hbar}{i}\nabla_x - a(x,t)\right)^2 + v(x,t). \tag{4.1}$$

The function a above represents a time-dependent vector field mapping $R^3_+ \times [0,T] \to R^3$ while v is a scalar potential from $R^3_+ \times [0,T] \to R$.

To solve this problem we shall employ method of images blended with the technique of parametrix solution developed in Chapter 3. In this section we construct an appropriate extended Hamiltonian $H^e(x,-i\hbar\nabla_x,t;m)$ from the one given in equation 4.1. This extended Hamiltonian is required for the application of method of images in this context.

Definition 4.1: *Let* $\hat{R}_1$ *be a mapping* $\hat{R}_1: R^3 \to R^3$ *given by*

$$\hat{R}_1 x = x^r \equiv (-x_1,x_2,x_3) \qquad x \in R^3.$$

The operator $\hat{R}$: $L^1_{loc}(R^3,C) \to L^1_{loc}(R^3,C)$ *associated with the transformation* $\hat{R}_1$ *is defined to be*

$$\hat{R}f = g; \qquad f,g \in L^1_{loc}(R^3,C) \tag{4.2}$$

where

$$g(x) = f(\hat{R}_1 x) \quad \text{a.e.}$$

Similarly, the operator $\hat{R}_V: L^1_{loc}(R^3,C^3) \to L^1_{loc}(R^3,C^3)$ *associated with* $\hat{R}_1$ *is defined to be*

$$\hat{R}_V f = g; \qquad f,g \in L^1_{loc}(R^3,C) \tag{4.3}$$

where

$$g(x) = (g_1(x), g_2(x), g_3(x)) = (-f_1(\hat{R}_1 x), f_2(\hat{R}_1 x), f_3(\hat{R}_1 x)) \text{ a.e.}$$

Note that $\hat{R}$ *and* $\hat{R}_V$ *when restricted to* $L^2(R^3,C)$ *and* $L^2(R^3,C^3)$ *define bounded operators. In particular they are involutions with the usual defining properties*

$$\hat{R} = \hat{R}^*; \quad \hat{R}^2 = I \quad \text{and} \quad \hat{R}_V = \hat{R}_V^*; \quad \hat{R}_V^2 = I.$$

Moreover, the Hilbert space $L^2(R^3,C)$ *can be divided into two orthogonal parts, i.e.,*

$$L^2(R^3,C) = S^{ev.} \oplus S^o$$

where $\frac{1}{2}(I+\hat{R})L^2(R^3,C) = S^{ev.}$ *and* $\frac{1}{2}(I-\hat{R})L^2(R^3,C) = S^0$. *Here the superscripts* 'ev.' *and* 'o' *stands for even and odd respectively.* □

__Definition 4.2__: Let a *and* v *be the vector and scalar potentials satisfying assumptions 1 and 2 of Chapter 2 on the half-space* $\Omega = R^3_+ \times [0,T]$, *then*

(a) The scalar operator $V^e: L^2(R^3,C) \to L^2(R^3,C)$ *is defined by multiplication by a real valued function* $v^e(\cdot,t): R^3 \to R$ *where*

$$v^e(x,t) = v(x,t) \qquad \textit{if } (x,t) \in R_+^3 \times [0,T] \tag{4.4a}$$

$$= \hat{R}v(x,t) = v(x^r,t) \textit{ if } (x,t) \in R_-^3 \times [0,T]. \tag{4.4b}$$

(b) The vector operator $a^e(t): L^2(R^3,C) \to L^2(R^3,C)$ *is a three-dimensional operator whose components* $a_i^e(t)$ *are operator mappings* $L^2(R^3,C) \to L^2(R^3,C)$. *Each* $a_i^e(t)$ *is defined by multiplication by a real valued function* $a_i^e(t): R^3 \to R$ *where*

$$a_i^e(t) = a_i(x,t) \qquad \textit{if } (x,t) \in R_+^3 \times [0,T] \tag{4.5a}$$

$$= \hat{R}a_i(x,t) \quad \textit{if } (x,t) \in R_-^3 \times [0,T]. \tag{4.5b}$$

Specifically, $\hat{R}_v a(x,t) = (-a_1(x^r,t), a_2(x^r,t), a_3(x^r,t))$. □

<u>*Definition 4.3*</u>*: We say that* $a,v \in A^+$ *if* $a,v \in A$ *for all* $x \in R_\pm^3$, *i.e.,* $a,v \in A$ *for the two separate half-spaces* R_+^3 *and* R_-^3. *Similarily* $a,v \in A^+(2M)$ *if* $a,v \in A(2M)$ *for all* $x \in R_\pm^3$. □

The extended potentials a^e, v^e of Definition (4.2) are members of class A^+. Furthermore, a_1^e and $\frac{\partial v^e}{\partial x_1}$ have jump discontinuities at $x = (0,x_2,x_3)$. At this stage we recall that the proof of self-adjointness [cf. Lemma 2.2] depends only on the L^∞-norms of the scalar and vector fields. Thus the results of Lemma (2.2) can be easily extended to include the potentials of class A^+ with the coordinate domain $\Omega = R^3$. In particular, for a^e, v^e we may conclude that the extended Hamiltonian $H^e(t)$ whose differential form is

$$H^e(x,-ih\nabla_x,t) = \frac{1}{2m}\left(\frac{h}{i}\nabla_x - a^e(x,t)\right)^2 + v^e(x,t) \tag{4.6}$$

is self-adjoint with a time invariant domain

$$D(H_0^e) = \{\psi \in L^2(R^3): |k|^2\hat{\psi} \in L^2(R^3)\}.$$

The construction of $H^e(t,m): D(H_0^e) \to L^2(R^3)$ defines the image charge extension (as induced by reflection $\hat{R}_1$) of $H_{0_+}(t,m): D(H_{0_+}) \to L^2(R_+^3)$.

REMARK 4.1: The extended Hamiltonian $H^e(t,m)$ commutes with the reflection operator $\hat{R}$. This can be shown by using the following simple identities and the definitions 4.1 and 4.2:

$$\begin{aligned}\hat{R}_V(\vec{\nabla}_x f) &= \left\{\frac{\partial f}{\partial x_1}(-x_1,x_2,x_3)(-\hat{e}_1) + \frac{\partial f}{\partial x_2}(-x_1,x_2,x_3)\hat{e}_2\right.\\ &\qquad\left. + \frac{\partial f}{\partial x_3}(-x_1,x_2,x_3)\hat{e}_3\right\}\\ &= \vec{\nabla}_{\hat{R}_1 x}(\hat{R}f)(x)\end{aligned} \tag{4.7}$$

$$\hat{R}(\vec{\nabla}_x\cdot\vec{a}^e(x,t))f(x) = \vec{\nabla}_x\cdot\vec{a}^e(x,t)(\hat{R}f)(x) \tag{4.8}$$

$$\hat{R}(\Delta_x f)(x) = \Delta_x(\hat{R}f)(x) \tag{4.9}$$

and

$$\hat{R}(-ih\nabla_x - a^e(x,t))^2 f(x) = (-ih\nabla_x - a^e(x,t))^2(\hat{R}f)(x). \tag{4.10}$$

With the mathematical definition of $H^e(t,m)$ complete we are now ready to determine the formal propagator for the problem of evolution on half-space.

4.2 The Formal Propagator

First consider the case when the scalar and vector fields are both absent. In this circumstance solution to

Schrödinger PDE (3.2) subjected to conditions (3.3a) and (3.3b) is known [Sc]. This solution can be interpreted in terms of the method of images in the following manner.

To each $x = (x_1, x_2, x_3)$ in R_+^3 we associate its reflection x^r through the plane $x_1 = 0$ and define

$$K_0^+(Q) = K_0(Q) - K_0(Q^r) \tag{4.11}$$

where $Q^r = (x,t;y^r,s)$ and K_0 is the familiar free propagator in R^3 [cf. equation 3.16]. Clearly, K_0^+ is a solution of (3.2) and it satisfies the initial-boundary condition (3.3a) and (3.3b). Moreover, K_0^+ has a useful symmetry, i.e.,

$$K_0^+(x,t;y,s) = K_0^+(y,t;x,s). \tag{4.12}$$

From equation (4.11) we can infer that the free propagator solution to the problem of quantum evolution on half-space is expressible in terms of the propagators in R^3. Guided by this interpretation of K_0^+ we propose that the exact propagator be of the form

$$K^+(Q) = K^e(Q) - K^e(Q^r) \quad \text{for} \quad Q \in R_+^3 \times R_+^3 \times T_\Delta. \tag{4.13}$$

In (4.13) it is assumed that the evolution problem defined by $H^e(t,m)$ has a propagator $K^e(Q)$ in the sense of Definition 3.1. A similar expression can be written for the other mixed boundary value problems. Note that the relative sign on the right hand side of (4.13) is determined by the boundary conditions [La].

In Chapter 3, we demonstrated that if the scalar and the vector potentials are finitely continuously differentiable [Assumption 3], then a formal truncated m^{-1}-asymptotic expansion can be worked out for $K(Q)$. Assume $a^e, v^e \in A^+(2M)$; then the formal $m \to \infty$ asymptotic expression

$$W_M^+(Q) = K_0(Q)\exp(-\frac{i}{\hbar} J^e(Q)) \sum_{i=0}^{M} m^{-i} T_i^e(Q)$$

$$- K_0(Q^r)\exp(-\frac{i}{\hbar} J^e(Q^r)) \sum_{i=0}^{M} m^{-i} T_i^e(Q^r)$$

$$\equiv W_M^e(Q) - W_M^e(Q^r) \qquad (4.14)$$

generalizes the R^3-expression (3.24). In the above expression $J^e(Q)$ is given by equation (3.18) while T_i^e's satisfy the recurrence relation (3.22). Since a^e and the $\frac{\partial}{\partial x_1}$-derivative of v^e are discontinuous at $x = (0, x_2, x_3)$, we cannot use the formulas (with the replacement $Q \to Q^r$) for $J^e(Q^r)$ and $T_i^e(Q^r)$ in [POM, equations 4.32-4.33] nor can we use the estimates of Lemma A1.

For the reasons above a new calculation of $J^e(Q^r)$ and $T_i^e(Q^r)$ is required. In doing so we shall require definition and properties of a linear path connecting

(x,t) and (y^r,s). Geometrically, the path $w(\xi;Q^r)$ has the structure shown in Figure 4.1.

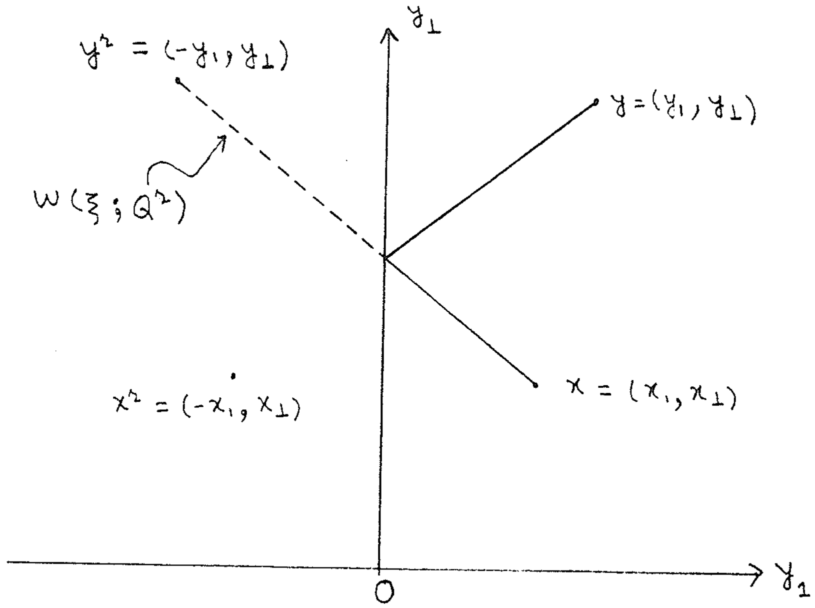

Fig. 4.1

Let τ be the running time variable and define the dimensionless parameter $\xi = \frac{\tau}{(t-s)}$; then the ξ-parametrized path $w(\xi;Q^r): [0,1] \to R^3$ for fixed x,y is given by

$$w(\xi;Q^r) = (y^r + \xi(x-y^r),\ s + \xi(t-s)); \quad \xi \in [0,1]. \tag{4.15}$$

At the boundary $\xi = \xi_c = \frac{y_1}{(x_1+y_1)}$. This is obtained by setting the 1-component of the space part w_x of w equal to zero. This point is of special importance because a^e and $\frac{\partial v^e}{\partial x_1}$ are both discontinuous at $x = (0,x_2,x_3)$.

