THE SCHRÖDINGER EQUATION

AS A VOLTERRA PROBLEM

A Thesis

by

FERNANDO DANIEL MERA

Submitted to the Office of Graduate Studies of
Texas A&M University
in partial fulfillment of the requirements for the degree of

MASTER OF SCIENCE

May 2011

Major Subject: Mathematics

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Committee Members,   Peter Kuchment
   Christopher Pope

Head of Department,   Al Boggess

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ABSTRACT

The Schrödinger Equation

as a Volterra Problem. (May 2011)

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Chair of Advisory Committee: Stephen Fulling

The objective of the thesis is to treat the Schrödinger equation in parallel with a standard treatment of the heat equation. In the books of the Rubensteins and Kress, the heat equation initial value problem is converted into a Volterra integral equation of the second kind, and then the Picard algorithm is used to find the exact solution of the integral equation. Similarly, the Schrödinger equation boundary initial value problem can be turned into a Volterra integral equation. We follow the books of the Rubinsteins and Kress to show for the Schrödinger equation similar results to those for the heat equation. The thesis proves that the Schrödinger equation with a source function does indeed have a unique solution. The Poisson integral formula with the Schrödinger kernel is shown to hold in the Abel summable sense. The Green functions are introduced in order to obtain a representation for any function which satisfies the Schrödinger initial-boundary value problem. The Picard method of successive approximations is to be used to construct an approximate solution which should approach the exact Green function as $n \to \infty$. To prove convergence, Volterra kernels are introduced in arbitrary Banach spaces, and the Volterra and General Volterra theorems are proved and used in order to show that the Neumann series for the L^1 kernel, the L^∞ kernel, the Hilbert-Schmidt kernel, the unitary kernel, and the WKB kernel converge to the exact Green function. In the WKB case, the solution of the Schrödinger equation is given in terms of classical paths; that is, the multiple

scattering expansions are used to construct from, the action S, the quantum Green function. Then the interior Dirichlet problem is converted into a Volterra integral problem, and it is shown that Volterra integral equation with the quantum surface kernel can be solved by the method of successive approximations.

To my parents Pedro Mera and Hilda Margarita Mera

and to my sister Hilda Alejandrina Mera

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the professor who told me what book to read on the topic of divergent integrals and Abel summability. I would also like to say, that without this reference, my progress would have been substantially slowed down.

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CHAPTER I

INTRODUCTION

The books of the Rubinsteins [1] and Kress [2] show how the heat equation is converted to a Volterra integral equation, which is then solved by the Picard algorithm. In this thesis we shall show that the Schrödinger equation has similar properties and results as the heat equation such as the existence of surface potentials and the Integral Representation Theorem. The similarities between the Schrödinger equation and the heat equation were used to create a theoretical framework which will give the solution to the Schrödinger problem. As much as possible, we use the books [1, 2] as guides to treat the quantum problem like a heat problem. However, the parallel between the heat equation and the Schrödinger is found to be a limited one, and we use the potential theory formalism that Kress laid down in his book in order to study the existence, and uniqueness of the solution of the Schrödinger equation. The difference between the heat operator and the quantum operator require different proofs for the uniqueness theorems, the surface integral theorems, and the Poisson Integral Theorem. As expected the Representation Theorem is formulated in terms of the source integral term, the surface integral term, and the initial integral term. The second chapter introduces the fundamental solution of the Schrödinger equation in $\mathbb{R}^n$. The representation theorem for the Schrödinger equation is proved in Chapter III. In the same chapter, the boundary-value problem is introduced, and the solution of the Schrödinger equation is formulated in terms of integral equations. In Chapter IV, the uniqueness of the solution to the Schrödinger equation is proved. Also in Chapter IV, the definition of a Green function is given and the complex Green function is shown to

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This thesis follows the style of the IEEE Journal of Quantum Electronics.

have reciprocity, and thus the Green functions have symmetry. The Green functions are defined to satisfy the Dirichlet, Neumann, and Robin boundary conditions.

In Chapter V, we consider the pure initial value problem. The initial value problem can be expressed as a Volterra integral equation of the second kind with respect to time. Our main task is to use the method of successive approximation in order to prove that there exists a unique solution to the integral equation. In Chapter V, the article focuses on linear integral operators in arbitrary Banach spaces. In Chapter VI, the article introduces the Volterra kernels and applies the Neumann series to give an approximation to the exact solution. The Volterra integral equation is shown to be solved by the method of successive approximations. In particular, we work with Volterra integral operators $\hat{Q}$ that go from $L^p(I; \mathcal{B})$ to itself, where $1 \leq p \leq \infty$. These Volterra integral operators $\hat{Q}$ are assumed to have uniformly bounded kernels such that $A : \mathcal{B} \to \mathcal{B}$. Furthermore, we only consider kernels A which are Volterra kernels in time. Then the Volterra theorem proves that Volterra integral equation with a uniform bounded kernel can be solved by successive approximations with respect to the topology $L^\infty(I; \mathcal{B})$. The general Volterra theorem proves the more general case when $L^p(I; \mathcal{B})$, and where $1 \leq p < \infty$. In Chapter VII, the article covers four specific kernels, the L^1 and L^∞ kernels, the Schrödinger kernel, and the Hilbert-Schmidt kernel. In the Schrödinger case, the perturbation expansion series contains a unitary operator and a uniformly bounded potential, and we prove that the Neumann series converges.

In Chapters VIII and IX we reach the projects that were the original motivation for this thesis: showing the convergence of the "classical paths" expansions for solutions of the Schrödinger equation with a potential and with a boundary, respectively. It turns out that these do not exaclty fit into the general Volterra theorems proved in Chapter V, but the fundamental idea continues to apply and enables the

proof to be carried out in the same way. In Chapter VIII a perturbation expansion is constructed by using the semiclassical propagator and a uniformly bounded potential $V(x,t)$. The solution of the Schrödinger equation is given in terms of classical paths, and the semiclassical propagator $G_{scl} = Ae^{iS/\hbar}$ to the Green function is considered as the building block for the exact Green function [3]. The semiclassical Neumann series will also be shown to have norm convergence, and thus the Neumann series converge to the exact Green function under some technical assumptions. In Chapter IX, the boundary-value problem is written in terms of Volterra integral equations of the second kind. Furthermore, the single-layer Schrödinger and double-layer Schrödinger potentials with continuous density functions are shown to be extended to $\partial U \times (0, T]$ with some limiting values. Finally, the interior Dirichlet problem is considered, and the double-layer Schrödinger operator is shown to be bounded from $L^\infty(I; \partial U)$ to itself. Thus Neumann series is shown to converge in the case of the quantum surface kernel with respect to the topology of $L^\infty(I; \partial U)$.

CHAPTER II

FUNDAMENTAL SOLUTION OF THE SCHRÖDINGER EQUATION

The wavefunction $\Psi(x,t)$ of a nonrelativistic particle in $\mathbb{R}^n$ is a solution to the Schrödinger equation

$$H\Psi(x,t) = i\hbar\partial_t\Psi(x,t) \tag{II.1}$$

where H is the Hamiltonian, given by

$$H = H_0 + V = \frac{1}{2m}p^2 + V(x,t) = -\frac{\hbar^2}{2m}\Delta_x + V(x,t) \tag{II.2}$$

The kinetic operator $T = \frac{1}{2m}p^2$, is also known as the free Hamiltonian H_0 in nonrelativistic quantum mechanics. The complex-valued function $\Psi(x,t)$ is the wavefunction, and $|\Psi(x,t)|^2$ represents a particle density function. First, we will consider the case when there is no potential, i.e, $V(x,t) = 0$. Therefore, the free Schrödinger equation becomes,

$$i\partial_t\Psi(x,t) = -a^2\Delta_x\Psi(x,t) \tag{II.3}$$

where $a^2 = \frac{\hbar}{2m}$. The fundamental solution to the equation (II.3) in $\mathbb{R}^n$ is the free propagator,

$$K_f(x,y,t) = \left(\frac{m}{2\pi\hbar it}\right)^{n/2} e^{im|x-y|^2/2\hbar t} \quad \forall x,y \in \mathbb{R}^n,\, t \neq 0 \tag{II.4}$$

Also, the fundamental solution $K_f(x,t;y,\tau)$ as a function of (x,t) satisfies(away from the origin) the equation

$$-a^2\Delta_x K_f(x-y,t-\tau) = i\partial_t K_f(x-y,t-\tau) \tag{II.5}$$

An important difference between the heat equation and the Schrödinger equation is that the latter is reversible in time. The following calculations are motivated by

Isaak and Lev Rubenstein's treatment on the heat operator and its adjoint operator [1]. In this article, our case deals with the Schrödinger equation, and we seek to explore what are the differences and similarities between the heat equation and the Schrödinger equation.

Suppose $G \subset \mathbb{R}^n$ is a bounded region with a lateral boundary ∂G. In this case the integer n is the spatial dimension. Let $u(x,t) \in C^{2,1}(G \times \mathbb{R}^+) \bigcap C^{1,0}(\bar{G} \times \mathbb{R}^+)$, i.e, the function $u(x,t)$ is twice differentiable on the spatial region G, and once differentiable with respect to time in the interval $(0,\infty)$. The Schrödinger operator and its complex conjugate can be rewritten as

$$L = a^2 \Delta_x + i\hbar \partial_t \tag{II.6}$$

and

$$L^* = a^2 \Delta_x - i\hbar \partial_t \tag{II.7}$$

where $a^2 = \frac{\hbar}{2m}$. Then the adjoint operator of L is

$$L^\dagger = L = a^2 \Delta_x + i\hbar \partial_t \tag{II.8}$$

with respect to the usual L^2 inner product and the imposed homogeneous boundary conditions. In other words the Schrödinger operator L is formally self-adjoint. An important difference to notice is that the heat operator is not formally self-adjoint because the time derivative term changes sign.

Also, the kernel $K_f(x - y, t - \tau)$ as a function of (y, τ) satisfies(away from the origin) the equation

$$a^2 \Delta_y K_f(x - y, t - \tau) = i\partial_\tau K_f(x - y, t - \tau) \tag{II.9}$$

and hence,

$$L^*_{y,\tau}K_f(x-y,t-\tau) = a^2\Delta_y K_f(x-y,t-\tau) - i\partial_\tau K_f(x-y,t-\tau) = 0 \qquad \text{(II.10)}$$

The solution to the Schrödinger equation can be given by a kernel that gives the solution of the homogeneous problem for $t > 0$ in terms of the initial data at $t = 0$:

$$u(x,t) = \int_{\mathbb{R}^n} K_f(x,y,t)f(y)\,dy \qquad \text{(II.11)}$$

The kernel that solves the nonhomogeneous problem for all t is an extension of the kernel $K(x,y,t)$ to negative t as identically 0 and then we introduce the difference time variable $t - \tau$ and define $\tilde{K}$ by:

$$\tilde{K}(x,y,t,\tau) \equiv \begin{cases} K_f(x,y,t-\tau) & \text{if } t > \tau \\ \delta^n(x-y) & \text{if } t = \tau \\ 0 & \text{if } t < \tau \end{cases} \qquad \text{(II.12)}$$

Thus the nonhomogenous kernel can also be expressed by $\tilde{K}(x,t,y,\tau) = \theta(t-\tau)K_f(x,y,t,\tau)$. Then the nonhomogeneous kernel $\tilde{K}(x,t,y,\tau)$ satisfies the partial differential equation:

$$(i\partial_t - H_x)\tilde{K}(x,t,y,\tau) = \delta(t-\tau)\delta^n(x-y) \qquad \text{(II.13)}$$

and the homogeneous kernel $K_f(x,t,y,\tau)$ satisfies the partial differential equation:

$$(i\partial_t - H_x)K_f(x,t,y,\tau) = 0 \qquad \forall (x,t) \in \mathbb{R}^n \times \mathbb{R} \qquad \text{(II.14)}$$

The solution $u(x,t)$ that we obtain is the one that vanishes when $t = 0$. The free propagator $K_f(x,y,t)$ makes perfect sense for $t < 0$. Furthermore, the free propagator is a kernel that solves the initial-value problem for the homogeneous Schrödinger

equation for any final time, and it is a distributional solution of the homogeneous equation (II.5) for all times.