The function $w(\xi;Q^r)$ has the following useful properties:

1°. $w(\xi;Q^r) \in C^\infty([0,1])$; $w(0,Q^r) = (y^r,s)$; $w(1;Q^r) = (x,t)$

2°. $\frac{\partial w_i}{\partial x_i}(\xi;Q^r) = \xi$ for $i = 1 \sim 3$ and $\frac{\partial^2 w}{\partial x_i \partial x_j} = 0$ for all i,j.

3°. Let $w_x(\xi;Q^r)$ and $w_t(\xi;Q^r)$ represent the space and time part of $w(\xi;Q^r)$; then

$$\frac{w_x(\xi;Q^r) - y^r}{w_t(\xi;Q^r) - s} = \frac{x-y^r}{t-s} .$$

The right hand side of the above equation is a velocity (in the sense of classical mechanics) of a particle. This velocity is independent of the value of $\xi \in [0,1]$.

4°. The linear path $w(\xi;Q^r)$ has the following semi-group property:

$$w(\xi;w(\xi',Q^r);y^r,s) = w(\xi'\xi;Q^r); \quad \xi,\xi' \in [0,1].$$

Let us now calculate $J^e(Q^r)$. The $m \to \infty$ asymptotic expansion of $K^e(Q^r)$ requires that $J^e(Q^r)$ satisfy the PDE [of (3.41)]

$$\frac{\partial}{\partial t} J^e(Q^r) + \frac{x-y^r}{t-s} \cdot \nabla_1 J^e(Q^r) = v^e(x,t) - \frac{x-y^r}{t-s} \cdot \vec{a}^e(x,t). \tag{4.16a}$$

Using the linear path substitution $(x,t) \to w(\xi;Q^r)$ [cf. 3.19] in (4.16a) we note that it becomes an ODE. In particular, using property 3° of $w(\xi;Q^r)$ we obtain from equation (4.16a)

$$\frac{1}{t-s}\frac{d}{d\xi} J^e(w(\xi;Q^r);y^r,s) = v^e(w(\xi;Q^r)) - (\frac{x-y^r}{t-s}) \cdot \vec{a}^e(w(\xi;Q^r)). \tag{4.16b}$$

The right hand side of (4.16b) is piecewise continuous in ξ and may therefore be integrated with respect to $d\xi$ giving

$$J^e(x,t;y^r,s) - J^e(y^r,s;y^r,s) = (t-s)\int_0^1 v^e(w(\xi;Q^r))d\xi$$

$$- (x-y^r)\cdot\int_0^1 a^e(w(\xi;Q^r))d\xi. \quad (4.17)$$

If the initial condition is taken to be

$$J^e(y^r,s;y^r,s) = 0$$

$W_0^+(Q)$ [cf. equation 4.14] satisfies the Dirichlet boundary condition. This is basically a consequence of the R_1-symmetry of the potentials v^e and a^e. The definitions of $J^e(Q)$ and $J^e(Q^r)$ now ensure that

$$J^e(x,t;y^r,s)\Big|_{x_1=0} = J^e(x,t;y,s)\Big|_{x_1=0}$$

which suffices to show that the direct and image charge parts of $W_0^+(Q)$ cancel on the boundary $x_1 = 0$. Moreover, formula (4.17) shows that the path averaged structure of $J^e(Q^r)$ is unaltered by the fact that $\frac{\partial v^e}{\partial x_1}$ and a^e are discontinuous along the path $w(\xi;Q^r)$. The calculation of $T_1^e(Q^r)$ will however show that this coefficient will alter its structure as a consequence of non-smooth behaviour of a^e and $\frac{\partial v^e}{\partial x_1}$.

To calculate $T_1^e(Q^r)$ we require expressions for $(\nabla_1 J^e+a^e)(Q^r)$ and $\nabla_1\cdot(\nabla_1 J^e+a^e)(Q^r)$. Using Leibnitz rule for differentiation under the integral sign we get

$$\frac{\partial J^e(Q^r)}{\partial x_1} = (t-s)\left(\int_0^{\xi_c^-} + \int_{\xi_c^+}^{1}\right) d\xi \left[\frac{\partial w_1}{\partial x_1}(\xi;Q^r)\right.$$

$$\times\left(\frac{\partial v^e}{\partial w_1} - \frac{x_1+y_1}{t-s}\frac{\partial a_1^e}{\partial w_1} - \sum_{k=2}^{3}\frac{(x-y^r)_k}{t-s}\frac{\partial a_k^e}{\partial w_1}\right)(w(\xi;Q^r))$$

$$\left. - \frac{1}{t-s}\, a_1^e(w(\xi;Q^r))\right]$$

$$+ (t-s)\frac{\partial \xi_c}{\partial x_1}\left[\left(v^e - \frac{w_x(\xi_c;Q^r)-y^r}{w_t(\xi_c;Q^r) - s}\cdot a^e\right)(w(\xi_c^-;Q^r))\right.$$

$$\left. - \left(v^e - \frac{w_x(\xi_c;Q^r)-y^r}{w_t(\xi_c;Q^r) - s}\cdot a^e\right)(w(\xi_c^+;Q^r))\right].$$

In the last expression ξ_c is the value of ξ at the boundary $x_1 = 0$ and $\xi_c^- \equiv \xi_c-0$; $\xi_c^+ \equiv \xi_c+0$. Using the definition of $w_1(\xi;Q^r)$, the property 3° of $w(\xi;Q^r)$, the continuous and discontinuous behaviour of v^e and a^e at the boundary respectively, we get

$$\frac{\partial J^e(Q^r)}{\partial x_1} = (t-s)\left(\int_0^{\xi_c^-} + \int_{\xi_c^+}^{1}\right) d\xi \left\{- \frac{1}{t-s}\, a_1^e(w(\xi;Q^r))\right.$$

$$\left. + \xi\left(\frac{\partial v^e}{\partial w_1} - \frac{x_1+y_1}{t-s}\frac{\partial a_1^e}{\partial w_1} - \sum_{k=2}^{3}\frac{(x-y^r)_k}{t-s}\frac{\partial a_k^e}{\partial w_1}\right)(w(\xi;Q^r))\right\}$$

$$- \frac{2y_1}{(x_1+y_1)}\, a_1^e(w(\xi_c^+;Q^r)). \tag{4.18a}$$

Since

$$\xi_c^- a_1^e(w(\xi_c^-;Q^r)) - \xi_c^+ a_1^e(w(\xi_c^+;Q^r)) = -\frac{2y_1}{x_1+y_1}\, a_1^e(w(\xi_c^+;Q^r))$$

we can express $a_1^e(x,t)$ as

$$a_1^e(x,t) = \left(\int_0^{\xi_c^-} + \int_{\xi_c^+}^{1}\right) d\xi \frac{d}{d\xi}[\xi a_1^e(w(\xi;Q^r))] + \frac{2y_1}{x_1+y_1} a_1^e(w(\xi_c^+)) . \tag{4.18b}$$

Thus from (4.18a) and (4.18b) we obtain

$$\frac{\partial J^e(Q^r)}{\partial x_1} + a_1^e(x,t) = (t-s) \int_0^1 d\xi\xi \left\{ \left(\frac{\partial v^e}{\partial w_1} + \frac{\partial a_1^e}{\partial t}\right)(w(\xi;Q^r)) + \sum_{k=1}^{3} \frac{(x-y^r)_k}{t-s} F_{k1}^e(w(\xi;Q^r)) \right\} \tag{4.19}$$

where

$$F_{k1}^e(w(\xi;Q^r)) = \left(\frac{\partial a_1^e}{\partial w_k} - \frac{\partial a_k^e}{\partial w_1}\right)(w(\xi;Q^r)) . \tag{4.20}$$

One note-worthy feature of the above calculation is seen in the equations (4.18a,b). We see that both $\frac{\partial J^e(Q^r)}{x_1}$ and $a_1^e(x,t)$ are discontinuous at the boundary $x_1 = 0$, but when added together the surface terms in (4.18a,b) cancel each other. Thus for any $j = 1 \sim 3$

$$\frac{\partial J^e(Q^r)}{\partial x_j} + a_j^e(x,t) = (t-s) \int_0^1 \xi d\xi \left\{ \left(\frac{\partial v^e}{\partial w_j} + \frac{\partial a_j^e}{\partial t}\right)(w(\xi;Q^r)) + \sum_{k=1}^{3} \frac{(x-y^r)_k}{t-s} F_{kj}^e(w(\xi;Q^r)) \right\}. \tag{4.21}$$

Next, we compute $(\nabla_1 \cdot (\nabla_1 J + a^e))(Q^r)$. Differentiating equation (4.19) with respect to x_1 and using the property 3° of $w(\xi;Q^r)$ we obtain

$$\frac{\partial}{\partial x_1}\left(\frac{\partial J^e(Q^r)}{\partial x_1} + a_1^e(x,t)\right) = (t-s)\int_0^1 d\xi\,\xi^2$$

$$\times \left[\left(\frac{\partial^2 v^e}{\partial w_1^2} + \frac{\partial^2 a_1^e}{\partial w_1 \partial t}\right)(w(\xi;Q^r)) + \sum_{k=1}^{3} \frac{(x-y^r)_k}{t-s} \frac{\partial}{\partial w_1} F_{k1}^e(w(\xi;Q^r))\right]$$

$$+ \xi_c(t-s)\frac{\partial \xi_c}{\partial x_1}\left\{\left(\frac{\partial v^e}{\partial w_1} + \frac{\partial a_1^e}{\partial t} + \sum_{k=1}^{3}\frac{(x-y^r)_k}{t-s}F_{k1}^e\right)(w(\xi_c^-;Q^r))\right.$$

$$\left. - \left(\frac{\partial v^e}{\partial w_1} + \frac{\partial a_1^e}{\partial t} + \sum_{k=1}^{3}\frac{(x-y^r)_k}{t-s}F_{k1}^e\right)(w(\xi_c^+;Q^r))\right\}.$$

But,

$$\frac{\partial v^e}{\partial w_1}(w(\xi_c^-;Q^r)) = -\frac{\partial v^e}{\partial w_1}(w(\xi_c^+;Q^r))$$

$$\frac{\partial a_1^e}{\partial t}(w(\xi_c^-;Q^r)) = -\frac{\partial a_1^e}{\partial t}(w(\xi_c^+;Q^r))$$

and

$$\frac{\partial \xi_c}{\partial x_1} = -\frac{y_1}{(x_1+y_1)^2}.$$

Also note that the $\{\ldots\}$ is non-zero only when the linear path $w(\xi;Q^r)$ goes beyond the origin. This is due to the fact that functions $\frac{\partial v^e}{\partial x_1}$ and a_1^e have jump discontinuities only at the point $x = (0,x_2,x_3)$. Thus for $\xi < \xi_c$ the two terms in {...} cancel each other whereas for $\xi > \xi_c$ the two terms are added. Let $\Theta(\xi > \xi_c)$ denote the standard Heaviside function, then using the properties listed above we obtain

$$\frac{\partial}{\partial x_1}\left(\frac{\partial J^e(Q^r)}{\partial x_1} + a_1^e(x,t)\right) = (t-s)\int_0^1 d\xi\,\xi^2$$
$$\times\left[\left(\frac{\partial^2 v^e}{\partial w_1^2} + \frac{\partial^2 a_1^e}{\partial w_1 \partial t}\right)(w(\xi;Q^r)) + \sum_{k=1}^{3}\frac{(x-y^r)_k}{t-s}\frac{\partial}{\partial w_1}F_{k1}^e(w(\xi;Q^r))\right]$$
$$+\Theta(\xi > \xi_c)\frac{2y_1^2}{(x_1+y_1)^3}(t-s)\left[\left(\frac{\partial v^e}{\partial w_1} + \frac{\partial a_1^e}{\partial t} + \sum_{k=1}^{3}\frac{(x-y^r)_k}{t-s}F_{k1}^e\right)(w(\xi_c^+;Q^r))\right]$$

(4.22a)

Now for $j \neq 1$, there are no boundary terms and we have

$$\frac{\partial}{\partial x_j}\left(\frac{\partial J^e(Q^r)}{\partial x_j} + a_j^e(x,t)\right) = (t-s)\int_0^1 d\xi\,\xi^2$$
$$\times\left[\left(\frac{\partial^2 v^e}{\partial w_j^2} + \frac{\partial^2 a_j^e}{\partial w_j \partial t} + \sum_{k=1}^{3}\frac{(x-y^r)_k}{t-s}\frac{\partial}{\partial w_j}F_{kj}^e\right)(w(\xi;Q^r))\right]. \qquad (4.22b)$$

Thus we have shown that $g_0(w(\xi;Q^r);y^r,s)$ [cf. equation 3.23] is piecewise continuous in $\xi \in [0,1]$, and therefore the equation (3.22) remains valid for $T_1^e(Q^r)$ provided $T_1^e(t,y^r;s,y^r) = 0$. It is this condition that ensures that W_1^+ satisfies Dirichlet boundary conditions. Recall that

$$T_1^e(Q^r) = \frac{t-s}{2} \int_0^1 d\xi\{(i\hbar)^{-1}[(\nabla_1 J^e + a^e)(w(\xi;Q^r))]^2$$

$$+ \nabla_1 \cdot (\nabla_1 J^e + a^e)(w(\xi;Q^r))\}. \qquad (4.23)$$

Define

$$f_j^e(x,t) = -(\nabla^j v^e)(x,t) - \frac{\partial a_j^e}{\partial t}(x,t); \qquad j = 1 \sim 3$$

and

$$\Omega_j^e(x,t) = f_j^e(x,t) + \frac{(x-y^r)_k}{t-s} F_{jk}^e(x,t).$$

The first term in the right hand side of (4.23) can be calculated in a manner identical to the one shown in [POM, equation 4.32]. The result is

$$\frac{t-s}{2ih} \int_0^1 d\xi(\nabla_1 J^e + a^e)^2(w(\xi;Q^r))$$

$$= \frac{(t-s)^3}{2ih} \int_{I^2} d\xi_1 d\xi_2 g(\xi_1,\xi_2)\Omega_j^e(w(\xi_1))\Omega_j^e(w(\xi_2)). \qquad (4.24a)$$

Here $I^n = [0,1]^n$ and g is the one-dimensional Green's function given by

$$g(\xi_1,\xi_2) = \min.(\xi_1,\xi_2) \times (1 - \max.(\xi_1,\xi_2)).$$

Using (4.22a,b) the second term in (4.23) can also be calculated in a straightforward fashion. In this case we have a boundary term B,

$$B \equiv \frac{(t-s)^2}{2}\left[\left(\frac{\partial v^e}{\partial w_1}+\frac{\partial a_1^e}{\partial t}+\sum_{k=1}^{3}\frac{(x-y^r)_k}{t-s}F^e_{k1}\right)(w(\xi_c^+;Q^r))\right]$$
$$\times \int_0^1 d\xi\xi \frac{y_1^2}{(w_1+y_1)^2}\,\Theta(\xi > \xi_c).$$

Observe that [...] in the last expression is the component of Lorentz force parallel to the 1-axis and

$$\int_0^1 d\xi\xi \frac{y_1^2}{(w_1+y_1)^3}\,\Theta(\xi > \xi_c) = \frac{x_1y_1}{(x_1+y_1)^3}.$$

Thus,

$$B = \frac{(t-s)^2}{2}\frac{x_1y_1}{(x_1+y_1)^3}\,[-F^{(1)}_{\mathrm{LOR.}}(w(\xi_c;Q^r))]. \tag{4.24b}$$

Finally from (4.23) and (4.24a,b) we get

$$\begin{aligned}T_1^e(Q^r) = &-\frac{(t-s)^2}{2}\frac{x_1y_1}{(x_1+y_1)^3}F^{(1)}_{\mathrm{LOR.}}(w(\xi_c;Q^r))\\ &-\frac{(t-s)^3}{2ih}\int_{I^2} d\xi_1 d\xi_2 g(\xi_1,\xi_2)\Omega_j^e(w(\xi_1;Q^r))\Omega_j^e(w(\xi_2;Q^r))\\ &-\frac{(t-s)^2}{2}\int_I d\xi\xi(1-\xi)\left\{(\nabla_1\cdot f^e)(w(\xi;Q^r))\right.\\ &\left.\qquad+\sum_{k=1}^{3}\frac{(x-y^r)_k}{t-s}(\nabla^j F^e_{jk})(w(\xi;Q^r))\right\}.\end{aligned} \tag{4.25}$$

In $T_1^e(Q)$ there appears no surface term and the resulting formula is the same as the sum of the last two terms in (4.25) with Q^r replaced by Q. Following a similar procedure one can calculate the higher order coefficients in (4.14) by using the recursion relation (3.22). The surface terms in $\{T_j^e(Q^r)\}_{j=2}^M$ exhibit a stronger algebraic singularity than the one seen in equation (4.25). In particular they grow as $0(1/x_1^j)$ near the boundary.

Next, we show that the singular surface term appearing in equation (4.25) is a common feature in asymptotic expansions with Dirichlet boundary condition. Let us first consider the WKB expansion. For simplicity set $a^e = 0$ and consider just the image charge term. Recall the formal WKB expansion for $K^e(Q^r)$ [OM].

$$K^e(Q^r) \sim \left(\frac{m}{2\pi i\hbar\Delta t}\right)^{3/2} \exp\left(\frac{i}{\hbar} S(Q^r) + \psi_1^e + i\hbar\psi_2^e + \ldots\right) \quad (4.26)$$

where $S(Q^r) = \dfrac{(x-y^r)^2}{t-s}$ is the free particle (image charge) action and the coefficient functions ψ_p are given by

$$\psi_p^e(Q^r) = \sum_{k=p}^{\infty} m^{-k} G_p^k(Q^r). \quad (4.27)$$

The coefficient of interest is $\psi_1^e(Q^r)$. The surface contribution to $\psi_1^e(Q^r)$ comes from the coefficient $G_1^1(Q^r)$ which is given by [OM]

$$G_1^1(Q^r) = \frac{t-s}{2} \int_I d\xi \; \Delta_1 G_0^0(w(\xi;Q^r);y^r,s) \quad (4.28)$$

where

$$G_0^0(Q^r) = (t-s) \int_I d\xi \; v^e(w(\xi;Q^r)). \quad (4.29)$$

Since $\frac{\partial v}{\partial x_1}$ has a jump discontinuity at $x_1 = 0$, it follows from (4.29) that

$$\Delta_1 G_0^0(Q^r) = \int_I d\xi\xi^2(\Delta_1 v^e)(w(\xi;Q^r)) + \theta(\xi > \xi_c)\frac{\partial v^e}{\partial x_1}(w(\xi_c^+;Q^r))\frac{2y_1^2}{(x_1+y_1)^3} .$$

Using the last expression in (4.28) and integrating we find

$$G_1^1(Q^r) = \frac{(t-s)^2}{2}\int_I d\xi\xi(1-\xi)(\Delta_1 v^e)(w(\xi;Q^r)) + (t-s)^2\frac{\partial v}{\partial x_1}(w(\xi_c^+;Q^r))\frac{x_1 y_1}{(x_1+y_1)^3} \tag{4.30}$$

Thus comparing (4.25) and (4.30) we see that the coefficient of $\hbar^0$ in WKB expansion has a surface term which is identical to the one found in the coefficient of m^{-1} in $m \to \infty$ expansion.

Another well studied asymptotic expansion is the short time expansion of the propagator, i.e.,

$$K^e(Q^r) \sim K_0(Q^r)[1 + (t-s)P_1^e(Q^r;m) + \frac{(t-s)^2}{2!}P_2^e(Q^r;m) + \ldots].$$

The coefficient functions P_n^e are known explicitly [WFO, OF]. In particular,

$$P_1^e(Q^r;m) = \int_0^1 d\xi\ v^e(w(\xi;Q^r))$$

$$P_2^e(Q^r;m) = 2\int_0^1 d\xi\ \xi\, v^e(w(\xi;Q^r)) - \frac{\hbar^2}{m}\int_0^1 d\xi\xi(\Delta_1 P_1^e)(Q^r;m) .$$

The term of interest is the coefficient of $\frac{1}{m}$ in $P_2^e(Q^r;m)$. A straightforward calculation shows that

$$(\Delta_1 P_1^e)(Q^r;m) = \int_0^1 d\xi\,\xi^2 (\Delta_1 v^e)(w(\xi;Q^r))$$

$$- \Theta(\xi > \xi_c) \frac{2y_1^2}{(x_1+y_1)^3} \frac{\partial v}{\partial w_1} (w(\xi_c;Q^r)).$$

Substituting this and using property 4^o of $w(\xi;Q^r)$ one obtains the singular term in $P_2^e(Q^r)$ which is identical to the one found in coefficient of m^{-1} in large mass expansion.

The above calculations clearly demonstrate that the appearance of singular terms is purely an effect of the presence of the boundary. Moreover, this special feature of coefficient functions is common to all the relevant semi-classical expansions.

4.3 Discussions: In this section we further elaborate on some of the key features of the analysis done in the previous sections. There are several points to be made.

(1) An alternative approach for calculating $T_M^e(Q^r)$:

In section (4.2) we used method of images to calculate $T_M^e(Q^r)$. There we saw that the surface terms in $T_M^e(Q^r)$ appear as a consequence of the jump discontinuity in $a_1^e(x,t)$ and $\frac{\partial}{\partial x_1} v^e(x,t)$ at the boundary. There exists an alternative approach to this calculation where $w(\xi;Q)$ is taken to be the classical one bounce linear path, i.e.,

$$w(\xi;Q) = (y+\xi(x^r-y),\ s+\xi(t-s)); \qquad \xi \in [0,\xi_c]$$

$$= (y^r+\xi(x-y^r),\ s+\xi(t-s)); \qquad \xi \in [\xi_c,1].$$

In this case the function $\frac{\partial w}{\partial x_1}(\xi;Q)$ has a jump discontinuity at the boundary whereas the potentials a and v are continuous in R^3_+. In comparison, this method is superior than the method of images, as far as the geometrical and physical interpretation is concerned. On the other hand, computations leading to the final result are relatively less tedious in the image charge approach. For this reason, we opted to display the calculations in the framework of the method of images.

(2) <u>The surface term singularity in $T^e_M(Q^r)$ is anamolous:</u> We illustrate this point by showing that the exact propagator $K^+(Q)$ is non-singular. For simplicity we assume that d = 1, time is purely imaginary and the vector potential a = 0 whereas the scalar potential v is time independent.