The free propagator K_f vanishes as a distribution as $t \to 0$ in the region $x \neq y$. As can be seen from equation (II.13), the function $\tilde{K}(x, y, t, \tau)$ satisfies the homogeneous Schrödinger equation distributionally except at the origin, where the time-dependent Schrödinger operator creates from it a delta function $\delta^n(x-y)\delta(t-\tau)$. The connection between K_f and $\tilde{K}$ will be proved and extended in the representation theorem in Chapter III.

The following definition is from G. H. Hardy's book on divergent series [4].

Definition 1 *If the integral*

$$P(\alpha) = \int_0^\infty f(x)e^{-\alpha x}\,dx \qquad (II.15)$$

is convergent for $\alpha > 0$, and approaches A when $\alpha \to 0$, then it is said that P is Abel summable to A and $P(0) = \int_0^\infty f(x)dx = A$.

The following theorem introduces the Poisson integral, which is a solution of the Schrödinger equation without a potential term.

Theorem 1 *Let $f(x)$ be a function on $\mathbb{R}^n$ with the following property: $(1+|y|^2)f(y) \in L^1(\mathbb{R}^n)$. Then the Poisson integral*

$$u(x, t) = K_f * f = \int_{\mathbb{R}^n} K_f(x - y, t)f(y)\,dy \qquad (II.16)$$

exists in the sense of Abel summability, and is a solution of the equation

$$Lu(x, t) = a^2\Delta_x u(x, t) + i\partial_t u(x, t) = 0 \qquad \forall (x, t) \in \mathbb{R}^n \times \mathbb{R}. \qquad (II.17)$$

with given initial data. The Poisson integral defines a solution of the free Schrödinger equation in $\mathbb{R}^n$, $\forall t \neq 0$, even $t < 0$. This solution can be extended into $\mathbb{R}^n \times [0, \infty)$

with the initial condition $u(x,0) = f(x)$ for all points x at which f is continuous.

Proof: If $|y|^2 f(y) \in L^1(\mathbb{R}^n)$, then the order of differentiation and integration in the equation (II.16) can be interchanged to show that the Poisson integral obeys Schrödinger equation. The hypothesis that $|y|^2 f(y) \in L^1(\mathbb{R}^n)$ implies that the function $u(x,t)$ solves the Schrödinger equation in $\mathbb{R}^n \times \mathbb{R}^+$. This hypothesis is obtained from Chapter IV of Lawrence C. Evans's book on partial differential equations [5]. Let $y = x + \gamma z$, where $\gamma^2 = \frac{2\hbar t}{m}$; then we can rewrite the Poisson integral as

$$u(x,t) = \left(\frac{1}{\pi i}\right)^{n/2} \int_{\mathbb{R}^n} e^{i|z|^2} f(x + \gamma z)\, dz \tag{II.18}$$

where $|z| = \frac{|x-y|}{\gamma}$. Let ϵ be any positive number. Then

$$(\pi i)^{n/2} u(x,t) = \int_{\mathbb{R}^n} e^{i|z|^2} f(x + \gamma z)\, dz = I_1 + I_2 + I_3, \tag{II.19}$$

where

$$I_1 = \int_{|z| \le \epsilon} e^{i|z|^2} \{f(x + \gamma z) - f(x)\}\, dz. \tag{II.20}$$

$$I_2 = \int_{|z| \ge \epsilon} e^{i|z|^2} f(x + \gamma z)\, dz \tag{II.21}$$

$$I_3 = \int_{|z| \le \epsilon} e^{i|z|^2} f(x)\, dz \tag{II.22}$$

Now, we do some calculations for I_1 in hyperspherical coordinates $(\rho, \phi_1, \ldots, \phi_{n-1})$. Equation (II.20) can be rewritten in the following manner:

$$I_1 = \int_{|z| \le \epsilon} e^{i|z|^2} \{f(x + \gamma z) - f(x)\}\, dz \tag{II.23}$$

The continuity of $f : \mathbb{R}^n \to \mathbb{R}^n$ at some point $y \in \mathbb{R}^n$ implies that $\forall \eta > 0\ \exists \delta > 0$ such that $\forall x \in \mathbb{R}^n$ with $|x - y| < \delta$ implies that $|f(x) - f(y)| < \eta$, and x, y are points where f is continuous. Given ϵ, choose γ such that $\varepsilon = \gamma \epsilon < \delta$, and let $\eta > 0$, then there exists a t so small such that $|f(x + \gamma z) - f(x)| < \eta$ for all z such that $|z| \le \epsilon$.

Therefore, by continuity, we obtain the following bounded estimate:

$$|I_1| \leq \eta \int_{|z| \leq \epsilon} dz \tag{II.24}$$

or, Thus

$$|I_1| \leq \eta \int_{|z| \leq \epsilon} dz \to 0 \tag{II.25}$$

as $\gamma |z| \to 0$ (i.e., $y \to x$) as $t \to 0$.

Then, since $f \in L^1(\mathbb{R}^n)$

$$|I_2| \leq \int_{|z| \geq \epsilon} |f(x + \gamma z)| \, dz \to 0 \tag{II.26}$$

(not necessarily uniformly in x) as $\epsilon \to \infty$. In order to handle I_3 we use the Fresnel integral formula

$$\int_{\mathbb{R}^n} e^{i|z|^2} dz = (\pi i)^{n/2} \tag{II.27}$$

A proof of the one-dimensional Fresnel integral formula is outlined on [6]. The one-dimensional Fresnel integral implies the product version

$$\int_{\mathbb{R}^n} e^{i|z|^2} \, dz = \int_{\mathbb{R}^n} \exp\left(i \sum_{k=1}^n z_k^2\right) dz = \prod_{k=1}^n \int_{-\infty}^{\infty} e^{i z_k^2} \, dz_k = \prod_{k=1}^n (\pi i)^{1/2} = (\pi i)^{n/2} \tag{II.28}$$

Therefore, we have

$$\lim_{\epsilon \to \infty} I_2 = (\pi i)^{n/2} f(x). \tag{II.29}$$

Then we consider computing the Fresnel integral in terms of polar coordinates instead of Cartesian coordinates. Thus, we can rewrite the equation (II.28) by

$$\int_{\mathbb{R}^n} e^{i|z|^2} \, dz = \int_0^\infty \int_{\partial B(0,1)} e^{i\rho^2} \rho^{n-1} \, d\rho d\Omega = \omega_n \int_0^\infty \rho^{n-1} e^{i\rho^2} \, d\rho \tag{II.30}$$

Then we make use of the substitution $t = \rho^2$, and hence we obtain

$$\int_{\mathbb{R}^n} e^{i|z|^2} \, dz = \frac{\omega_n}{2} \int_0^\infty t^{n-1} e^{it} \, dt \tag{II.31}$$

Then we insert the Abel factor $e^{-\alpha t}$ in the equation (II.31) and this gives

$$A(\alpha) = \frac{\omega_n}{2} \int_0^\infty e^{-\alpha t} t^{n-1} e^{it} \, dt \tag{II.32}$$

and ω_n is the surface area of the unit n-sphere. The surface area of the unit n-sphere is given by the following formula:

$$\omega_n = \frac{2\pi^{n/2}}{\Gamma(\frac{n}{2})} \tag{II.33}$$

The complex Gaussian integral (also known as the Gaussian Fresnel integrals) can be generalized for any positive integer, i.e. the Gaussian integral is a special case of $\int_0^\infty x^n e^{-x^2} \, dx$, when $n = 0$. The general Gaussian integral will be shown to be convergent when $n \in \mathbb{N}$. Then we consider the following complex integral

$$P_n = \int_0^\infty s^{n-1} e^{is^2} \, ds \tag{II.34}$$

where $|z| = s = \frac{|x-y|}{\gamma} = \frac{\rho}{\gamma}$. Let $t = s^2$, and substituting this change of variables into equation (II.36) we have

$$P_n = \frac{1}{2} \int_0^\infty t^m e^{it} \, dt \tag{II.35}$$

where, $m = \frac{n-2}{2}$ and hence,

$$\int_0^\infty t^m e^{it} \, dt = \lim_{r \to \infty} \int_0^r t^m e^{it} \, dt \tag{II.36}$$

Once again, the change of variables $t = iz$ is performed and we have

$$\int_0^r t^m e^{it} \, dt = i \int_0^{-ir} (iz)^m e^{-z} \, dz \tag{II.37}$$

Then we insert the Abel factor $e^{-\alpha t}$ into the left-hand side of equation (II.37) and this gives

$$\int_0^r t^m e^{-\alpha t} e^{it} \, dt = i \int_0^{-ir} (iz)^m e^{-i\alpha z} e^{-z} \, dz \tag{II.38}$$

Then the path of integration is shifted from 0 to $-i\infty$, to 0 to ∞. Therefore,

$$\lim_{r\to\infty} i \int_0^{-ir} (iz)^m e^{-\alpha z} e^{-z}\, dz = \lim_{r\to\infty} i \int_0^r (iz)^m e^{-\alpha z} e^{-z}\, dz \tag{II.39}$$

The integral in (II.39) is convergent for any positive $\alpha > 0$, and the integral over the semicircle at ∞ tends to 0. In order for the above limit to hold, the path of integration $(iz)^m$ must not go over a branch cut. Thus, if the integrand does not have any poles in the path of integration, then the integral in equation (II.36) is Abel summable and it is related to the gamma function $\Gamma(m+1)$. The integrand in equation (II.39) is an analytic function, and thus it does not have any poles or branch cuts in the path of integration. In other words,

$$\lim_{r\to\infty} i \int_0^{-ir} (iz)^m e^{-i\alpha z} e^{-z}\, dz = i^{m+1} \int_0^\infty z^m e^{-i\alpha z} e^{-z}\, dz \tag{II.40}$$

Then, we take the limit of $\alpha \to 0$, and the above equation becomes

$$\lim_{\alpha\to 0} i^{m+1} \int_0^\infty z^m e^{-i\alpha z} e^{-z}\, dz = i^{m+1} \int_0^\infty z^m e^{-z}\, dz \tag{II.41}$$

and this limit holds in the Abel sense, and we take $i^m = e^{i(\pi/2)m}$. Thus,

$$P_n = \frac{1}{2} i^{m+1} \Gamma(m+1) = \frac{i^{n/2}}{2} \Gamma\left(\frac{n}{2}\right) \tag{II.42}$$

and hence,

$$A(0) = \int_{\mathbb{R}^n} e^{i|z|^2}\, dz = \frac{i^{n/2} \omega_n}{2} \Gamma\left(\frac{n}{2}\right) \tag{II.43}$$

This confirms equation (II.28) in an alternative way.

This implies the continuity of $u(x, t)$ at $t = 0$. Therefore, the Poisson integral has the initial values $u(\cdot, 0) = f(x)$ for all points x at which f is continuous. $\blacksquare$

The fundamental solution of the Schrödinger operator has some specific filtering properties. Filtering properties refer to the ability of the Dirac delta function $\delta(t - \tau)$

to pick out the value of some function $\phi(t)$ at the point $t = \tau$. The filtering property is also called the sifting property. These filtering properties are shown in theorem 2. Theorem 2 is an extension of theorem 1

Theorem 2 *Let the boundary ∂U of U possess a tangent plane at each point. If $f(x)$ is a function continuous in the closure $\bar{U}$ of U, then*

$$\eta(x,t) = \lim_{t \to 0} \int_U K_f(x,y,t)f(y)\,dy = \begin{cases} f(x) & \text{if } x \in U, \forall t > 0 \\ \frac{f(x)}{2} & \text{if } x \in \partial U, \forall t > 0 \\ 0 & \text{if } x \notin \bar{U}, \forall t > 0 \end{cases} \tag{II.44}$$

and this limit exists in the Abel summability sense.