Let $\beta = +\frac{it}{h}$ and take $\{U(\beta) \equiv e^{-\beta H_+};\ \beta > 0\}$ to be the analytic semigroup generated by H on $L^2(R_+)$. Then the iteration of equation (3.10) gives the operator valued Dyson's series for the Dirichlet problem on $L^2(R_+)$.

$$U(\beta) = U_0(\beta) + \sum_{n=1}^{\infty} (-\beta)^n \int_{>}^{1} d^n\xi U_0(\beta\xi_n)\, V\, U_0(\beta(\xi_{n-1}-\xi_n))\, V \times \ldots \times$$

$$V\, U_0(\beta(\xi_1-\xi_2))\, V\, U_0(\beta(1-\xi_1)). \tag{4.31}$$

Let $U(\beta)$ have the kernel $K^+(x,y;\beta)$, then the kernel valued Dyson's series corresponding to (4.31) is

$$K^+(x,y;\beta) = K_0^+(x,y;\beta) + \sum_{n=1}^{\infty} (-\beta)^n \int_>^1 d^n\xi \int_{R_+} dy_1 \ldots$$

$$\ldots \int_{R_+} dy_n \{\ldots\} \tag{4.32a}$$

where

$$\{\ldots\} = K_0^+(x,y_1;\beta\xi_n)v(y_1)K_0^+(y_1,y_2;\beta(\xi_{n-1}-\xi_n))v(y_2) \ldots$$

$$\ldots v(y_{n-1})K_0^+(y_{n-1},y_n;\beta(\xi_1-\xi_2))$$

$$\times\, v(y_n)K_0^+(y_n,y;\beta(1-\xi_1)) \tag{4.32b}$$

and

$$\int_>^1 d^n\xi \equiv \int_{0\le\xi_n\le\ldots\le\xi_1\le 1} d\xi_1 \ldots d\xi_n .$$

Note that for a given n each term in (4.32a) satisfies the Dirichlet boundary condition. In the following lemma we will show that the Dyson's series (4.32) is uniformly convergent in $x,y \in R_+ \times R_+$.

<u>*LEMMA 4.1*</u>. *If* $\sup_{x\ge 0} |v(x)| \equiv \|v\|_\infty < \infty$, *then the Dyson series (4.32a) is uniformly convergent in* $x,y \in R_+ \times R_+$. *Moreover,*

$$|K^+(x,y;\beta)| \le 2 \exp(2\beta\|v\|_\infty)\, K_0(x,y;\beta) . \tag{4.33}$$

<u>Proof</u>: Let $n \geq 1$ and consider the n^{th} term in (4.32a).

$$|D_n^+(x,y;\beta)| \leq \beta^n \int_{>}^{1} d^n\xi \int_{R_+} dy_1 \ldots \int_{R_+} dy_n \; |\{\ldots\}|.$$

From (3.16) it is clear that

$$K_0(x_1,x_2;\beta) \geq K_0(x_1,-x_2;\beta); \qquad x,y \in R_+ \times R_+.$$

Therefore, using (4.11) we get

$$|K_0^+(x_1,x_2;\beta')| \leq 2\, K_0(x_1,x_2;\beta'); \qquad x,y \in R_+ \times R_+.$$

Thus

$$|D_n^+(x,y;\beta)| \leq 2(2\beta\|v\|_\infty)^n \int_{>}^{1} d^n\xi \int_R dy_1 \ldots \int_R dy_n K_0(x,y_1;\beta\xi_n)$$
$$\times\, K_0(y_1,y_2;\beta(\xi_{n-1}-\xi_n)) \times \ldots \times K_0(y_n,y;\beta(1-\xi_1)).$$

Now using the semi-group property of $U_0(\beta')$ in H we get

$$|D_n^+(x,y;\beta)| \leq \frac{2}{n!}\,(2\beta\,\|v\|_\infty)^n\, K_0(x,y;\beta). \tag{4.34}$$

Estimate (4.33) follows by using (4.34) in (4.32a). □

From (4.32a) and (4.13) it can be shown that $K^+(x,y;\beta)$ goes uniformly to zero in the neighbourhood of boundary ∂R_+, i.e., $K^+(x,y;\beta)$ satisfies Dirichlet boundary condition. In particular, the diagonal $K^+(x,x;\beta)$ is uniformly bounded for all $x \in R_+$ and vanishes as $x \to 0$. This is possible only if $K^+(x,x;\beta)$ is nonsingular as $x \quad 0$. For this reason the surface term singularity ($\sim x_1^{-1}$) appearing in (4.25) has an analytic behaviour incompatible with the exact kernel and is thus termed 'anomalous'. Note that this anomaly disappears if both the potentials **a** and v are assumed to be constants in the neighbourhood of the boundary. We will deal with this surface anomaly in more general situations in Chapter 5.

(3) <u>The $m \to \infty$ expansion and the Dirichlet boundary conditions</u>: The large mass ($m \to \infty$) semi-calssical expansion expresses in an analytic form with the remainder estimates the way in which the Laplacian in the Hamiltonian dominates the contribution to the propagator coming from $\vec{a}\cdot\vec{\nabla}$ and the scalar potential terms [POM]. However, at the pointwise level the Dirichlet boundary condition has a profound effect on the expansion. If the Dirichlet boundary condition is interpreted as an infinite potential at the boundary then its contribution to evolution is of the same order in mass as that of leading partial derivative in the Hamiltonian (i.e., the Laplacian). For example, the presence of infinite potential at the boundary gives rise to a new essential singularity in m^{-1} via $K_0(\Omega^r)$ which does not exist in the absence of boundary.

(4) The analysis presented in sections 4.1-4.2 was worked out for the case of a single particle moving in a 3-dimensional half-space R_+^3. All the results of these sections can be extended to the case of N-particles moving in a 3N-dimensional half-space R_+^{3N},

$$R_+^{3N} = \underbrace{R_+^3 \times R_+^3 \times \ldots \times R_+^3}_{\text{N-times}}.$$

This generalization is straightforward and thus the details are not given here.

(5) Motion in an interval: Consider a particle whose one degree of freedom is constrained to be the interval $[0,a]$ subjected to the periodic boundary conditions. The dynamics of this system is governed by the Schrödinger equation (3.2, 3.3a) with the boundary condition (3.3b) replaced by

$$K^P(0,t;y,s) = K^P(a,t;y,s). \tag{4.35}$$

For simplicity we assume that $a \equiv 0$ and the scalar potential v is time independent. The differential form of the Hamiltonian corresponding to the perturbed $H_{0\mathcal{S}}$; $\mathcal{S} = (\cdot,\cdot,\ldots,\cdot)$ [cf. Lemma 2.1] is given by

$$H(x,-i\hbar\nabla_x,m) = -\frac{\hbar^2}{2m}\Delta_x + v(x) \tag{4.36}$$

In the special case when $v = 0$, the propagator for the system (4.36) is known [Sc]. It is given by the formula

$$K_0^P(Q) = \sum_{n=-\infty}^{+\infty} K_n^0(Q) \tag{4.37}$$

where n is the winding number which represents the number of times the path goes past a particular point moving in a particular direction (say left) minus the number of times it passes that same point in the opposite direction (say right). The function $K_n^0(Q)$ in (4.37) is given by

$$K_n^0(Q) = \left(\frac{m}{2\pi i\hbar\Delta t}\right)^{\frac{1}{2}}\exp[i(2\hbar\Delta t)^{-1}m(x-y+na)^2 + in\delta]. \tag{4.38}$$

Here δ is some phase factor [Sc].

In the general situation when $v \neq 0$, we appeal to the method of images to construct the formal propagator. Consider a classical particle moving in the interval $[0,a]$. The periodic boundary conditions imply that when particle encounters one end of the interval it re-appears on the other end. Thus a particle can start from a fixed initial position $y \in [0,a]$ and arrive at some final point x in a number of different ways. The most general situation would be when particle (starting from y) goes "around" the interval n number of times before arriving at x. The total distance is computed by projecting the final point x to the nearest interval, every time particle goes "around" the original interval. This amounts to the following coordinate transformation:

$$y \rightarrow y; \qquad x \rightarrow x+na \ . \tag{4.39}$$

This can be easily generalized to higher dimensions. For example, in the two dimensional rectangular boundary $[0,a] \times [0,b]$ there will appear a two dimensional periodic lattice characterized by a pair of integers (n_1,n_2). The resulting transformation is:

$$y \equiv (y_1,y_2) \rightarrow (y_1,y_2); \quad x \equiv (x_1,x_2) \rightarrow (x_1+n_1a, x_2+n_2b) \ . \tag{4.40}$$

Next we must define the extended Hamiltonian corresponding to the one given in (4.36). This is done in the same way as shown in Definition 4.2. The extended potential

v^e: $L^2(R,C) \to L^2(R,C)$ is defined by multiplication by a real valued function $v^e(\cdot)$: $R \to R$. The function v^e is given by

$$v^e(x) = v_0(x-na) \quad \text{for all} \quad x-na \in [-a,a] \tag{4.41a}$$

where

$$\begin{aligned} v_0(x) &= v(x) \quad \text{for} \quad x \in [0,a] \\ &= v(-x) \;\text{for} \quad x \in [-a,0]. \end{aligned} \tag{4.41b}$$

Thus the motion of a particle in the interval [0,a] is equivalent to that of a particle moving on an entire real line under the influence of a periodic potential. Note that the velocity vector does not change direction at the end points. Thus the coefficient functions T_j^e are not singular at the boundary. On the other hand if the Dirichlet boundary conditions are imposed at the end points, the particle suffers a perfectly elastic collision with the boundary. Thus the x-derivative of the classical path [cf. figure 4.1] has a jump discontinuity which is responsible for the anomalous singular behaviour of the coefficient functions T_j^e.

From the above discussion it is clear that the appearance of the surface-term singularity is solely due to the effect of the instantaneous momentum transfer associated with particle reflection from a hard wall (Dirichlet boundary). Boundary conditions not associated with momentum transfer, such as periodic boundary conditions, do not give rise to singularities in the expansion coefficients in any of the physicslly interesting asymptotic expansions (i.e., small $\hbar$, m^{-1} or (t-s)).

CHAPTER 5

ERROR ANALYSIS

5.0 Introduction

In this chapter we show that the parametrix method (developed in Chapter 3) can be used to obtain the L^2-approximate solution of a general mixed boundary value problem in quantum mechanics. For simplicity we first select the problem of quantum evolution in the half-space R^3_+ to display the necessary computational details.

We begin by constructing a suitable parametrix kernel for the half-space problem in Section 5.1. It will be shown that the image charge term $W^e_M(\Omega^r)$ [cf. equation (4.14)] does not contribute to the L^2-approximate solution of the Schrodinger equation (3.2) subjected to initial-boundary conditions (3.3a,b). Section (5.1) concludes with the derivation of the pointwise PDE identity satisfied by the parametrix $K^+_M(\Omega)$. In section (5.2) we will show that for sufficiently smooth initial data, the PDE identity of section 5.1 determines an abstract inhomogeneous equation of motion in $L^2(R^3_+)$. This abstract equation will be solved in section (5.3) and consequently the L^2-norm difference between the exact and the approximate wave function will be computed. Finally, in section (5.4) we provide a prescription for extending these results to solve a general mixed boundary value problem. Some of the lengthy computational details of section (5.1) are placed in an appendix at the end of this chapter.

5.1 The Parametrix

For a parametrix we are interested in a function which is twice continuously differentiable in space-time variables. To find such a parametrix we begin by defining a special smooth cutoff function suitable for use in the neighbourhood of the boundary ∂R_+^3.

Definition 5.1: Let n *be a non-negative integer and denote by* α *a characteristic distance along* 1*-axis, then we define a function* $\lambda: R \to R_+$ *by setting*

$$\lambda(x,\alpha;n) = \frac{1}{\Lambda(n,\alpha)} \int_0^x (x')^n \exp\left[\frac{\alpha^2}{(x'-\alpha)^2-\alpha^2}\right] dx' \; ; \qquad x \le 2\alpha \qquad (5.1a)$$

$$= 1 \; ; \qquad x > 2\alpha \qquad (5.1b)$$

$$= 0 \; ; \qquad x \le 0 \qquad (5.1c)$$

where the normalization factor $\Lambda(n,\alpha)$ *is determined from* (5.1a) *by requiring that* $\lambda(2\alpha,\alpha;n) = 1$. □

The function λ defined above has the following useful properties.

1°. $\lambda(0,\alpha;n) = 0$

2°. $\lambda(x,\alpha;n) = 0(|x|^{n+1})$ and

3°. $(\frac{\partial}{\partial x})^p \lambda(x,\alpha;n) = 0(|x|^{n-p+1})$ if $x \le 2\alpha$

$= 0$ if $x \ge 2\alpha$.

The pointwise calculations of Chapter 4 suggest the following candidate parametrix,

$$K_M^+(Q;\alpha,n) = \Gamma(x_1,y_1;\alpha,n)[K_M^e(Q) - K_M^e(Q^r)] \tag{5.2a}$$

where

$$\Gamma(x_1,y_1;\alpha,n) = \lambda(x_1,\alpha;n)\lambda(y_1,\alpha;n) \tag{5.2b}$$

$$K_M^e(Q) = (\chi_D * \rho_\ell)(d(Q))W_M(Q) \tag{5.2c}$$

and

$$K_M^e(Q^r) = (\chi_D * \rho_\ell)(d(Q^r))W_M(Q^r). \tag{5.2d}$$

In the above expressions W_M and $(\chi_D * \rho_\ell)$ are given by equations (4.14) and (3.26) respectively. The symbols $d(Q)$ and $d(Q^r)$ denote the metric distances $|x-y|$ and $|x-y^r|$ respectively.

Next we show that the second term in equation (5.2a) does not contribute to the L^2-approximate solution to the leading order in mass (i.e., m^{-M}). In doing so we will make the parameter α a function of mass. In particular α will be assumed to be of the order of $m^{-1/k}$; $k \geq 4$. This allows for no restriction on the support of initial data ϕ. Even though all the forthcoming calculations can be performed for an arbitrary $k \geq 4$, we will set $k = 4$ for the sake of convenience.

In the following analysis the initial data ϕ will be assumed to be a member of Sobolev space $H_n(R_+^3)$,

$$\mathcal{H}_n(R^3_+) = \{\phi \in L^2(R^3_+) : |||\phi|||_n \equiv \sup_{|\gamma|\le n} ||\nabla^\gamma \phi||_2 < \infty\}.$$

LEMMA 5.1: Let $\alpha \sim O(m^{-\frac{1}{4}})$ *and assume that the initial data* $\phi \in \mathcal{H}_N(R^3_+) \cap D(H_{0+}(m))$. *Further suppose that the potentials* a, v *belong to the class* A(N+3).
For $n \ge N$, *define*

$$f(x,t) = \int_{R^3_+} \Gamma(x_1,y_1;\alpha,n) K^e_1(Q^r)\phi(y)dy. \tag{5.3}$$

With χ^+_N *as given in Definition 3.2, then*

$$||f(\cdot,t)|| \le \text{const.}(D,\ell) m^{-\frac{1}{4}(3N-7)} ||\chi^+_N||_1 |||\phi|||_N .$$

Proof: Let $\beta = \frac{m}{2\hbar\Delta t}$ and rewrite equation (5.3) as

$$f(x,\beta) = \left(\frac{\beta}{\pi i}\right)^{\frac{3}{2}} \int_{R^2} d^2y \int_{R_+} dy_1 \exp[i\beta(x-y^r)^2] g(x,y)\phi(y) \tag{5.4}$$

where

$$g(x,y) = \lambda(x_1,n,\alpha)(\chi_D * \rho_\ell)(x-y^r)$$
$$\times \exp\left(-\frac{i}{\hbar} J^e(Q^r)\right)\lambda(y_1;n,\alpha)\left[1+\frac{1}{m} T^e_1(Q^r)\right]. \tag{5.5}$$

Consider the y_1-integral in (5.4), i.e.,

$$I(\beta) \equiv \left(\frac{\beta}{\pi i}\right)^{\frac{1}{2}} \int_0^\infty dy_1 \exp[i\beta(x_1+y_1)^2] g(x,y)\phi(y).$$

Introduce a change of variable by setting

$$u_1 = (x_1+y_1).$$

Then,

$$I(\beta) = \left(\frac{\beta}{\pi i}\right)^{\frac{1}{2}} \int_{x_1}^{\infty} du_1 \exp(i\beta u_1^2) h(u_1) \tag{5.6}$$

where

$$h(u_1) = g(x_1, u_1 - x_1; y_2, y_3)\, \phi(u_1 - x_1; y_2, y_3). \tag{5.7a}$$

Note that $h(0) = h(x_1) = 0$ and $h(u) = 0$ for large u. (5.7b)

Integrating by parts in (5.6) we get

$$I(\beta) = \left(\frac{\beta}{\pi i}\right)^{\frac{1}{2}} \left(\frac{i}{2\beta}\right) \int_{x_1}^{\infty} du_1 \exp(i\beta u_1^2) \frac{d}{du_1} \left(\frac{h(u_1)}{u_1}\right). \tag{5.8}$$

The surface term in (5.8) vanishes on account of properties of $h(u_1)$ listed in (5.7b). Repeating this process N-times we get

$$I(\beta) = \left(\frac{\beta}{\pi i}\right)^{\frac{1}{2}} \left(\frac{i}{2\beta}\right)^N \int_{x_1}^{\infty} du_1 \exp(i\beta u_1^2) h_N(u_1) \tag{5.9a}$$

where

$$h_0(u_1) = h(u_1) \; ; \quad h_N(u_1) = \frac{d}{du_1} \left(\frac{h_{N-1}(u_1)}{u_1}\right). \tag{5.9b}$$

Now since $\lambda(x_1; \alpha, n) = 0$ for $x_1 \leq 0$, it follows from (5.4) and (5.9a) that

$$f(x,\beta) = \left(\frac{\beta}{\pi i}\right)^{\frac{3}{2}} \left(\frac{i}{2\beta}\right)^N \int_{R_+^3} d^2y\, du_1 h_N(u_1)$$

$$\times \exp\left[i\beta\left(\sum_{j=2}^{3} (x_j - y_j)^2 + u_1^2\right)\right]. \tag{5.10}$$

From Definition (5.1) we note that for $n \geq N$,

$(\frac{d}{dy_1})^N \lambda(y_1;\alpha,n) \frac{x_1 y_1}{(x_1+y_1)^3}$ is non-singular. With this observation it can be shown [cf. Appendix 5.1] that

$$|h_N(u_1)| \leq \text{const.}\ (2\alpha)^{-(N+1)} \chi_N^+(u_1,x_2-y_2,x_3-y_3) \times \sup_{|\gamma|\leq N} \left|(\frac{d}{du_1})^\gamma \phi(u_1)\right|. \qquad (5.11)$$

Using the above estimate and the Young inequality in (5.10) we obtain

$$||f(\cdot,\beta)|| \leq \text{const.}(D,\ell)\beta^{\frac{3}{2}-N} (2\alpha)^{-(N+1)} ||\chi_N^+||_1 |||\phi|||_N.$$

Since $\alpha \sim 0(m^{-\frac{1}{4}})$ it follows that

$$||f(\cdot,\beta)|| = 0(m^{-\frac{1}{4}(3N-7)}). \qquad \square$$

<u>REMARK 5.1</u>: The above result was established for the special case when $M = 1$ [cf. equation (5.2a)]. This can be generalized to the case when M is arbitrary by noting that for sufficiently large n, the function $\Gamma(x_1,y_1;\alpha,n)$ neutralizes the singular behaviour of coefficient functions $\{T_j^e(Q^r)\}_{j=1}^M$. In particular we observe from Lemma 5.1 that for $N \geq \frac{4M+7}{3}$, the L^2-norm of the function $f(\cdot,t)$ in equation (5.3) is of the order $m^{-M-\epsilon}$, for some $\epsilon > 0$.

From here we may conclude that the second term in equation (5.2a) does not contribute to the L^2-approximate wave function to the leading order in mass. Thus the most appropriate parametrix for the problem at hand can be written as

$$K_M^+(\Omega;\alpha,n) = \Gamma(x_1,y_1;\alpha,n)K_M^e(\Omega). \qquad \square \quad (5.12)$$

In the remainder of this section we state and prove some of the useful properties of $K_M^+(\Omega)$. To begin with we have the following result.

LEMMA 5.2: *Let* $a(\cdot,t)$ *and* $v(\cdot,t)$ *belong to the potential class* $A(2M+2)$. *For* $\phi \in D(H_+(t,m)) = D(H_{0_+}(m))$ *and* $n \geq 0$ *define*

$$\psi_M(x,t) = \int_{R_+^3} K_M^+(\Omega;\alpha,n)\phi(y)\,dy.$$

Then

$$\psi_M(\cdot,t) \in C^2(R_+^3) \qquad t \in (s,T]$$

$$\psi_M(x,\cdot) \in C^1(s,T) \qquad \textit{for each } x \in R_+^3.$$

Furthermore suppressing α, n *dependence in* $K_M^+(\Omega;\alpha;n)$

(a) $$\nabla_x^\gamma \psi_M(x,t) = \int_{R_+^3} \nabla_x^\gamma K_M^+(\Omega)\phi(y)\,dy, \quad 2 \geq |\gamma| > 0.$$

(b) $$\frac{\partial \psi_M}{\partial t}(x,t) = \int_{R_+^3} \frac{\partial}{\partial t} K_M^+(\Omega)\phi(y)\,dy.$$

(c) *For* $\phi \in C_0^3(R_+^3) \cap D(H_{0_+})$

$$\lim_{t\to s^+} \int K_M^+(\Omega)\phi(y)\,dy = \phi(x); \quad (x,t) \in R_+^3 \times [0,T].$$

(d) *The Dirichlet boundary condition:*

$$K_M^+(\Omega)\Big|_{x\in\partial\Omega} = K_M^+(\Omega)\Big|_{y\in\partial\Omega} = 0, \quad (t,s) \in T_\Delta.$$

Proof: A slight modification of the argument presented in the proof of Lemma 3.3 can be used to prove (a), (b) and (c). The property (d) on the other hand, is a direct consequence of the definition of $\Gamma(x_1,y_1;\alpha,n)$. □

Next we use the result of Lemma 5.2 to show that $K_M^+(Q)$ generates a family of bounded operators which shares many of the abstract properties of the evolution family $\{U(t,s): (t,s) \in T_\Delta\}$. Once again we will find that the analysis bears very strong resemblance to the one presented in Chapter 3. Thus only the new features, if any, of the analysis will be mentioned.

Proposition 5.1: Let $a(\cdot,t)$ *and* $v(\cdot,t)$ *be as in Lemma 5.2. Then*

(i) The parametrix kernel $\{K_M^+(Q;\alpha,n);\ n \geq 0\}$ *generates a family of uniformly bounded operators* $\{U_M(t,s) \in \mathcal{B}(L^2(R_+^3)): (t,s) \in T_\Delta\}$ *via the relation*

$$[U_M(t,s)\phi](x) = \int_{R_+^3} K_M^+(Q)\phi(y)\,dy; \quad \phi \in L^2(R_+^3);\ x \in R_+^3.$$

(ii) The restriction of $U_M(t,s)$ *to the domain* $D(H_{0_+})$ *is strongly continuously differentiable in* $t \in (s,T]$.