Proof: Suppose there exist a function $g(x)$ defined in the following way

$$g(x) = \begin{cases} f(x) & \text{if } x \in U, \forall t > 0 \\ 0 & \text{if } x \notin \bar{U}, \forall t > 0 \end{cases} \tag{II.45}$$

where f is a continuous function almost everywhere. By applying Theorem 1 to g, then we obtain the following result

$$\eta(x,t) = \lim_{t \to 0} \int_U K_f(x,y,t)g(y)\,dy = \begin{cases} f(x) & \text{if } x \in U, \forall t > 0 \\ 0 & \text{if } x \notin \bar{U}, \forall t > 0 \end{cases} \tag{II.46}$$

Suppose $x \in \partial U$. Then we introduce the hyperspherical coordinates $(\rho, \phi_1, \ldots, \phi_{n-1})$ with the origin at x. Let us consider an n-sphere $S(x, \varepsilon)$ with its center at x and radius $\varepsilon > 0$. Let D be the intersection between the n-sphere S and the region U, i.e, $D = S(x, \varepsilon) \cap U$. Thus, we can represent the region U as the following:

$$U = D \cup (U \setminus D) \tag{II.47}$$

Therefore,

$$Q(x,t) = Q_1(x,t) + Q_2(x,t) = \int_U K_f(x,y,t)f(y)\,dy + \int_{U \setminus D} K_f(x,y,t)f(y)\,dy \quad \text{(II.48)}$$

Since $x \notin U \setminus D$,

$$\lim_{t \to 0} Q_2(x,t) = \lim_{t \to 0} \int_{U \setminus D} K_f(x,y,t)f(y)\,dy = 0 \quad \text{(II.49)}$$

Therefore,

$$Q_1(x,t) = F(x,t) + H(x,t) = f(x)\int_D K_f(x,y,t)\,dy + \int_D K_f(x,y,t)\{f(y) - f(x)\}\,dy$$
$$\text{(II.50)}$$

or,

$$
\begin{aligned}
Q_1(x,t) &= f(x)\int_D \left(\frac{m}{2\pi i \hbar t}\right)^{n/2} e^{im|x-y|^2/2\hbar t}\,dy + \int_D \left(\frac{m}{2\pi i \hbar t}\right)^{n/2} e^{im|x-y|^2/2\hbar t}\{f(y) - f(x)\}\,dy \\
&= \frac{f(x)}{(\pi i)^{n/2}}\int_D e^{i|x-y|^2/\gamma^2}\frac{1}{\gamma^n}\,dy + \frac{1}{(\pi i)^{n/2}}\int_D e^{i|x-y|^2/\gamma^2}\{f(y) - f(x)\}\frac{1}{\gamma^n}\,dy \\
&= \frac{f(x)}{(\pi i)^{n/2}}\int_{D(z)} e^{i|z|^2}\,dz + \frac{1}{(\pi i)^{n/2}}\int_{D(z)} e^{i|z|^2}\{f(y) - f(x)\}\,dz
\end{aligned}
$$
$$\text{(II.51)}$$

where, $y = x + \gamma z$, and $\gamma^2 = \frac{2\hbar t}{m}$.

Then, the limit $\gamma \to 0$ is taken, and since f is continuous almost everywhere, then the above estimate becomes

$$|H(x,t)| \leq \frac{\eta}{\pi^{n/2}}\int_{D(z)}\,dz \to 0 \quad \text{(II.52)}$$

as $\gamma \to 0$. Then, as $\varepsilon \to 0$, the region D approaches half the surface area of the n-sphere $S(x,\varepsilon)$. This is true because of the fact that the boundary $\partial D = S(x,\varepsilon) \cap U$ is required to have a tangent plane at each point. Thus, in this limit we can use the tangent plane approximation to see that the ∂D becomes ∂K, which is the boundary

of a half n-sphere $K(x, \varepsilon)$.

Then we take the limit of $\gamma \to 0$ and of $\epsilon \to 0$ of the function $I(x,t)$. Hence

$$
\begin{aligned}
\lim_{\delta(\gamma) \to \infty} I(x,t) &= \lim_{\delta(\gamma) \to \infty} \int_0^{\delta(\gamma)} \int_{\partial D} \sigma^{n-1} e^{i\sigma^2} \, d\sigma d\Omega \\
&= \lim_{\delta(\gamma) \to \infty} \int_0^{\delta(\gamma)} \sigma^{n-1} e^{i\sigma^2} \, d\sigma \cdot \lim_{\delta(\gamma) \to \infty} \int_{\partial D} d\Omega = \frac{\omega_n}{2} \int_0^{\infty} \sigma^{n-1} e^{i\sigma^2} \, d\sigma
\end{aligned}
\tag{II.53}
$$

where, $\sigma = \frac{\varrho}{\gamma}$. The summability of the function $I(x,t)$ is understood to hold and exist in the Abel sense. Now, we use the Fresnel integral formula

$$
P_n = \int_0^{\infty} \sigma^{n-1} e^{i\sigma^2} \, d\sigma = \frac{i^{1/2}}{2} \Gamma\left(\frac{n}{2}\right)
\tag{II.54}
$$

into the equation (II.53). Therefore, we get

$$
\lim_{\delta(\gamma) \to \infty} F(x,t) = \frac{f(x)}{(\pi i)^{n/2}} \lim_{\delta(\gamma) \to \infty} I(x,t) = \frac{f(x)}{2(\pi i)^{n/2}} \left(\frac{i^{n/2} \omega_n}{2} \Gamma\left(\frac{n}{2}\right) \right)
\tag{II.55}
$$

Therefore,

$$
\lim_{\delta(\gamma) \to \infty} F(x,t) = \frac{f(x)}{2(\pi i)^{n/2}} \frac{2\pi^{n/2}}{\Gamma(\frac{n}{2})} \left(\frac{i^{n/2}}{2} \Gamma\left(\frac{n}{2}\right) \right) = \frac{f(x)}{2}
\tag{II.56}
$$

In other words, if $f(x)$ is a continuous function, then

$$
\eta(x,t) = \lim_{t \to 0} \int_U K_f(x,y,t) f(y) dy = \frac{f(x)}{2} \qquad \forall x \in \partial U, \forall t > 0. \quad \blacksquare
\tag{II.57}
$$

Next, we cite some material that is found in Chapter IV of Evans' book on partial differential equations [5]. The Poisson integral formula can also be expressed as

$$
u(x,t) = \frac{e^{\frac{i|x|^2}{4t}}}{(4\pi it)^{n/2}} \int_{\mathbb{R}^n} e^{\frac{-ix \cdot y}{2t}} g(y) \, dy
\tag{II.58}
$$

Lemma 1 *If the solution $u(x,t)$ is given by the above formula, and if $g(x) \in L^1(\mathbb{R}^n) \cap$*

$L^2(\mathbb{R}^n)$, *then*

$$\|u(t)\|_{L^2(\mathbb{R}^n)} = \|g\|_{L^2(\mathbb{R}^n)} \qquad \forall t > 0 \qquad\qquad\qquad \text{(II.59)}$$

Thus, the mapping $g \mapsto u(t)$ is unitary with respect to the L^2-norm.

CHAPTER III

REPRESENTATION THEOREM

The boundary-value problem for the nonhomogeneous Schrödinger equation with non-homogeneous initial conditions can be reduced to the analogous problem with homogeneous initial condition by using the integral fundamental representation

$$u(x,t) = \Gamma(x,t) + U(x,t) + \Pi(x,t) \tag{III.1}$$

where $u(x,t)$ is the solution of the nonhomogeneous problem, and as detailed below $U(x,t)$ is the source term, $\Gamma(x,t)$ is the surface term, and $\Pi(x,t)$ is the Poisson integral term(initial term). The following theorem gives the fundamental integral representations for the Schrödinger equation.

Theorem 3 *(Representation Theorem)*

The solution of the boundary-value problem for the Schrödinger equation can be represented as the following integral formula:

$$u(x,t) = \Gamma(x,t) + U(x,t) + \Pi(x,t) \tag{III.2}$$

The initial term, the source term, and the surface boundary terms are given by the following integral formulas:

$$\Pi(x,t) = \int_U K_f(x,t;y,t_0)h(y)\,dy \tag{III.3}$$

$$U(x,t) = i \int_{t_0}^t \int_U K_f(x,t;y,\tau)Lu(y,\tau)\,dyd\tau \tag{III.4}$$

and,

$$\Gamma(x,t) = ia^2 \int_{t_0}^t \int_{\partial U} \left(K_f(x,t;y,\tau)\partial_{\nu(y)}u(y,\tau) - u(y,\tau)\partial_{\nu(y)}K_f(x,t;y,\tau) \right) ds(y)d\tau \tag{III.5}$$

where, $K_f(x, t; y, \tau)$ is the fundamental solution and $a^2 = \frac{\hbar}{2m}$, and $u(x, t_0) = h(x)$.

Remark: The upper limit t in equation (III.4) enforces the fact that the K_f in that formula is effectively $\tilde{K}$.

Proof: Let $u(x, t)$, and $w(x, t)$ be solutions to the Schrödinger equation. Furthermore, assume that $u(x, t), w(x, t) \in C^{2,1}(U \times \mathbb{R}^+) \bigcap C^{1,0}(\bar{U} \times \mathbb{R}^+)$.

Remark: The above smooth conditions are required in order to justify all the integrations by parts. Since, the functions $u(x, t)$ and $v(x, t)$ are solutions of the Schrödinger equation, we require these solutions to be at twice differentiable on the region U because Greens' second formula applies to C^2 functions. Similarly, the temporal differentiability conditions are also needed for analogous reasons.

The Schrödinger operator L^* acts on the (y, τ) variables, and not the (x, t) variables. Then, we subtract the term containing the $w^*(y, \tau)Lu(y, \tau)$ minus the other term $u(y, \tau)L^*w^*(y, \tau)$, and we obtain

$$
\begin{aligned}
w^*(y, \tau)Lu(y, \tau) - u(y, \tau)L^*w^*(y, \tau) = a^2 w^*(y, \tau)\Delta_y u(y, \tau) \\
+ i\left(w^*(y, \tau)\partial_\tau u(y, \tau)\right) - a^2 u(y, \tau)\Delta_y w^*(y, \tau) + i\left(u(y, \tau)\partial_\tau w^*(y, \tau)\right)
\end{aligned}
\tag{III.6}
$$

and then integrating with respect to time τ and the spatial region U gives

$$
\begin{aligned}
\int_{t_0}^{t} \int_U w^*(y, \tau)Lu(y, \tau) - u(y, \tau)L^*w^*(y, \tau)\, dyd\tau = \\
a^2 \int_{t_0}^{t} \int_U [w^*(y, \tau)\Delta_y u(y, \tau) - u(y, \tau)\Delta_y w^*(y, \tau)]\, dyd\tau \\
+ i\int_{t_0}^{t} \int_U w^*(y, \tau)\partial_\tau u(y, \tau)\, dyd\tau + \int_{t_0}^{t} \int_U u(y, \tau)\partial_\tau w^*(y, \tau)\, dyd\tau
\end{aligned}
\tag{III.7}
$$