<u>Proof</u>: Since $|\Gamma(x_1,y_1;\alpha,n)| \le 1$, the proof of Proposition (3.3) is valid in establishing (i) and (ii). □

Next step in our analysis is to determine the PDE identity satisfied by the parametrix kernel $K_M^+(Q;\alpha)$. The derivation is identical to the one seen in Chapter 3 and thus we only quote the result here. Dropping α, n dependence in K_M^+,

$$LK_M^+(Q) = \Gamma(x_1,y_1)[m^{-M-1}R_M^0(Q) + \sum_{i=1}^{3} R_M^i(Q)] + \sum_{i=1}^{4} S_M^i(Q). \quad (5.13)$$

In the above identity functions $\{R_M^j(Q);\ j = 0 \sim 3\}$ are given by equations (3.43)-(3.47). The additional terms S_M^i come from the derivations of $\Gamma(x_1,y_1)$ and are given below:

$$S_M^1(Q) = \frac{\hbar^2}{2m}(\chi_D * \rho_\ell)(d(Q))(\Delta_x\Gamma(x_1,y_1))W_m(Q) \quad (5.14)$$

$$S_M^2(Q) = \frac{\hbar^2}{m}[\nabla_x\Gamma(x_1,y_1)\cdot\nabla_x(\chi_D*\rho_\ell)(d(Q))]W_M(Q) \quad (5.15)$$

$$S_M^3(Q) = \frac{\hbar^2}{m}(\chi_D*\rho_\ell)(d(Q))[\nabla_x\Gamma(x_1,y_1)\cdot\nabla_x]W_M(Q) \quad (5.16)$$

$$S_M^4(Q) = \frac{i\hbar}{m}(\chi_D*\rho_\ell)(d(Q))[a^e(x,t)\cdot\nabla_x\Gamma(x_1,y_1)]W_M(Q). \quad (5.17)$$

The task of the next section (5.2) is to show that the inhomogeneous PDE identity (5.13) defines an inhomogeneous abstract equation of motion in $L^2(R_+^3)$.

5.2 The Abstract Equation of Motion

Let ϕ be a sufficiently smooth function in $L^2(R_+^3)$; then from (5.13),

$$\int_{R_+^3} LK_M^+(Q;\alpha)\,\phi(y)\,dy = \int_{R_+^3} E_M(Q;\alpha)\,\phi(y)\,dy \tag{5.18}$$

where $E_M(Q;\alpha)$ represents the right hand side of (5.13).

By following an argument identical to the one shown in section (3.3), the left hand side of (5.18) can be written as

$$\int_{R_+^3} LK_M^+(Q;\alpha)\,\phi(y)\,dy = L\int_{R_+^3} K_M^+(Q)\,\phi(y)\,dy$$

$$= [i\hbar\,\frac{d}{dt} - H(t,m)]U_M(t,s)\,\phi. \tag{5.19}$$

Next we show that $E_M(Q;\alpha)$ generates a strongly t-differentiable bounded operator in $L^2(R_+^3)$. In the following analysis we shll denote by $\{E_M^k(Q;\alpha)\}_{k=0}^7$ the individual terms on the RHS of equation (5.13) indexed from left to right. The operators generated by these kernels will be denoted by $\{E_M^k(t,s;\alpha)\}_{k=0}^7$. The new feature in the following analysis is the presence of $\Gamma(x_1,y_1;\alpha,n)$. From here on α, n dependence will be displayed only when necessary.

<u>*LEMMA 5.3*</u>: *Let $\phi \in H_3(R_+^3)$ and assume that* a *and* v *belong to the potential class* A(2M+3), *then for* $n \geq 0$ *the kernel* $E_M^0(Q) \equiv m^{-(M+1)}\Gamma(x_1,y_1)R_M^0(Q)$ *generates a strongly continuously t-differentiable bounded operator* $E_M^0(t,s)$ *in* $L^2(R_+^3)$. *Moreover,*

$$\|E_M^0(t,s)\phi\| \le C(D,\ell,\tilde{c}_i)m^{-(M+1)}(\Delta t)^M(2\alpha)^{-1}\|\chi_3^+\|_1 |||\phi|||_3.$$

Proof: From Definition (4.2) we observe that

$$\left|\frac{d}{dx_1}\lambda(x_1;n,\alpha)\right| \le \text{const.}(2\alpha)^{-1} \qquad \text{for all } n \ge 0.$$

Using this result and the proof of Lemma (3.5) we get the desired result. □

Next we analyze $\Gamma(x_1,y_1)\sum_{i=1}^{3} R_M^i(Q)$.

LEMMA 5.4: Let $p \ge 2$ *and suppose that* $\phi \in H_{p+1}(R_+^3)$. *Further assume that potentials* a *and* v *belong to the potential class* A(2M+p+1), *then for all* $n \ge 0$ *the kernels* $\{\Gamma(x_1,y_1)R_M^i(Q)\}_{i=1}^3$ *generate bounded operators* $\{E_M^i(t,s)\}_{i=1}^3$ *in* $L^2(R_+^3)$. *Furthermore*

$$\|E_M^1(t,s)\phi\| \le \text{const. } m^{-p+\frac{1}{2}}(2\alpha)^{-p}(\Delta t)^{p-3/2}\|\chi_{p+2}^+\|_1 |||\phi|||_p$$

$$\|E_M^2(t,s)\phi\| \le \text{const. } m^{-p+\frac{1}{2}}(2\alpha)^{-p-1}(\Delta t)^{p-3/2}\|\chi_{p+2}^+\|_1 |||\phi|||_{p+1}$$

$$\|E_M^3(t,s)\phi\| \le \text{const. } m^{-p+\frac{1}{2}}(2\alpha)^{-p}(\Delta t)^{p-3/2}\|\chi_{p+1}^+\| \; |||\phi|||_p$$

Proof: Follow the argument of Lemma (3.4) and use the estimate

$$\left|\left(\frac{d}{dy_1}\right)^N \lambda(y_1;\alpha,n)\right| \le \text{const.}(2\alpha)^{-N} \qquad \text{for } n \ge 0. \quad \square$$

Next, we analyze the kernels $\{S_M^j(Q)\}_{j=1}^4$. The new feature in this part of analysis is the presence of derivates of the smooth cut-off function $\Gamma(x_1,y_1)$. Note that $S_M^2(Q)$ is nonzero only when $D-\ell \le |x-y| \le D+\ell$. Thus this particular term can be analyzed by using the procedure presented in Lemma (3.4). For the other terms we follow an argument similar to the one seen in Lemma (5.1). The result of this calculation is quoted in the following lemma.

LEMMA 5.5: Let $p \ge 2$, $n \ge 0$ *and suppose that* $\phi \in H_{p+1}(R_+^3)$. *Further assume that* a *and* v *are the same as in Lemma (5.4). Then* $\{S_M^j(Q)\}_{j=1}^4$ *generate bounded operators* $\{E_M^j(t,s)\}_{j=4}^7$.

$$||E_M^4(t,s)\phi|| \le \text{const. } m^{-p+\frac{1}{2}}(2\alpha)^{-p-2}(\Delta t)^{p-3/2}||\chi_p^+||_1 |||\phi|||_p$$

$$||E_M^5(t,s)\phi|| \le \text{const. } m^{-p+\frac{1}{2}}(2\alpha)^{-p-1}(\Delta t)^{p-3/2}||\chi_{p+1}^+||_1 |||\phi|||_p$$

$$||E_M^6(t,s)\phi|| \le \text{const. } m^{-p+\frac{1}{2}}(2\alpha)^{-p-2}(\Delta t)^{p-3/2}||\chi_{p+2}^+||_1 |||\phi|||_{p+1}$$

$$||E_M^7(t,s)\phi|| \le \text{const. } m^{-p+\frac{1}{2}}(2\alpha)^{-p-1}(\Delta t)^{p-3/2}||\chi_p^+||_1 |||\phi|||_p.$$

<u>Proof</u>: Using the results and procedure of Lemmas 5.1, A3 [Appendix 3.1] and the estimate

$$\left|\left(\frac{d}{dy_1}\right)^p \lambda(y_1;\alpha,n)\right| \le \text{const.}(2\alpha)^{-p} \qquad \text{for } n \ge 0$$

the above result follows. □

From Lemmas (5.3), (5.4) and (5.5) we have shown that the kernel $E(Q;\alpha)$ generates a bounded operator in $L^2(R^3_+)$. Thus the PDE identity (5.13) defines an abstract equation of motion in $L^2(R^3_+)$. In the next section we will solve this equation and consequently compute the L^2-norm difference between the exact and the approximate solutions of Schrödinger equation.

5.3 The Error Analysis

The following theorem is the main result of this chapter.

THEOREM 5.1: *Let* $p \ge \frac{4M+6}{3}$ *and assume that* $\alpha \sim O(m^{-1/4})$. *Further suppose that the initial data* $\phi \in H_{p+1}(R^3_+) \cap D(H_{0_+})$ *and the potentials* a *and* v *belong to the potential class* $A(2M+p+1)$; *then for some* $\epsilon > 0$

$$||U_M(t,s)\phi - U(t,s)\phi|| \le C(D,\ell,\tilde{c}_i)m^{-M-\epsilon}(\Delta t)^{p-3/2}||\chi^+_{p+2}||_1|||\phi|||_{p+1}.$$

where $\tilde{c}_i$ *are the constants defined in Assumption 3 [Chapter 3].*

Proof: The existence of exact evolution operator $U(t,s)$ for the problem of evolution on half space was established in Chapter 2. The operator $E_M(t,s): H_{p+1}(R^3_+) \to L^2(R^3_+)$ has a strong continuous t-derivative. This can be easily shown by using Lemma A2 [Appendix 3.1].

Let

$$A(t) = \frac{1}{ih} H(t) - cI \tag{5.20}$$

where c $(= 1 + \alpha/h)$ is a constant and H(t) is obtained by perturbing the free Hamiltonian $H_{0_+}(m)$ [cf. Lemma 2.1]. It was also shown in Chapter 2 that the Cauchy problem associated with H(t) is uniformly correct. Now recall the inhomogeneous equation in $L^2(R^3_+)$, i.e.,

$$[ih \frac{d}{dt} - H(t,m)]U_M(t,s)\phi = E_M(t,s)\phi. \tag{5.21}$$

According to Proposition 3.4, the above equation has a unique solution

$$U_M(t,s)\phi = U(t,s)\phi + \int_s^t U(t,\tau)E_M(t,\tau)\phi.$$

It follows that

$$||U_M(t,s)\phi - U(t,s)\phi|| \leq \int_s^t ||U(t,\tau)||\ ||E_M(t,\tau)||d\tau. \tag{5.22}$$

The mass dependence in α $(= 0(m^{-1/4}))$ ensures that the Dirichlet boundary condition is satisfied in the limit $m \to \infty$. This allows one to consider initial data with support up to the boundary. A careful scan of estimates in Lemmas (5.3), (5.4) and (5.5) reveals that for $p \geq \frac{4M+6}{3}$, the bound for (5.22) becomes

$$||U_M(t,s)\phi - U(t,s)\phi|| \leq \text{const.}\, m^{-M-\epsilon}(\Delta t)^{p-3/2}||\chi^+_{p+2}||\ |||\phi|||_{p+1}.$$

□

Observe that the above theorem also provides the following strong limit

$$\underset{t\to s}{\text{s-lim}}\ U_M(t,s)\phi = U(s,s)\phi = \phi,$$

for $\phi \in H_{p+1}(R^3) \cap D(H_{0_+})$. Observe that the function ϕ has support up to the boundary. This is a consequence of mass dependence in α. In the event that α was independent of mass, the above strong limit will be valid only for those initial states which are supported away from the boundary.

5.4 Generalization to Bounded Regions

The goal in this section is to show that the result of Theorem 5.1 can be extended to include bounded regions of Definitions (2.4) and (2.5). To begin with we define a smooth cut-off function suitable for use in the neighbourhood $\partial\Omega$ of a bounded set Ω in R^d.