Therefore, we get

$$
\begin{aligned}
\int_{t_0}^{t} \int_U w^*(y, \tau)Lu(y, \tau) - u(y, \tau)L^*w^*(y, \tau)\, dyd\tau = \\
a^2 \int_{t_0}^{t} \int_U [w^*(y, \tau)\Delta_y u(y, \tau) - u(y, \tau)\Delta_y w^*(y, \tau)]\, dyd\tau + J
\end{aligned}
\tag{III.8}
$$

where,

$$J = i \int_{t_0}^{t} \int_{U} \partial_\tau [u(y,\tau)w^*(y,\tau)] \, dy d\tau \tag{III.9}$$

Green's second formula is the following identity:

$$\int_{U} [v(y,\tau)\Delta_y u(y,\tau) - u(y,\tau)\Delta_y v(y,\tau)] \, dy = \int_{\partial U} \left(v(y,\tau)\partial_{\nu(y)} u(y,\tau) - u(y,\tau)\partial_{\nu(y)} v(y,\tau) \right) ds(y) \tag{III.10}$$

where, U is a region in $\mathbb{R}^3$ with lateral boundary ∂U. This lateral boundary is defined by

$$\partial U = \{x,y,z : F(x,y,z) = 0\} \tag{III.11}$$

where (x,y,z) are the Cartesian coordinates in $\mathbb{R}^3$ and F is a continuously differentiable function. Therefore, by Green's second formula, we obtain the following result:

$$a^2 \int_{t_0}^{t} \int_{U} [w^*(y,\tau)\Delta_y u(y,\tau) - u(y,\tau)\Delta_y w^*(y,\tau)] \, dy d\tau$$
$$= a^2 \int_{t_0}^{t} \int_{\partial U} \left(w^*(y,\tau)\partial_{\nu(y)} u(y,\tau) - u(y,\tau)\partial_{\nu(y)} w^*(y,\tau) \right) ds(y) d\tau \tag{III.12}$$

Then, the second term of the right-hand side in equation (III.8) can be expressed in the following manner:

$$J = i \int_{t_0}^{t} \int_{U} \partial_\tau [u(y,\tau)w^*(y,\tau)] \, dy d\tau$$
$$= i \int_{t_0}^{t} \partial_\tau \int_{U} u(y,\tau)w^*(y,\tau) \, dy d\tau - \int_{\partial U} u(y,\tau)w^*(y,\tau)\partial_\tau \nu(y) \, ds(y) d\tau$$
$$= i \int_{t_0}^{t} \left(\partial_\tau \int_{U} u(y,\tau)w^*(y,\tau) \, dy \right) d\tau = i \int_{U} u(y,t)w^*(y,t) \, dy - i \int_{U} u(y,t_0)w^*(y,t_0) \, dy \tag{III.13}$$

where the integral term containing the time derivative of the normal vector vanishes because the boundary ∂U is assumed to be static. Finally, we obtain the following

equation:

$$\int_{t_0}^t \int_U w^*(y,\tau) Lu(y,\tau) - u(y,\tau) L^* u^*(y,\tau) \, dy d\tau$$

$$= i \int_U u(y,t) w^*(y,t) \, dy - i \int_U u(y,t_0) w^*(y,t_0) \, dy \qquad \text{(III.14)}$$

$$+ a^2 \int_{t_0}^t \int_{\partial U} \left(w^*(y,\tau) \partial_{\nu(y)} u(y,\tau) - u(y,\tau) \partial_{\nu(y)} w^*(y,\tau) \right) ds(y) d\tau$$

Suppose that $L^* w^*(y,\tau) = 0$, $\forall (y,\tau) \in U \times (t_0, \infty)$. Then, equation (III.14) becomes

$$\int_{t_0}^t \int_U w^*(y,\tau) Lu(y,t) \, dy d\tau = i \int_U u(y,t) w^*(y,t) \, dy - i \int_U u(y,t_0) w^*(y,t_0) \, dy$$

$$+ a^2 \int_{t_0}^t \int_{\partial U} \left(w^*(y,\tau) \partial_{\nu(y)} u(y,\tau) - u(y,\tau) \partial_{\nu(y)} w^*(y,\tau) \right) ds(y) d\tau$$

$$\text{(III.15)}$$

or,

$$i \int_U u(y,t) w^*(y,t) \, dy = i \int_U u(y,t_0) w^*(y,t_0) \, dy$$

$$- a^2 \int_{t_0}^t \int_{\partial U} \left(w^*(y,\tau) \partial_{\nu(y)} u(y,\tau) - u(y,\tau) \partial_{\nu(y)} w^*(y,\tau) \right) ds(y) d\tau + \int_{t_0}^t \int_U w^*(y,\tau) Lu(y,\tau) \, dy d\tau$$

$$\text{(III.16)}$$

Let $w^*(y,\tau) = K_f(x,y,t-\tau+\epsilon)$, and thus the solution $w^*(y,\tau)$ is a solution of equation (II.9) i.e, $L^* w^* = 0$. By substituting this equation into equation (III.16) we have

$$i \int_U K_f(x,y,\epsilon) u(y,t) \, dy = i \int_U K_f(x,y,t-t_0+\epsilon) u(y,t_0) \, dy$$

$$- a^2 \int_{t_0}^t \int_{\partial U} \left(K_f(x,y,t-\tau+\epsilon) \partial_{\nu(y)} u(y,\tau) - u(y,\tau) \partial_{\nu(y)} K_f(x,y,t-\tau+\epsilon) \right) ds(y) d\tau$$

$$+ \int_{t_0}^t \int_U K_f(x,y,t-\tau+\epsilon) Lu(y,\tau) \, dy d\tau$$

$$\text{(III.17)}$$

or,

$$\int_U K_f(x, y, \epsilon) u(y, t) \, dy = \int_U K_f(x, y, t - t_0 + \epsilon) u(y, t_0) \, dy$$

$$+ ia^2 \int_{t_0}^t \int_{\partial U} \left(K_f(x, y, t - \tau + \epsilon) \partial_{\nu(y)} u(y, \tau) - u(y, \tau) \partial_{\nu(y)} K_f(x, y, t - \tau + \epsilon) \right) ds(y) d\tau$$

$$- i \int_{t_0}^t \int_U K_f(x, y, t - \tau + \epsilon) Lu(y, \tau) \, dy d\tau$$

$$\text{(III.18)}$$

Then, we take the limit $\epsilon \to 0$ of equation (III.18), and by theorem 2

$$u(x, t) = \int_U K_f(x, y, t - t_0) u(y, t_0) \, dy$$

$$+ ia^2 \int_{t_0}^t \int_{\partial U} \left(K_f(x, y, t - \tau) \partial_{\nu(y)} u(y, \tau) - u(y, \tau) \partial_{\nu(y)} K_f(x, y, t - \tau) \right) ds(y) d\tau$$

$$- i \int_{t_0}^t \int_U K_f(x, y, t - \tau) Lu(y, \tau) \, dy d\tau$$

$$\text{(III.19)}$$

Therefore, we can write equation (III.19) as the representation formula

$$u(x, t) = \Pi(x, t) + \Gamma(x, t) + U(x, t) \tag{III.20}$$

where $\Pi(x, t)$ is the Poisson integral, $\Gamma(x, t)$ is the surface integral and $U(x, t)$ is the source integral. ∎

The definition of the Green function will be given in this section in order to prove the Representation Theorem for a more general Green function in place of K_f.

Definition 2 *A Green function for the Schrödinger equation is a function $G(x, t; y, \tau)$ satisfying*

$$LG(x, t; y, \tau) = 0 \qquad \forall (x, t) \in U \times \mathbb{R} \tag{III.21}$$

and the filtering property

$$\lim_{t \to \tau} \int_U G(x, t; y, \tau) f(y) \, dy = f(x) \tag{III.22}$$

for $x \in U$, and one of these boundary conditions

$$G(x, t; y, \tau) = 0 \qquad \forall (x, t) \in \partial U \times \mathbb{R} \tag{III.23}$$

or,

$$\partial_{\nu(x)} G(x, t; y, \tau) = 0 \qquad \forall (x, t) \in \partial U \times \mathbb{R} \tag{III.24}$$

or,

$$\partial_{\nu(x)} G(x, t; y, \tau) + \beta(x, t) G(x, t; y, \tau) = 0 \qquad \forall (x, t) \in \partial U \times \mathbb{R} \tag{III.25}$$

Thus the function $G(x, t; y, \tau)$ satisfies the homogeneous Dirichlet, Neumann, or Robin boundary conditions.

Recall that the function $K_f(x, t; y, \tau)$, the fundamental solution, satisfies

$$LK_f(x, t; y, \tau) = 0 \qquad \text{in } U \times \mathbb{R} \tag{III.26}$$

and the filtering property

$$K_f(x, \tau; y, \tau) = \delta(x - y) \tag{III.27}$$

In other words the function $G(x, t; y, \tau)$ is the response of the system at a field point(variable point) (x, t) due to a delta function δ at the source point(field point) (y, τ).

Lemma 2 *The Green function is the sum of a particular integral of the homogeneous equation and of the fundamental solution of the homogeneous equation*

$$G(x, t; y, \tau) = F(x, t; y, \tau) + K_f(x, t; y, \tau) \qquad \forall (x, t) \in \partial U \times \mathbb{R} \tag{III.28}$$

where $F(x, t; y, \tau)$ satisfies

$$LF(x, t; y, \tau) = 0 \qquad \forall (x, t) \in U \times \mathbb{R} \tag{III.29}$$

and it also satisfies one of the following boundary conditions

$$F(x, t; y, \tau) = -K_f(x, t; y, \tau) \quad \forall (x, t) \in \partial U \times \mathbb{R} \tag{III.30}$$

or,

$$\partial_{\nu(x)} F(x, t; y, \tau) = -\partial_{\nu(x)} K_f(x, t; y, \tau) \quad \forall (x, t) \in \partial U \times \mathbb{R} \tag{III.31}$$

or,

$$\left[\partial_{\nu(x)} + \beta(x, t) \right] F(x, t; y, \tau) = -\left[\partial_{\nu(x)} + \beta(x, t) \right] K_f(x, t; y, \tau) \quad \forall (x, t) \in \partial U \times \mathbb{R}$$
$$\tag{III.32}$$

and it also obeys the filtering property

$$F(x, \tau; y, \tau) = 0 \quad in\, U \times \{\tau = t\} \tag{III.33}$$

The following corollary will not be proved until Chapter IV, after we present the Reciprocity Theorem. In the meantime, the corollary serves to show that the Representation Theorem can be applied to any Green function which satisfies the Schrödinger equation and the boundary conditions.

Corollary 1 *The solution of the boundary-value problem for the Schrödinger equation can be represented as the following integral formula:*

$$u(x, t) = \Gamma(x, t) + U(x, t) + \Pi(x, t) \tag{III.34}$$

The initial term, the source term, and the surface boundary terms are given by the

following integral formulas:

$$\Pi(x,t) = \int_U G(x,t;y,t_0)h(y)\,dy \tag{III.35}$$

$$U(x,t) = i\int_{t_0}^t \int_U G(x,t;y,\tau)Lu(y,\tau)\,dyd\tau \tag{III.36}$$

and,

$$\Gamma(x,t) = ia^2 \int_{t_0}^t \int_{\partial U} \left(G(x,t;y,\tau)\partial_{\nu(y)}u(y,\tau) - u(y,\tau)\partial_{\nu(y)}G(x,t;y,\tau) \right) ds(y)d\tau \tag{III.37}$$

where, $G(x,t;y,\tau)$ is any Green function and $a^2 = \frac{\hbar}{2m}$, and $u(x,t_0) = h(x)$.

As an application of the representation theorem, let us consider the following linear boundary-value problem:

$$L\psi(y,\tau) = V(y,\tau)\psi(y,\tau) \qquad \forall (y,\tau) \in U \times \mathbb{R} \tag{III.38}$$

with the initial and boundary conditions

$$\psi(x,0) = f(x), \forall x \in U, \qquad \alpha(x,t)\psi(x,t)+\beta(x,t)\partial_{\nu(x)}\psi(x,t)\Big|_{\partial U} = h(x,t) \qquad \forall t \in \mathbb{R}. \tag{III.39}$$

In this case, the boundary conditions can determine the Dirichlet, Neumann or the Robin boundary-value problem. The first case to be considered is the Dirichlet case. Suppose $\psi(x,t)$ is a solution to the given initial and boundary value problem. Then, we apply the fundamental identity for the Dirichlet boundary-value problem, and we obtain the following integral equation:

$$\psi(x,t) = \int_U G(x,t;y,0)f(y)\,dy + ia^2 \int_0^t \int_{\partial U} G(x,t;y,\tau)\partial_{\nu(y)}\psi(y,\tau)\,ds(y)d\tau$$
$$- ia^2 \int_0^t \int_{\partial U} h(y,\tau)\partial_{\nu(y)}G(x,t;y,\tau)\,ds(y)d\tau - i\int_0^t \int_U G(x,t;y,\tau)V(y,\tau)\psi(y,\tau)\,dyd\tau \tag{III.40}$$

Then, we treat the Neumann boundary-value problem:

$$\alpha(x,t) = 0, \qquad \beta(x,t) = 1, \qquad \partial_{\nu(x)}\psi(x,t)\bigg|_{\partial U} = h(x,t) \quad \forall t > 0 \qquad \text{(III.41)}$$

and once again apply the fundamental identity in order to obtain the following integral equation:

$$\psi(x,t) = \int_U G(x,t;y,0)f(y)\,dy + ia^2\int_0^t\int_{\partial U} G(x,t;y,\tau)h(y,\tau)\,ds(y)d\tau$$

$$- ia^2\int_0^t\int_{\partial U}\psi(y,\tau)\partial_{\nu(y)}G(x,t;y,\tau)\,ds(y)d\tau - i\int_0^t\int_U G(x,t;y,\tau)V(y,\tau)\psi(y,\tau)\,dyd\tau$$

$$\text{(III.42)}$$

Finally, we treat the Robin boundary-value problem:

$$\beta(x,t) = 1, \qquad \alpha(x,t)\psi(x,t) + \partial_{\nu(x)}\psi(x,t)\bigg|_{\partial U} = h(x,t) \quad \forall t > 0 \qquad \text{(III.43)}$$

and once again we use the representation theorem in order to obtain the following integral equation:

$$\psi(x,t) = \int_U G(x,t;y,0)f(y)\,dy + ia^2\int_0^t\int_{\partial U} G(x,t;y,\tau)h(y,\tau)\,ds(y)d\tau$$

$$- ia^2\int_0^t\int_{\partial U}\psi(y,\tau)\Big(\partial_{\nu(y)}G(x,t;y,\tau) + \alpha(y,\tau)G(x,t;y,\tau)\Big)\,ds(y)d\tau \qquad \text{(III.44)}$$

$$- i\int_0^t\int_U G(x,t;y,\tau)V(y,\tau)\psi(y,\tau)\,dyd\tau$$

CHAPTER IV

GREEN FUNCTIONS AND THE RECIPROCITY THEOREM

Unlike [1], the boundary ∂U is considered to be a static boundary, and thus

$$\partial_t \nu(x) = 0 \qquad \forall x \in \partial U, \forall t > 0 \tag{IV.1}$$

Theorem 4 *Let U be an open and bounded domain in $\mathbb{R}^n$, i.e., $U \subset \mathbb{R}^n$. Consider the following boundary-value problem: Find a function $u(x,t) \in C^{2,1}(U \times \mathbb{R}^+) \bigcap C^{1,0}(\bar{U} \times \mathbb{R}^+)$, such that*

$$Lu(x,t) + F(x,t) = 0 \qquad \forall x \in U \ \forall t > 0, \tag{IV.2}$$

$$u(x,0) = \varphi(x) \qquad \forall x \in U, \tag{IV.3}$$

$$u(x,t) = f_1(x,t) \qquad x \in \partial U_1, \forall t > 0 \tag{IV.4}$$

$$\partial_{\nu(x)} u(x,t) = f_2(x,t) \qquad x \in \partial U_2, \forall t > 0 \tag{IV.5}$$

where, $\partial U_1 \cup \partial U_2$. If the solution of problem (IV.2)-(IV.3) exists, it is also unique.

Proof: If, u_1 and u_2 are two solutions of the problem, then their difference

$$u = u_1 - u_2 \tag{IV.6}$$

is a solution of the corresponding homogeneous problem. First, we consider the following equation,

$$\int_0^t \int_U w^*(y,\tau) Lu(y,\tau) \, dy d\tau = \int_0^t \int_U w^*(y,\tau) \left(a^2 \Delta_y u(y,\tau) + i \partial_\tau u(y,\tau) \right) dy d\tau \tag{IV.7}$$

where, L is the Schrödinger operator. Let $w(x,t) = u(x,t)$ and substitute $v(x,t) \equiv w^*(x,t)$ into Green's first identity, to obtain

$$\int_U u^*(y,\tau)\Delta_y u(y,\tau)\, dy + \int_U \nabla u^*(y,\tau) \cdot \nabla u(y,\tau)\, dy = \int_{\partial U} u^*(y,\tau)\partial_{\nu(y)} u(y,\tau)\, ds(y).$$

$$(IV.8)$$

Therefore, equation (IV.7) becomes,

$$\int_0^t \int_U u^*(y,\tau)Lu(y,\tau)\, dyd\tau = -a^2 \int_0^t \int_U \nabla u^*(y,\tau) \cdot \nabla u(y,\tau)\, dyd\tau$$
$$+ a^2 \int_0^t \int_{\partial U} u^*(y,\tau)\partial_{\nu(y)} u(y,\tau)\, ds(y)d\tau + i \int_0^t \int_U u^*(y,\tau)\partial_\tau u(y,\tau)\, dyd\tau$$

$$(IV.9)$$

The left-hand side of equation (IV.9) equals zero. Thus,

$$0 = -a^2 \int_0^t \int_U \nabla u^*(y,\tau) \cdot \nabla u(y,\tau)\, dyd\tau + a^2 \int_0^t \int_{\partial U} u^*(y,\tau)\partial_{\nu(y)} u(y,\tau)\, ds(y)d\tau$$
$$+ i \int_0^t \int_U u^*(y,\tau)\partial_\tau u(y,\tau)\, dyd\tau$$

$$(IV.10)$$

The second integral in the right-hand side of the above equation is equal to zero because of the Neumann or Dirichlet boundary condition. Then

$$I = i \int_0^t \int_U u^*(y,\tau)\partial_\tau u(y,\tau)\, dyd\tau$$
$$= \frac{i}{2} \int_0^t \int_U \left(u^*(y,\tau)\partial_\tau u(y,\tau) - \left(\partial_\tau u^*(y,\tau) \right) u(y,\tau) \right) dyd\tau$$
$$+ \frac{i}{2} \int_0^t \int_U \left(u^*(y,\tau)\partial_\tau u(y,\tau) + \left(\partial_\tau u^*(y,\tau) \right) u(y,\tau) \right) dyd\tau$$
$$= I_1 + I_2$$

$$(IV.11)$$

Then, the first term in equation (IV.11) can be expressed in the following way,

$$I_1 = \frac{i}{2} \int_0^t \int_U \left(u^*(y,\tau)\partial_\tau u(y,\tau) - \left(u^*(y,\tau)\partial_\tau u(y,\tau) \right)^* \right) dyd\tau$$
$$= -\int_0^t \int_U \Im\left\{ u^*(y,\tau)\partial_\tau u(y,\tau) \right\} dyd\tau$$

$$(IV.12)$$

The second term in equation (IV.11) is:

$$
\begin{aligned}
I_2 &= \frac{i}{2} \int_0^t \int_U \left(u^*(y,\tau)\partial_\tau u(y,\tau) + \partial_\tau u^*(y,\tau) \Big) u(y,\tau) \right) dyd\tau \\
&= \frac{i}{2} \int_0^t \int_U \partial_\tau [u^*(y,\tau)u(y,\tau)]\, dyd\tau = \frac{i}{2} \int_U |u(y,t)|^2\, dy - \frac{i}{2} \int_U |u(y,0)|^2\, dy
\end{aligned}
\tag{IV.13}
$$

In this equation the second term vanishes from the fact that $u(y,\tau = 0) = 0$. Then equation (IV.10) can be rewritten in the following manner,

$$
\begin{aligned}
a^2 \int_0^t \int_U [\nabla u^*(y,\tau) \cdot \nabla u(y,\tau)]\, dyd\tau &= - \int_0^t \int_U \mathfrak{Im}\left\{ u^*(y,\tau)\partial_\tau u(y,\tau) \right\} dyd\tau \\
&+ \frac{i}{2} \int_U |u(y,t)|^2\, dy
\end{aligned}
\tag{IV.14}
$$

Thus, we take the real part of equation (IV.14),and we get the following expression,

$$
a^2 \int_0^t d\tau \int_U [\nabla u^*(y,\tau) \cdot \nabla u(y,\tau)]\, dy = - \int_0^t \int_U \mathfrak{Im}\left\{ u^*(y,\tau)\partial_\tau u(y,\tau) \right\} dyd\tau
\tag{IV.15}
$$

Also, if we take the imaginary part of the equation (IV.14), we get the following expression,

$$
\frac{1}{2} \int_U |u(y,t)|^2\, dy = 0
\tag{IV.16}
$$

The above equation implies that the function $u(y,\tau) \equiv 0, \forall (y,\tau) \in U \times \mathbb{R}^+$. Then the real part of equation (IV.14) is satisfied trivially. $\blacksquare$

Remark: In the case of the heat equation, the Rubinsteins' proof went in a different direction. A difference between the heat operator and the Schrödinger operator is that the Schrödinger operator has a complex number in front of the partial derivative with respect to time. There is no analogue of equation (IV.15) in the heat equation case.

In the rest of this section, the method of Green function will be introduced as an important method for solving different types of boundary-value problems such as

the initial and boundary value problem. In this section, the Green's function will be shown to have reciprocity.

The following theorem is based on a similar theorem found on Chapter 15 on Rubinstein book, but in this case it is proved for the Schrödinger case.