Definition 5.2: Let Ω be an open bounded set in R^d and define two sets Ω_α and G_α such that $\Omega \supset \Omega_\alpha \supset G_\alpha$ by setting

$$\Omega_\alpha \equiv \{x \in \Omega: \inf_{y\in\partial\Omega} |x-y| > \alpha\}, \tag{5.23a}$$

$$G_\alpha = \{x \in \Omega_\alpha: \inf_{y\in\partial\Omega_\alpha} |x-y| > \alpha\}. \tag{5.23b}$$

Let α denote the supremum of the values of α for which Ω_α and G_α are non-empty with $\dim \Omega_\alpha = \dim G_\alpha = \dim \Omega$.
We define a smooth cut-off function $\zeta: R^d \times [0,\alpha_0] \to R_+$

$$\zeta(x,\alpha) = \frac{1}{\alpha^d} \int_{\Omega_\alpha} dy \ \rho\left(\frac{x-y}{\alpha}\right) \tag{5.24a}$$

where

$$\begin{aligned} \rho(x) &= 0 \quad , \qquad |x| \geq 1 \\ &= c \exp[(|x|^2 - 1)^{-1}], \qquad |x| \leq 1. \end{aligned} \tag{5.24b}$$

The constant c *is such that* $\int_{R^d} \rho(x)dx = 1$. *The function* ζ *has the following easy-to-prove properties:*

1°. $\zeta(\cdot,\alpha) \in C^\infty(R^d)$.

2°. $\nabla_x^\beta \zeta(x,\alpha) = 0$ *if* $x \in \partial\Omega$.

3°. $\zeta(x,\alpha) = 1$ *if* $x \in G_\alpha$.

4°. $|\nabla_x^\beta \zeta(x,\alpha)| \leq \text{const.}\ \alpha^{-d-|\beta|}(\text{vol}\ \Omega)\|\nabla^\beta \rho\|_\infty$, $x \in R^d$

where the constant depends on β *but not on* x. □

The parametrix kernel $K_M(\Omega;\alpha)$, for the cases where $\Omega \subset R^d$ is a bounded region [cf. Definitions 2.4, 2.5], has the common structure

$$K_M(\Omega;\alpha) = \Gamma(x,y;\alpha)(\chi_D * \rho_\ell) d(\Omega) W_M(\Omega) \tag{5.25a}$$

where

$$\Gamma(x,y;\alpha) = \zeta(x;\alpha)\zeta(y;\alpha), \tag{5.25b}$$

and the functions $\chi_D * \rho_\ell$ and W_M are given by equations (3.26) and (4.14) respectively. The presence of $\Gamma(x,y;\alpha)$ guarantees that the parametrix $K_M(\Omega;\alpha)$ satisfies Dirichlet boundary conditions.

In the special case when $\Omega \in$ HR [cf. Definition 2.4] one may also choose

$$\Gamma(x,y;n,\alpha) = \zeta(x,n;\alpha)\zeta(\ell-x,n;\alpha)\zeta(y,n;\alpha)\zeta(\ell-y,n;\zeta) \qquad (5.25c)$$

where

$$\zeta(x,n;\alpha) = \prod_{i=1}^{d} \lambda(x_i,n;\alpha). \qquad (5.25d)$$

Here, the function $\lambda(x_i,n;\alpha)$ is the same as given by Definition (5.1). If one chooses to impose periodic boundary condition, the boundary cut-off function is not required and consequently we set $\Gamma = 1$.

Observe that the parametrix (5.25a) has the same form as in (5.12) and thus by following the same argument it can be shown that $K_M(\Omega;\alpha)$ satisfies a PDE identity, identical in structure to equation (5.13). Likewise, the analysis of Lemmas (5.3), (5.4) and (5.5) can be repeated to obtain the required error estimates. We thus have the folllowing result.

<u>THEOREM 5.2:</u> *Let* $\Omega \subseteq R^d$ *be as in Definition (2.4) or (2.5) and assume that* H(t) *is the Hamiltonian obtained by pertur-*

bing the free Hamiltonian $H_0 \in \{H_{0\Omega}, H_{0s}\}$. *Further, suppose that the initial data* $\phi \in H_{p+1}(\Omega) \cap D(H_0)$ *and the potentials* $a, v \in A(2M+p+1)$, *then for* $p > \frac{4M}{3} + d - \frac{2}{3}$; $\alpha \sim 0(m^{-\frac{1}{4}})$ *and some* $\epsilon > 0$

$$\|U_M(t,s)\phi - U(t,s)\phi\|$$

$$\leq C(D,\ell,\tilde{c}_i)m^{-M-\epsilon}(\Delta t)^{p-d/2}\|\chi^{+}_{p+2}\|_1 |||\phi|||_{p+1}$$

where $\tilde{c}_i$ *are constants defined in Assumption 3 of Chapter 3.*

□

<u>Conclusions</u>: In the preceding discussion we have developed a bonafide scheme to determine L^2-approximate solution of the Schrödinger evolution equation (1.1, 1.3) for sufficiently smooth interactions and initial data. □

APPENDIX 5.1

LEMMA: Let $n \geq N$ *and suppose that* $\phi \in H_N(R^3_+)$. *Define the function* $h_{N+1}: R^3_+ \to R$ *by*

$$h_0(u_1) = h(u_1) = g(x, u_1 - x_1; y_2, y_3)\,\phi(u_1 - x_1; y_2, y_3)$$

and

$$h_N(u_1) = \frac{d}{du_1}\left(\frac{h_{N-1}(u_1)}{u_1}\right)$$

where

$$g(x,y) = \lambda(x_1; n, \alpha)\,(\chi_D * \rho_\ell)(x - y^r)$$

$$\times \exp\left(-\frac{i}{\hbar} J^e(Q^r)\right)\lambda(y_1; n, \alpha)\left(1 + \frac{1}{m} T_1^e(Q^r)\right).$$

Then

$$|h_N(u_1)| \leq \text{const.}(2\alpha)^{-N+1}\chi_N^+(u_1; x_2 - y_2, x_3 - y_3)$$

$$\times \sup_{|\gamma| \leq N}\left|\left(\frac{d}{du_1}\right)^\gamma \phi(u_1)\right|.$$

<u>Proof</u>: We first prove the result for $N = 1$:

$$h_1(u_1) = \frac{d}{du_1}\left(\frac{h(u_1)}{u_1}\right) = -\frac{h(u_1)}{u_1^2} + \frac{h'(u_1)}{u_1} \quad . \tag{1}$$

Consider first term on the right hand side. Suppressing α, n dependence and using equation (4.25) for $T_1^e(Q^r)$, we have

$$\frac{h(u_1)}{u_1^2} = \lambda(x_1)(\chi_D * \rho_\ell)(u_1)\exp\left(-\frac{iJ^e(Q^r)}{\hbar}\right)\frac{\lambda(u_1)}{u_1^2}$$

$$\times\left[1 + m^{-1}\left(\tilde{T}_1^e(Q^r) + (\Delta t)^2 F_1^{LOR}\frac{x_1 u_1}{(u_1+x_1)^3}\right)\right]|\phi(y)| \qquad (2)$$

From Definition (5.1) we observe that for $n \geq 2$, $\frac{\lambda(u_1)}{u_1^3}$ is non singular. Moreover using property 2^o of λ we note that

$$\left|\frac{\lambda(u_1)}{u_1^b}\right| \leq \text{const. } |u_1|^{n-b+1}.$$

Using this result in (2) we get

$$\left|\frac{h(u_1)}{u_1^2}\right| \leq (\chi_D * \rho_\ell)(u_1)[C_1(2\alpha)^{-2} + m^{-1}(C_2(2\alpha)^{-2}$$

$$+ C_3(2\alpha)^{-3})]|\phi(y)|. \qquad (3)$$

In the last inequality we have used the fact that the normalization constant $\Lambda(n,\alpha) = 0((2\alpha)^{n+1})$, C_1, C_2 and C_3 are constants independent of α. A similar procedure works for the second term on the right hand side of (1). The result is

$$\left|\frac{h'(u_1)}{u_1}\right| \leq \chi_1^+(u_1)[C_1'(2\alpha)^{-2} + m^{-1}(C_2'(2\alpha)^{-2} + C_3'(2\alpha)^{-3})]$$

$$\times \sup_{|\gamma|\leq 1}\left|\left(\frac{d}{du_1}\right)^\gamma \phi(u_1)\right|. \qquad (4)$$

Using (3) and (4) the desired result is easily established.

For arbitrary $N \geq 1$, we prove this result by induction. Let the estimates (3) and (4) be true for $h_N(u_1)$ and consider

$$h_{N+1}(u_1) = -\frac{h_N(u_1)}{u_1^2} + \frac{h_N'(u_1)}{u_1}$$

$$\Rightarrow \quad |h_{N+1}(u_1)| \leq \left|\frac{h_N(u_1)}{u_1^2}\right| + \left|\frac{h_N'(u_1)}{u_1}\right|$$

$$\leq \text{const.}\ \chi_N^+(u_1)(2\alpha)^{-2} \sup_{|\gamma|\leq N} \left|\left(\frac{d}{du_1}\right)^\gamma \phi(u_1)\right|$$

$$\times [C_1(2\alpha)^{-N} + m^{-1}(C_2(2\alpha)^{-N} + C_3(2\alpha)^{-N-1})]$$

$$+ \text{const.}\ \chi_{N+1}^+(u_1)(2\alpha)^{-1} \sup_{|\gamma|\leq N+1} \left|\left(\frac{d}{du_1}\right)^\gamma \phi(u_1)\right|$$

$$\times [C_1'(2\alpha)^{-N-1} + m^{-1}(C_2'(2\alpha)^{-N-1} + C_3(2\alpha)^{-N-2})]$$

$$\leq \text{const.}\ \chi_{N+1}^+(u_1) \sup_{|\gamma|\leq N+1} \left|\left(\frac{d}{du_1}\right)^\gamma \phi(u_1)\right| \times (2\alpha)^{-(N+2)} .$$

$\square$

SUPPLEMENT

Introduction

In this section we will provide answers to the questions and suggestions of Prof. S.A. Fulling.

In proving the self-adjointness of Hamiltonians for a bounded region [cf. Lemma 2.1] we attempted to provide a unified description for problems with a variety of boundary conditions. But as indicated by Prof. Fulling, such a scheme doesn't work for Dirichlet Problem. First of all the momentum lattice Λ [cf. Definition 2.6] is not the same for Periodic and Dirichlet boundary conditions. Moreover, in Dirichlet's case the operator a.P is an infinite dimensional non-diagonal matrix, thereby disallowing the validity of estimate used in proving Lemma 2.2. This problem clearly does not arise in the regions with periodic boundary conditions. Thus in the following analysis we provide a new method of proving the self-adjointness of Dirichlet problem in which all the computations and estimations are done in $\mathcal{H} = L^2(\Omega)$.

On page 121 we demonstrated (formally) that the problem of motion in an interval subjected to periodic boundary condition is equivalent to the motion of a particle in a periodic potential [cf. eqn. 4.41]. Same can be shown to be true in case of Dirichlet problem but in this case the period of the extended potential V^e is twice the size of the given interval, i.e.,

$$V^e(x) = v_0(x-2na) \quad \text{for all } x-na \in [-a,a]. \tag{4.41c}$$

"On the Self-Adjointness of Dirichlet Hamiltonian for Hypercube $\Omega \subset R^d$"

NOTATION: 1. $\Omega \equiv \{0 < x_i < \pi;\ i = 1 \sim d\} \subseteq R^d$; $\partial\Omega$ = Boundary of Ω

$\bar{\Omega}$ = closure of Ω

2. $H = L^2(\bar{\Omega})$

3. $\vec{n} = (n_1, \ldots, n_d) \in N^d$; $N = \{1,2,3,\ldots.\}$

4. For convenience, set $\hbar = 2m = 1$

FREE HAMILTONIAN H_0:

Define an operator $T: D \to H$ by

$$(Tf)(x) = -(\Delta f)(x) \tag{1}$$

where

$$f \in D \equiv \{f \in C^\infty(\bar{\Omega}): f(x) = 0 \text{ for } x \in \partial\Omega\}. \tag{2}$$

LEMMA 1:

(a) *T is essentially self-adjoint on H.*

(b) *Let $H_0 \equiv \bar{T}$ be the unique self-adjoint extension of T and let*

$$D_0 \equiv \{f \in H: \sum_{\vec{n}\in N^d} |\vec{n}|^4 |\langle\beta_{\vec{n}}, f\rangle|^2 < \infty\} \tag{3}$$

where

$$|\vec{n}|^4 = (\vec{n}\cdot\vec{n})^2 = \left(\sum_{i=1}^{d} n_i^2\right)^2 \tag{4}$$

and

$$\beta_{\vec{n}}(x) = \left(\sqrt{\frac{2}{\pi}}\right)^d \prod_{i=1}^{d} \sin(n_i x_i) . \tag{5}$$

Then,

$$H_0 = T^{**} \qquad \textit{and} \qquad D(H_0) = D_0 . \tag{6}$$

Proof: We consider (a) and (b) together. Note that $\{\beta_{\vec{n}}\}_{N^d}$ forms a complete orthonormal basis in H. We first show that T is symmetric. Observe that $C_0^\infty(\Omega) \subset D$ and thus D is clearly dense in H. Let $f,g \in D$ and consider

$$<f,Tg> = \int_\Omega dx\ \bar{f}(x)(-\Delta g)(x) . \tag{7}$$

Recall the vector identity

$$\vec{\nabla}\cdot(\vec{\alpha}\beta) = \beta(\vec{\nabla}\cdot\vec{\alpha}) + \vec{\alpha}\cdot(\vec{\nabla}\beta) . \tag{8}$$

Set $\vec{\alpha} = (-\vec{\nabla}g)(x)$ and $\beta = \bar{f}(x)$, then

$$(-\Delta g)(x)\bar{f}(x) = \vec{\nabla}\cdot((-\vec{\nabla}g)(x)f(x)) + (\vec{\nabla}g)(x)\cdot(\vec{\nabla}\bar{f})(x) . \tag{9}$$

Substituting (9) in (7) and using divergence theorem we obtain

$$\begin{aligned} <f,Tg> &= \int_{\partial\Omega} -(\vec{\nabla}g)(x)\bar{f}(x)\cdot d\vec{s} + \int_\Omega (\vec{\nabla}g)(x)\cdot(\vec{\nabla}\bar{f})(x)dx \\ &= \int_\Omega (\vec{\nabla}g)(x)\cdot(\vec{\nabla}\bar{f})(x)dx \\ &= \int_\Omega dx\ (-\Delta\bar{f})(x)g(x) = <Tf,g> \\ &= <T^*f,g> \end{aligned}$$

$\Rightarrow\ T^* \supset T$, i.e., T is symmetric and T^* is densely defined.

Now, by Proposition (2.7) of [AJS] it follows that $\bar{T} = T^{**}$. Thus to complete the proof of part (b) it remains to show that $D(T^{**}) = D_0$. Let $f \in D(T^{**})$ and set

$$\sigma \equiv \sum_{\vec{n}\in N^d} |\vec{n}|^4 \ |\langle \beta_{\vec{n}}, f\rangle|^2 = \sum_{\vec{n}\in N^d} |\langle n^2 \beta_{\vec{n}}, f\rangle|^2 . \tag{10}$$

Observe that $\beta_{\vec{n}} \in D$ and

$$|\vec{n}|^2 \beta_{\vec{n}}(x) = T\beta_{\vec{n}}(x) \tag{11}$$

Therefore, since $T^* \supset T$, we have

$$\begin{aligned}\sigma &= \sum_{\vec{n}\in N^d} |\langle T\beta_{\vec{n}}, f\rangle|^2 = \sum_{\vec{n}\in N^d} |\langle T^*\beta_{\vec{n}}, f\rangle|^2 \\ &= \sum_{\vec{n}\in N^d} |\langle \beta_{\vec{n}}, T^{**}f\rangle|^2 \\ &< \infty .\end{aligned}$$

The last inequality follows because $T^{**}f \in H$ and that $\{\beta_{\vec{n}}\}$ forms an orthonormal basis in H. This shows that $D(T^{**}) \subset D_0$. To prove the converse, we let $f \in D_0$ and set

$$g \equiv \sum_{\vec{n}\in N^d} |\vec{n}|^2 \ \langle \beta_{\vec{n}}, f\rangle \beta_{\vec{n}} . \tag{12}$$

Clearly, $g \in H$. Define

$$\ell_M \equiv \sum_{\substack{\vec{n}\in N^d \\ (|\vec{n}|^2 \le M)}} \langle \beta_{\vec{n}}, f\rangle \beta_{\vec{n}} . \tag{13}$$

Note that $\ell_M \in D$ and by completeness $\lim_{M\to\infty} \ell_M = f$. If $h \in D(T^*)$, then

$$\begin{aligned} \langle T^*h, f\rangle &= \lim_{M\to\infty} \langle T^*h, \ell_M\rangle \\ &= \lim_{M\to\infty} \langle h, T\ell_M\rangle \quad \text{as } h \in D(T^*) \text{ and } \ell_M \in D . \end{aligned} \tag{14}$$

Now,

$$T\ell_M = \sum_{|\vec{n}|^2 \le M} \langle \beta_{\vec{n}}, f\rangle T\beta_{\vec{n}} = \sum_{|\vec{n}|^2 \le M} n^2 \beta_{\vec{n}} \langle \beta_{\vec{n}}, f\rangle .$$

Since $g \in \mathcal{H}$ and $\lim_{M\to\infty} T\ell_M = g$, we have

$$\langle T^*h, f\rangle = \langle h, g\rangle .$$

This implies that $f \in D(T^{**})$. This establishes that $D(T^{**}) = D_0$.

Recall [AJS, Problem 2.23] that if T is a densely defined symmetric operator then T is essentially self-adjoint iff $T^* = T^{**}$. We will show $T^* = T^{**}$. We have shown earlier that $T^* \supset T$ which implies that $T^{**} \subset T^*$, so it remains to show that $D(T^*) \subseteq D(T^{**}) = D_0$. To do this, let $f \in D(T^*)$ and consider

$$\begin{aligned} \sum_{\vec{n}\in N^d} |\vec{n}|^4 |\langle \beta_{\vec{n}}, f\rangle|^2 &= \sum_{\vec{n}\in N^d} |\langle n^2 \beta_{\vec{n}}, f\rangle|^2 \\ &= \sum_{\vec{n}\in N^d} |\langle T\beta_{\vec{n}}, f\rangle|^2 \\ &= \sum_{\vec{n}\in N^d} |\langle \beta_{\vec{n}}, T^*f\rangle|^2 < \infty . \end{aligned}$$

The inequality follows that $T^*f \in H$. Thus $f \in D_0$. Since $T^* = T^{**}$ we have that T is essentially self-adjoint. This completes the proof of Lemma 1. □

Total Hamiltonian:

Let $W: D \to H$ be the perturbation

$$W = 2i\, \vec{a}\cdot\vec{\nabla} + i(\vec{\nabla}\cdot\vec{a}) + a^2 + v\,.$$

LEMMA 2:

Let $a, v \in A$ *[see Chapter 2],*

(a) W *is symmetric on* D *and* $D(W) = D \subset D_0$.

(b) There exist constants $\alpha > 0$, $\beta > 0$ *such that*

$$||Wf|| \le \alpha\,||f|| + \beta\,||H_0 f||\,, \quad \textit{for all } f \in D\,.$$

Proof: (b) Let $f \in D$ and consider

$$\begin{aligned} ||a\cdot\nabla f||^2 &\le ||a||_\infty^2\ ||\nabla f||^2 \\ &\le M^2 \int_\Omega (\nabla f)(x)\cdot(\nabla\bar{f})(x)\,dx \\ &= M^2\left[\int_{\partial\Omega} \bar{f}(x)(\vec{\nabla} f)(x)\cdot d\vec{s} - \int_\Omega \bar{f}(x)(\Delta f)(x)\,dx\right] \\ &= -M^2 \int_\Omega \bar{f}(x)(\Delta f)(x)\,dx\,. \end{aligned} \tag{15}$$

Let $E_\delta \equiv \{x \in \Omega: \delta > 0,\ \delta^{-1}|f(x)| \ge \delta|\Delta f(x)|\}$.

Thus from (15)

$$||a\cdot\nabla f||^2 \le M^2\left[\int_{E_\delta} |\delta^{-1} f(x)|^2 dx + \int_{\Omega\setminus E_\delta} |\delta\Delta f(x)|^2 dx\right]$$

$$\le M^2[\delta^{-2}||f||^2 + \delta^2||\Delta f||^2]$$

$$= M^2[\delta^{-2}||f||^2 + \delta^2||H_0 f||^2] .$$

Since δ can be made arbitrary small, we have the result that $a\cdot\nabla$ is H_0-bounded on D with H_0-bound less than 1. Finally, for potentials of class A, $\nabla\cdot a$, a^2 and v are bounded and therefore are H_0-bounded with H_0-bound less than 1 on D. This completes the part (b) of the lemma. Part (a) is straightforward and thus the details are avoided. □

To establish the self-adjointness of total Hamiltonian we wish to make use of Kato-Rellich theorem. This requires a unique symmetric extension of W to domain D_0. We define this extention W_1: $D \to H$ by setting

$$W_1 f = \underset{j\to\infty}{\text{s-lim}}\, Wf_j \tag{16}$$

where $\{f_j\} \subseteq D$ is an H_0-convergent sequence [K, page 164], i.e., there exists an $f \in D_0$ such that $\{f_j, H_0 f_j\} \underset{j\to\infty}{\to} \{f, H_0 f\}$ or in short $f_j \underset{H_0}{\to} f$. To establish the uniqueness of W_1, let $\{f_j\} \subseteq D$ and $\{f_j'\} \subseteq D$ be two different H_0-convergent sequences with limit point $f = f'$, then

$$\|W_1 f_j - W_1 f'_j\| = \|W(f_j - f'_j)\|$$

$$\leq \alpha \|f_j - f'_j\| + \beta \|H_0(f_j - f'_j)\| \underset{j\to\infty}{\to} 0 . \quad (17)$$

The last step follows by using Lemma (2b). This proves that $W_1 f_j = W_1 f'_j$, i.e., W_1 is a unique extension of W to D_0.

To show that W_1 is symmetric, let $g \in D$ and consider

$$(g,W_1 f) = \lim_{j\to\infty} (g,Wf_j)$$

$$= \lim_{j\to\infty} (Wg,f_j) = (Wg,f) = (W_1 g,f) . \quad (18)$$

In the above derivation we have used (16) in the first step followed by symmetry of W in the second step. Now, let $h \in D_0$ and suppose $\{h_i\} \subseteq D$ is an H_0-convergent sequence with limit h. Then for $f \in D_0$,

$$(h,W_1 f) = \lim_{j\to\infty} (h_j,W_1 f) = \lim_{j\to\infty} (W_1 h_j,f) .$$

The last equality follows from (18). But from (17) we know that $\{W_1 h_j\}$ is a Cauchy sequence with limit $W_1 h$. Thus,

$$(h,W_1 f) = (W_1 h,f), \quad \text{for all } g,f \in D_0 .$$

Finally, a straightforward application of Kato-Rellich theorem yields the following result.

THEOREM

Let $a,v \in A$, *then the total Hamiltonian* $H(t)\colon D(H(t)) \to H$, $H(t) = H_0 + W_1$ *is self-adjoint having the domain* $D(H(t)) = D_0$.

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