Theorem 5 *(The Reciprocity of Green's Functions)*

Suppose (x,t) is a fixed point and $(y,\tau) \in U \times \mathbb{R}$ is a variable point. The function $G(y,\tau;x,t)$ is considered a function of the first variables, and is a solution of the Schrödinger equation satisfying boundary conditions of Dirichlet, Neumann, or Robin boundary value problem respectively. Therefore, we obtain the reciprocity of Greens functions, i.e.,

$$G(y,\tau;x,t) = G^*(x,t;y,\tau). \tag{IV.17}$$

Proof: Suppose, $G(y,\tau;x,t) = K(y,\tau;x,t) + F(y,\tau;x,t)$, where

$$LF(y,\tau;x,t) = 0 \qquad \forall(y,\tau) \in U \times \mathbb{R} \tag{IV.18}$$

such that,

$$F(y,\tau;x,t) = -K(y,\tau;x,t) \qquad \forall(y,\tau) \in \partial U \times \mathbb{R} \tag{IV.19}$$

or,

$$\partial_{\nu(y)}F(y,\tau;x,t) = -\partial_{\nu(y)}K(y,\tau;x,t) \qquad \forall(y,\tau) \in \partial U \times \mathbb{R} \tag{IV.20}$$

or,

$$\left(\partial_{\nu(y)} + \beta(y,\tau)\right)F(y,\tau;x,t) = -\left(\partial_{\nu(y)} + \beta(y,\tau)\right)K(y,\tau;x,t) \qquad \forall(y,\tau) \in \partial U \times \mathbb{R} \tag{IV.21}$$

and also

$$F(x,t;y,t) = 0 \quad \text{in } U \times \{\tau = t\} \tag{IV.22}$$

Green's second formula is given by

$$\int_U [u(y,\tau)\Delta_y v(y,\tau) - v(y,\tau)\Delta_y u(y,\tau)]\, dy = \int_{\partial U}\left(u(y,\tau)\partial_{\nu(y)}v(y,\tau) - v(y,\tau)\partial_{\nu(y)}u(y,\tau)\right) ds(y)$$

(IV.23)

Then, we integrate the term $[G^*(y,\tau;x,t)LG(y,\tau;\rho,\theta) - G(y,\tau;\rho,\theta)(LG(y,\tau;x,t))^*]$
over the spacetime region $U \times (\theta,t)$, and we have

$$\int_\theta^t \int_U G^*(y,\tau;x,t)L_{y,\tau}G(y,\tau;\rho,\theta) - G(y,\tau;\rho,\theta)L^*_{y,\tau}G^*(y,\tau;x,t)\, dyd\tau$$
$$= a^2 \int_\theta^t \int_U G^*(y,\tau;x,t)\Delta_y G(y,\tau;\rho,\theta) - G(y,\tau;\rho,\theta)\Delta_y G^*(y,\tau;x,t)\, dyd\tau$$
$$+ i \int_\theta^t \int_U G^*(y,\tau;x,t)\partial_\tau G(y,\tau;\rho,\theta)\, dyd\tau + i \int_\theta^t \int_U G(y,\tau;\rho,\theta)\partial_\tau G^*(y,\tau;x,t)\, dyd\tau$$

(IV.24)

Then, Green's second formula is used in equation (IV.24), and we obtain

$$\int_\theta^t \int_U G^*(y,\tau;x,t)LG(y,\tau;\rho,\theta) - G(y,\tau;\rho,\theta)L^*G^*(y,\tau;x,t)\, dyd\tau$$
$$= a^2 \int_\theta^t \int_{\partial U}\left(G^*(y,\tau;x,t)\partial_{\nu(y)}G(y,\tau;\rho,\theta) - G(y,\tau;\rho,\theta)\partial_{\nu(y)}G^*(y,\tau;x,t)\right) ds(y)d\tau$$
$$+ i \int_\theta^t \int_U \partial_\tau[G^*(y,\tau;x,t)G(y,\tau;\rho,\theta)]\, dyd\tau$$

(IV.25)

The surface integrals vanish in the Dirichlet boundary problem because $G^*(y,\tau;x,t)$
and $G(y,\tau;x,t)$ vanish on $\partial U \times \mathbb{R}^+$. The surface integrals also vanish when we have
Neumann boundary conditions because $\partial_{\nu(y)}G(y,\tau;x,t) = 0$, on $\partial U \times \mathbb{R}^+$. Then,
equation (IV.25) becomes

$$\int_\theta^t \int_U G^*(y,\tau;x,t)LG(y,\tau;\rho,\theta) - G(y,\tau;\rho,\theta)L^*G^*(y,\tau;x,t)\, dyd\tau$$
$$= i \int_\theta^t \int_U \partial_\tau[G^*(y,\tau;x,t)G(y,\tau;\rho,\theta)]\, dyd\tau$$

(IV.26)

or,

$$\int_\theta^t \int_U G^*(y,\tau;x,t)LG(y,\tau;\rho,\theta) - G(y,\tau;\rho,\theta)L^*G^*(y,\tau;x,t)\,dyd\tau$$
$$= i\int_U G^*(y,t;x,t)G(y,t;\rho,\theta)\,dy - i\int_U G^*(y,\theta;x,t)G(y,\theta;\rho,\theta)\,dy \tag{IV.27}$$

Therefore, by using the definition of the Green function, we obtain

$$0 = i\int_U G^*(y,t;x,t)G(y,t;\rho,\theta)\,dy - i\int_U G^*(y,\theta;x,t)G(y,\theta;\rho,\theta)\,dy \tag{IV.28}$$

or,

$$i\int_U \delta(x-y)G(y,t;\rho,\theta)\,dy = i\int_U \delta(\rho-y)G^*(y,\theta;x,t)\,dy \tag{IV.29}$$

or,

$$G(x,t;\rho,\theta) = G^*(\rho,\theta;x,t) \tag{IV.30}$$

Therefore, $G^*(\rho,\theta;x,t) = G(x,t;\rho,\theta)$ and the quantum Green function has reciprocity. ∎

Remark: The reciprocity of the Green function basically expresses the unitarity of e^{-itH}.

Finally, we present the corollary 2 which was introduced back in Chapter III. This time we provide a proof to the corollary.

Corollary 2 *The solution of the boundary-value problem for the Schrödinger equation can be represented as the following integral formula:*

$$u(x,t) = \Gamma(x,t) + U(x,t) + \Pi(x,t) \tag{IV.31}$$

The initial term, the source term, and the surface boundary terms are given by the following integral formulas:

$$\Pi(x,t) = \int_U G(x,t;y,t_0)h(y)\,dy \tag{IV.32}$$

$$U(x,t) = i \int_{t_0}^t \int_U G(x,t;y,\tau) Lu(y,\tau)\, dy d\tau \qquad (\text{IV.33})$$

and,

$$\Gamma(x,t) = ia^2 \int_{t_0}^t \int_{\partial U} \left(G(x,t;y,\tau)\partial_{\nu(y)}u(y,\tau) - u(y,\tau)\partial_{\nu(y)}G(x,t;y,\tau) \right) ds(y) d\tau$$
$$(\text{IV.34})$$

where, $G(x,t;y,\tau)$ is any Green function and $a^2 = \frac{\hbar}{2m}$, and $u(x,t_0) = h(x)$.

Proof: Suppose there exists a function $G(x,t;y,\tau)$ such that

$$L_{y,\tau}^* G^*(x,t;y,\tau) = 0, \qquad \forall (x,t) \in U \times \mathbb{R} \qquad (\text{IV.35})$$

where (y,τ) is a variable point and (x,t) is a fixed point. In other words, the partial differential operator L^* acts on the (y,τ) variables. Also, by hypothesis the function $G(x,t;y,\tau)$ satisfies the same filtering properties as the free propagator $K_f(x,t;y,\tau)$. In this proof, the function is assumed to satisfy the filtering property. Thus, we can write $G(x,t;y,\tau)$ as the sum of $K_f(x,y,t-\tau)$ and $E(x,t;y,\tau)$. The function $E(x,t;y,\tau)$ satisfies the homogeneous equation

$$LE(x,t;y,\tau) = 0, \qquad \forall (x,t) \in U \times \mathbb{R} \qquad (\text{IV.36})$$

and vanishes when $t = \tau$, i.e $E(x,\tau;y,\tau) = 0$ in $U \times \{t = \tau\}$. This Green function satisfies the same properties and equations as K_f, and thus we can replace $w^*(y,\tau)$ by $G^*(y,\tau;x,t)$ in equation (III.14), and we obtain

$$\int_{t_0}^t \int_U G^*(y,\tau;x,t)Lu(y,\tau) - u(y,\tau)L^*G^*(y,\tau;x,t)\, dy d\tau$$
$$= i \int_U u(y,t)G^*(y,t;x,t)\, dy - i \int_U u(y,t_0)G^*(y,t_0;x,t)\, dy \qquad (\text{IV.37})$$
$$+ a^2 \int_{t_0}^t \int_{\partial U} \left(G^*(y,\tau;x,t)\partial_{\nu(y)}u(y,\tau) - u(y,\tau)\partial_{\nu(y)}G^*(y,\tau;x,t) \right) ds(y) d\tau$$

and by the Reciprocity Theorem, we can rewrite equation (IV.37) as

$$
\begin{aligned}
u(x,t) = & \int_U G(x,t;y,t_0)u(y,t_0)\,dy \\
& + ia^2 \int_{t_0}^t \int_{\partial U} \Big(G(x,t;y,\tau)\partial_{\nu(y)}u(y,\tau) - u(y,\tau)\partial_{\nu(y)}G(x,t;y,\tau) \Big)\, ds(y)d\tau \\
& - i \int_{t_0}^t \int_U G(x,t;y,\tau)Lu(y,\tau)\,dyd\tau
\end{aligned}
$$

$$\text{(IV.38)}$$

Therefore, we can write equation (IV.38) as the representation formula

$$
u(x,t) = \Pi(x,t) + \Gamma(x,t) + U(x,t) \tag{IV.39}
$$

where $\Pi(x,t)$ is the Poisson integral, $\Gamma(x,t)$ is the surface integral and $U(x,t)$ is the source integral. $\blacksquare$

CHAPTER V

GREEN FUNCTIONS AND INITIAL VALUE PROBLEMS

A.   Green Functions and Volterra Integral Equations

The boundary-value problem for the nonhomogeneous Schrödinger equation with non-homogeneous initial conditions can be reduced into a problem with homogeneous initial conditions by use of Theorem 3:

$$u(x,t) = \Gamma(x,t) + U(x,t) + \Pi(x,t) \tag{V.1}$$

where $u(x,t)$ is the solution of the nonhomogeneous problem, $U(x,t)$ is the volume potential, $\Gamma(x,t)$ is the surface integral and $\Pi(x,t)$ is the Poisson integral.

Let us consider the Schrödinger initial-value problem with a bounded potential term:

$$-\Delta_x u(x,t) + V(x,t)u(x,t) = i\partial_t u(x,t) \tag{V.2}$$

$$u(x,0) = f(x) \qquad \forall x \in \mathbb{R}^n \tag{V.3}$$

In this problem, we assume that $V(x,t)$ is a continuously differentiable function on $\mathbb{R}^n \times \mathbb{R}$. Let $V(x,t)$ be a bounded function such that

$$|V(x,t)| \leq M \qquad \forall (x,t) \in \mathbb{R}^n \times \mathbb{R} \tag{V.4}$$

Suppose the function $V(x,t)$ is a piecewise continuous and a piecewise smooth function on $\mathbb{R}^n \times \mathbb{R}$.

Then by equation (V.1) the solution $u(x,t)$ can be written as the following inte-

gral equation:

$$u(x,t) = \Pi(x,t) + U(x,t) \equiv \hat{U}f(x) + \hat{Q}u(x,t)$$
$$= \int_{\mathbb{R}^n} K_f(x,t;y,0)f(y)\,dy - i\int_0^t \int_{\mathbb{R}^n} K_f(x,t;y,\tau)V(y,\tau)u(y,\tau)\,dyd\tau \tag{V.5}$$

where $\hat{U}$ is a unitary operator and where $K_f(x,t;y,\tau)$ is the fundamental solution of the Schrödinger problem. We are applying the integral representation theorem in a case where $V(x,t)$ is a bounded function. Thus,

$$u(x,t) + iSVu(x,t) = \hat{U}f(x) \tag{V.6}$$

and where

$$\hat{Q}u(x,t) = -iSVu(x,t) = -i\int_0^t \hat{U}(t-\tau)V(\tau)u(\tau)\,d\tau \tag{V.7}$$

In more detail, we can express equation (V.6) as

$$u(x,t) + i\int_0^t \hat{U}(t-\tau)V(\tau)u(\tau)\,d\tau = \hat{U}f(x) \tag{V.8}$$

where,

$$\hat{U}(t-\tau)V(\tau)u(\tau) = \int_{\mathbb{R}^n} K_f(x,t;y,\tau)V(y,\tau)u(y,\tau)\,dy \tag{V.9}$$

Therefore, equation (V.5) is a Volterra integral equation of the second kind with respect to time. In order to find the solution to the Volterra integral equation of the second kind, we let the kernel satisfy the following condition:

$$K(x,y,t,\tau) = 0 \qquad \text{if } t < \tau \tag{V.10}$$

A Volterra integral equation of the second kind with respect to time, has the following form:

$$\phi(x,t) - \lambda\int_0^t \int_{\mathbb{R}^n} K(x,t;y,\tau)\phi(y,\tau)\,dyd\tau = f(x,t) \tag{V.11}$$

By defining $\hat{A}\phi(t) = \int_{\mathbb{R}^n} K(x,t;y,\tau)\phi(y,\tau)\,dy$, we rewrite equation (V.11) in a more

compact form,

$$\phi(t) - \lambda \int_0^t A(t,\tau)\phi(\tau)\, d\tau = f(t) \tag{V.12}$$

In this article, we will work only on the Euclidean spacetime $\mathbb{R}^{n+1}$. In this case, we are trying to generalize the kernel and the linear integral operator. The kernel $K(x,t;y,\tau)$ in equation (V.11) can be a Schrödinger kernel, a bounded kernel, or a Hilbert-Schmidt kernel. The Volterra integral equation of the second kind can be solved by Picard's method of successive approximations. For a detailed treatment of the Picard's method of successive approximations, I will refer the reader to the Tricomi reference [7]. The idea is to create an infinite sequence of functions, $\{\phi_n(x,t)\}_{n=0}^\infty$ that satisfy the following recurrence relations:

$$\phi_n(t) = f(t) + \lambda \int_0^t A(t,\tau)\phi_{n-1}(\tau)\, d\tau \qquad \forall n = 1, 2, \ldots \tag{V.13}$$

Then, let

$$\phi_n(x,t) = \sum_{m=0}^n \lambda^m \psi_m(x,t) \qquad \forall m = 1, 2, \ldots \tag{V.14}$$

The function $\psi_m(x,t)$ can be expressed in the following way:

$$\psi_m(x,t) = \int_0^t \int_{\mathbb{R}^n} K_m(x,t;y,\tau) f(y,\tau)\, dy d\tau \qquad \forall m = 1, 2, \ldots \tag{V.15}$$

or,

$$\psi_m(t) = \hat{Q}^m f(t) = \int_0^t A_m(t,\tau) f(\tau)\, d\tau \qquad \forall m = 1, 2, \ldots \tag{V.16}$$

Then, we can write the first term in the following manner,

$$\psi_1(t) = \int_0^t A(t,\tau) f(\tau)\, d\tau \tag{V.17}$$

and,

$$A_{n+1}(t,\tau) = \int_0^t A(t,\theta) A_n(\theta,\tau)\, d\theta \qquad \forall n = 1, 2, \ldots \tag{V.18}$$

where

$$A_1(t, \tau) = A(t, \tau) \qquad \text{(V.19)}$$

B.   Integral Equations and Neumann Series

In the previous subsection, the Volterra integral equations of the second kind were introduced. In this subsection, we introduce the integral operators in arbitrary Banach spaces in order to find a solution to the Schrödinger equation in $\mathbb{R}^{n+1}$. Section A is an informal preview of the Volterra and General Volterra Theorems which will be proved in Chapter VI. In the following analysis of integral operators, this article will use as a foundation Rainer Kress' treatment on linear integral equations [2]. In operator notation, the Volterra integral equation of the second kind is written in the following manner:

$$\phi - \hat{Q}\phi = f \qquad \text{(V.20)}$$

where $\hat{Q}$ is a bounded linear operator from a Banach space $\mathcal{B}$ to itself and $\phi, f \in \mathcal{B}$. The existence and uniqueness of a solution to an integral operator equation can be found via the inverse operator $(I - \hat{Q})^{-1}$, and whose existence will become clear below.

Definition 3 *Let $\mathcal{B}(\mathcal{H}; \mathcal{H})$ be the collection of bounded linear transformations from $\mathcal{H}$ into $\mathcal{H}$. Also, we denote the space $B(\mathcal{H}, \mathbb{F})$ as the set of bounded linear functionals on $\mathcal{H}$, where $\mathbb{F} = \{\mathbb{R}, \mathbb{C}\}$.*

Important Banach spaces which we will be dealing with are the Lebesgue spaces $L^p(\mu)$. This article will cover the case when $p = \infty$, in order to create bounded estimates of the Volterra operator $\hat{Q}$ with respect to the norm $\| \cdot \|$. In the next section, the Volterra Theorem will prove that the spectral radius of the Volterra operator is zero using the L^∞-estimates.

Definition 4 *The collection of all essentially bounded measurable functions is denoted by $L^\infty(\mu)$. The essential supremum of a function φ is given by*

$$\|\varphi\|_{L^\infty(\mu)} = \inf\{M \geq 0 : |\varphi(x)| \leq M \text{ holds for almost all } x\}. \qquad \text{(V.21)}$$

If φ does have an essential bound, then it is said to belong to $L^\infty(\mu)$.

Definition 5 *Let $A : X \to X$ be a bounded linear operator, where X is a Banach space, and let Ω be some measurable space. The norm of a bounded operator $A(x,y)$ is given by*

$$
\begin{aligned}
\|A\|_{L^\infty(\Omega^2)} &\equiv \inf\{M \geq 0 : \|A(x,y)\| \leq M, \text{for almost all } (x,y) \in \Omega^2\} \\
&= \sup_{(x,y)\in\Omega^2} \|A(x,y)\|
\end{aligned}
\qquad \text{(V.22)}
$$

where,

$$\|A(x,y)\| = \inf\{M \geq 0 : \|A(x,y)\phi\| \leq M\|\phi\|, \forall \phi \in \mathcal{B}\} \qquad \text{(V.23)}$$

and where $\mathcal{B}$ is also a Banach space.

The operator equation of the second kind was obtained by reformulating the Schrödinger equation as an integral equation. The existence and uniqueness of the operator equations of the second kind can be found by the Neumann series. In operator notation, we can write the Volterra equation of the second kind, in the following way

$$\phi - \hat{Q}\phi = f \qquad \text{(V.24)}$$

The integral operator $\hat{Q}$ is a bounded linear operator in an arbitrary Banach space $\mathcal{B}$. The solution to an operator equation can be found by the inverse operator $(I - \hat{Q})^{-1}$, where I is the identity operator. In other words, the solution of the Volterra integral

equation can be given by successive approximations. The successive approximations

$$\phi_{n+1} = \hat{Q}\phi_n + f \qquad (\text{V}.25)$$

converge to the exact solution of the integral equation, $\phi - \hat{Q}\phi = f$.

In this section, it will be assumed that the integral operators are bounded linear operators on a Banach space $\mathcal{B}$. The above integral equations are given for an arbitrary Banach space $\mathcal{B}$ that will be used in Picard's algorithm of successive approximation. Then, equation (V.25) is converging to the solution ϕ if the following conditions are satisfied:

1)the integral operator $\hat{Q}$ is a bounded linear operator in the Banach space $\mathcal{B}$.

2)the function f belongs to a Banach space $\mathcal{B}$,

3)and finally, the infinite series $\varphi = \sum_{j=0}^{\infty} \hat{Q}^j f$ is a convergent series with respect to the topology of L^∞ in time and of $\mathcal{B}$ in space.

If these three conditions are satisfied, then it is possible to use the Neumann series to obtain the exact solution to the original problem, which is the initial value problem of the Schrödinger equation with a potential term $V(x,t)$. The three conditions turn out be the necessary hypotheses to prove the Volterra and General Volterra theorems. Once again, we want to solve the Volterra integral equation $\phi - \hat{Q}\phi = f$, and the first initial term in the approximation is f. Then, we have,

$$(I - \hat{Q})\phi = f, \qquad (\text{V}.26)$$

and the formal solutions is

$$\phi = (I - \hat{Q})^{-1}f \qquad (\text{V}.27)$$

with the following Neumann series,

$$\phi = f + \hat{Q}f + \hat{Q}^2 f + \cdots \qquad (\text{V}.28)$$

Therefore, we obtain the partial sums

$$\phi_m = \sum_{j=0}^{m} \hat{Q}^j f \tag{V.29}$$

of the Neumann series which satisfy the recurrence relation $\phi_{n+1} = \hat{Q}\phi_n + f$, $\forall n \geq 0$.

Finally, in our case, we have, $f(t) = \hat{U}g(x) = \int_{\mathbb{R}^n} K_f(x, t; y, 0)g(y)\, dy$, and

$$\hat{Q}f(t) = -iSVf(t) = -i\int_0^t \int_{\mathbb{R}^n} K_f(x, t; y, \tau)V(y, \tau)f(y, \tau)\, dyd\tau, \tag{V.30}$$

and the first-order approximation to the exact solution is,

$$\phi_1(t) = f(t) + \hat{Q}f(t) = f(t) - i\int_0^t \int_{\mathbb{R}^n} K_f(x, t; y, \tau)V(y, \tau)f(y, \tau)\, dyd\tau \tag{V.31}$$

Even though we have extra dimensions, specifically, the spatial dimensions, the partial sums still converge since the spatial linear integral is bounded in a Banach space $\mathcal{B}$, and the temporal integration has the Volterra property which makes it converge.

CHAPTER VI

VOLTERRA KERNELS AND SUCCESSIVE APPROXIMATIONS

In this section we will revisit the method of successive approximations. We assume that A is a bounded linear operator in a Banach space $\mathcal{B}$. Physicists are especially interested in Hilbert spaces which are special cases of Banach spaces because Hilbert spaces have applications in quantum mechanics. If the spectral radius of the integral operator $r(A)$ is less than 1, then we are guaranteed that the Neumann series converges in the operator norm. Theorems 6 and 7 are from Rainer Kress' book [2].

Theorem 6 *Let $A : \mathcal{B} \to \mathcal{B}$ be a bounded linear operator mapping a Banach space $\mathcal{B}$ into itself. Then the Neumann series*

$$(\lambda I - A)^{-1} = \sum_{k=0}^{\infty} \lambda^{-k-1} A^k \qquad (VI.1)$$

converges in the operator norm for all $|\lambda| > r(A)$ and diverges for all $|\lambda| < r(A)$.

Theorem 7 *Let $\hat{V} : \mathcal{B} \to \mathcal{B}$ be a bounded linear operator in a Banach space $\mathcal{B}$ with spectral radius $r(A) < 1$. Then the successive approximations*

$$\varphi_{n+1} = \hat{V}\varphi_n + f, \quad n = 0, 1, 2, \ldots \qquad (VI.2)$$

converge for each $f \in \mathcal{B}$ and each $\varphi_0 \in \mathcal{B}$ to the unique solution of $\varphi - \hat{V}\varphi = f$.

The following theorem will prove that the Volterra integral operator of the second kind has an spectral radius of zero. This theorem is not found in Rainer Kress' book *Integral Equations*. In this case, we assume that A is a bounded linear operator in a Banach space $\mathcal{B}$. If the spectral radius of the integral operator $r(A)$ is less than 1, then we are guaranteed that the Neumann series is a convergent series. However, the proof of the Volterra and General Volterra theorems will not use the spectral radius

to prove that the Neumann series converges. The Volterra operator is known to have a nice property, known as the simplex structure. It is the simplex structure which make the infinite Neumann series converge. It follows from the convergence of the Neumann series that the spectral radius is zero.

It is a well-known fact that most kernels $K(x, t; y, \tau)$ usually do not belong to a function space such as $L^{\infty,1}(I^2; \mathbb{R}^{2n})$. Therefore, the most natural conditions to impose are those of the sort assumed in the Generalized Young's inequality as stated by Folland [8]. In Chapter VII, we use the theorem in the form stated by Folland, but in this chapter, we need it in a generalized form such that it takes values in a Banach space. Examination of Folland's proof show that it extends to our generalized case. The following inequality theorem is mentioned in Gerald Folland's book *Introduction to Partial Differential Equations*. The Generalized Young's Inequality theorem can be found in the preliminary chapter of Folland's book [8].

Theorem 8 *(Generalized Young's Inequality) Let $\mathcal{B}$ be a Banach space. Suppose (X, μ) is a σ- finite measure space, and let $1 \leq p \leq \infty$ and $C > 0$. Furthermore assume that K is a measurable operator-valued function on $\Omega \times \Omega$ such that*

$$\int_\Omega \|K(x, y)\| \, d\mu(y) \leq C \qquad \text{(VI.3)}$$

where $\| \cdot \|$ denotes the norm of an operator mapping $\mathcal{B}$ into $\mathcal{B}$. If $f \in L^p(\Omega; \mathcal{B})$, the function $Af(x)$ defined by

$$Af(x) = \int_\Omega K(x, y) f(y) \, d\mu(y) \qquad \text{(VI.4)}$$

is well-defined almost everwhere and is in $L^p(\Omega; \mathcal{B})$, and $\|Af\|_{L^p(\Omega;\mathcal{B})} \leq C\|f\|_{L^p(\Omega;\mathcal{B})}$.

If the space operator $A(t, \tau)$ turns out to be a bounded Volterra operator, then it follows that the Volterra property will make the norm of A_n to be bounded by $\frac{1}{n!}$. In

other words, we obtain the following corollary:

Lemma 3 *Suppose $A(t,\tau)$ is a uniformly bounded operator. If $A(t,\tau)$ is also a Volterra kernel, then by mathematical induction, $\|A_n\|_{L^\infty(I^2;\mathcal{B})} \leq \|A\|_{L^\infty(I^2;\mathcal{B})}^n \dfrac{T^{n-1}}{(n-1)!}$, $\forall n \in \mathbb{N}$.*

Proof: Suppose $A(t,\tau)$ is a Volterra kernel, and $A_2(t,\tau)$

$$A_2(t,\tau) = \int_0^t A(t,\theta)A(\theta,\tau)\,d\theta \tag{VI.5}$$

then $A_2(t,\tau)$ is also a Volterra kernel. Therefore, we obtain the following L^∞ norm estimates:

$$\|A_2(t,\tau)\| \leq \int_0^t \|A(t,\theta)\|\,\|A(\theta,\tau)\|\,d\theta \leq \int_0^t \|A\|_{L^\infty(I^2;\mathcal{B})}^2\,d\theta = \|A\|_{L^\infty(I^2;\mathcal{B})}^2 t \tag{VI.6}$$

Then,

$$\|A_2\|_{L^\infty(I^2;\mathcal{B})} = \max_{(t,\tau)\in[0,T]^2} |\,\|A_2(t,\tau)\|\,| \leq \|A\|_{L^\infty(I^2;\mathcal{B})}^2 T \tag{VI.7}$$

We continue by mathematical induction: Assume $\|A_n\|_{L^\infty(I^2;\mathcal{B})} \leq \|A\|_{L^\infty(I^2;\mathcal{B})}^n \dfrac{T^{n-1}}{(n-1)!}$, $\forall n \in \mathbb{N}$. Then, we assume that the following inequality holds $\forall n \in \mathbb{N}$,

$$\|A_n(t,\tau)\| \leq \|A\|_{L^\infty(I^2;\mathcal{B})}^n \frac{t^{n-1}}{(n-1)!} \tag{VI.8}$$

Then,

$$\begin{aligned}
\|A_{n+1}(t,\tau)\| &\leq \int_0^t \|A(t,\theta)\|\|A_n(\theta,\tau)\|\,d\theta \leq \|A\|_{L^\infty(I^2;\mathcal{B})} \int_0^t \|A_n(\theta,\tau)\|\,d\theta \\
&\leq \|A\|_{L^\infty(I^2;\mathcal{B})}^{n+1} \int_0^t \frac{\theta^{n-1}}{(n-1)!}\,d\theta \\
&\leq \|A\|_{L^\infty(I^2;\mathcal{B})}^{n+1} \frac{t^n}{n!}
\end{aligned} \tag{VI.9}$$

and hence,

$$\|A_{n+1}\|_{L^\infty(I^2;\mathcal{B})} \leq \|A\|_{L^\infty(I^2;\mathcal{B})}^{n+1} \frac{T^n}{n!} \qquad \blacksquare \tag{VI.10}$$

The following theorem is the main theorem of the master thesis. And, it is also used in the examples of Chapter VII. The General Volterra Theorem is simply just a variant of the Volterra Theorem, i.e. it is the L^p-analogue.

Theorem 9 *(Volterra Theorem) Let the kernel $A(t, \tau)$ be a measurable and uniformly bounded linear operator such that $A : \mathcal{B} \to \mathcal{B}$ where $\mathcal{B}$ is a Banach space. Suppose that the kernel satisfies the following condition, $A(t, \tau) = 0$, when $\tau < t$. The Volterra integral operator, $\hat{Q} : L^\infty(I; \mathcal{B}) \to L^\infty(I; \mathcal{B})$, is defined by*

$$\hat{Q}\varphi(t) = \int_0^T A(t, \tau)\varphi(\tau)\, d\tau = \int_0^t A(t, \tau)\varphi(\tau)\, d\tau, \qquad \text{(VI.11)}$$

where $\varphi \in \mathcal{B}$. Then, the Volterra integral equation with the above kernel $A(t, \tau)$ can be solved by successive approximations. That is, the Neumann series converges in the topology of $L^\infty(I; \mathcal{B})$.

Proof: Let $\mathcal{H} = L^\infty(I; \mathcal{B})$ be the Banach space with norm $\| \cdot \|_{L^\infty(I;\mathcal{B})}$, where $I = (0, T)$. Suppose that the function $\phi : I \to L^\infty(I; \mathcal{B})$ is a bounded function with norm $\|\phi\|_{L^\infty(I;\mathcal{B})} = \sup_{\tau \in [0,T]} |\,\|\phi(\tau)\|\,|$. Thus there exists a number D such that

$$\|A(t, \tau)\|_{\mathcal{B} \to \mathcal{B}} \leq D < \infty \quad \forall (t, \tau) \in \bar{I}^2 \qquad \text{(VI.12)}$$

Furthermore, $A(t, \tau) = 0$ when $\tau < t$. Then $A(t, \tau)$ satisfies the hypothesis of the Generalized Young's Inequality with $C = Dt$. Thus, by Theorem 8, we have that $\|A\phi\|_{L^\infty(I;\mathcal{B})} \leq C\|\phi\|_{L^\infty(I;\mathcal{B})}$. Therefore, we obtain an estimate of the Volterra operator $\hat{Q}$ acting on the function $\phi(t)$,

$$\|\hat{Q}\phi(t)\| \leq \int_0^t \|A(t, \tau)\|\, \|\phi(\tau)\|\, d\tau \leq \|A\|_{L^\infty(I^2;\mathcal{B})}\|\phi\|_{L^\infty(I;\mathcal{B})} \int_0^t d\tau \leq \|A\|_{L^\infty(I^2;\mathcal{B})}\|\phi\|_{L^\infty(I;\mathcal{B})} t$$

$$\text{(VI.13)}$$

or,

$$\|\hat{Q}\phi\|_{L^\infty(I;\mathcal{B})} \leq \|A\|_{L^\infty(I^2;\mathcal{B})}\|\phi\|_{L^\infty(I;\mathcal{B})} T \qquad \text{(VI.14)}$$

where $\phi \in L^\infty(I; \mathcal{B})$. Then we try to solve the Volterra integral of the second kind via the Picard algorithm(successive approximations). The first term of the Neumann series is given by

$$\psi_1(t) = \hat{Q}\phi(t) = \int_0^t A(t, \tau)\phi(\tau)\, d\tau \tag{VI.15}$$

and the second term is given by

$$\psi_2(t) = \hat{Q}\psi_1(t) = \hat{Q}^2\phi(t) = \int_0^t A(t, \tau_1)\psi(\tau_1)\, d\tau_1 \tag{VI.16}$$

Then, we compute the bounded norm estimates for the second term of the Neumann series and we obtain

$$\|\psi_2(t)\| = \|\hat{Q}^2\phi(t)\| \leq \int_0^t \|A(t, \tau_1)\|\, \|\psi_1(\tau_1)\|\, d\tau_1 \leq \|A\|_{L^\infty(I^2;\mathcal{B})}^2 \|\phi\|_{L^\infty(I;\mathcal{B})} \int_0^t \tau_1\, d\tau_1$$
$$= \|A\|_{L^\infty(I^2;\mathcal{B})}^2 \|\phi\|_{L^\infty(I;\mathcal{B})} \frac{t^2}{2}$$

$$\tag{VI.17}$$

Thus we obtain using equation (VI.14) the following symplex structure with respect to the L^∞ norm estimate for the Volterra equation $\hat{Q}^2\phi(t)$:

$$\|\psi_2\|_{L^\infty(I;\mathcal{B})} \leq \|A\|_{L^\infty(I^2;\mathcal{B})}^2 \|\phi\|_{L^\infty(I;\mathcal{B})} \frac{T^2}{2} \tag{VI.18}$$

Then by mathematical induction, we see that the nth term of the Neumann series ψ_n gives the simplex structure:

$$\|\psi_n(t)\| \leq \|A\|_{L^\infty(I^2;\mathcal{B})}^n \|\phi\|_{L^\infty(I;\mathcal{B})} \frac{t^n}{n!} \tag{VI.19}$$

and hence,

$$\|\psi_n\|_{L^\infty(I;\mathcal{B})} \leq \|A\|_{L^\infty(I^2;\mathcal{B})}^n \|\phi\|_{L^\infty(I;\mathcal{B})} \frac{T^n}{n!} \tag{VI.20}$$

Therefore the series $\sum_{n=0}^{\infty} \psi_n$ is majorized by

$$\|\phi\|_{L^\infty(I;\mathcal{B})} + \|\phi\|_{L^\infty(I;\mathcal{B})} \sum_{n=1}^{\infty} \|A\|_{L^\infty(I^2;\mathcal{B})}^n \frac{T^n}{n!} = \|\phi\|_{L^\infty(I;\mathcal{B})} \sum_{n=0}^{\infty} \|A\|_{L^\infty(I^2;\mathcal{B})}^n \frac{T^n}{n!}$$

$$= \|\phi\|_{L^\infty(I;\mathcal{B})} e^{\|A\|_{L^\infty(I^2;\mathcal{B})} T} \quad \text{(VI.21)}$$

Therefore, the Neumann series converges in the topology of $L^\infty(I;\mathcal{B})$. ■

Theorem 10 *(General Volterra Theorem) Let the kernel $A(t,\tau)$ be a measurable and uniformly bounded linear operator such that $A : \mathcal{B} \to \mathcal{B}$ where $\mathcal{B}$ is a Banach space. Suppose that the kernel satisfies the following condition, $A(t,\tau) = 0$, when $\tau < t$. The Volterra integral operator, $\hat{Q} : L^p(I;\mathcal{B}) \to L^p(I;\mathcal{B})$, is defined by*

$$\hat{Q}\varphi(t) = \int_0^T A(t,\tau)\varphi(\tau)\,d\tau = \int_0^t A(t,\tau)\varphi(\tau)\,d\tau, \quad \text{(VI.22)}$$

where $\varphi \in \mathcal{B}$ and $1 \le p < \infty$. Then, the Volterra integral equation with the above kernel $A(t,\tau)$ can be solved by successive approximations. That is, the Neumann series converges in the topology of $L^p(I;\mathcal{B})$.

Proof: Let $\mathcal{H} = L^p(I;\mathcal{B})$ be the Banach space with norm $\|\cdot\|_{L^p(I;\mathcal{B})}$ and where $I = (0,T)$. Suppose that the function $\psi : I \to L^p(I;\mathcal{B})$, is a bounded function with norm

$$\|\psi\|_{L^p(I;\mathcal{B})} = \left(\int_0^t \|\psi(\tau)\|^p \,d\tau \right)^{1/p}, \quad \text{(VI.23)}$$

and where $1 \le p < \infty$. Define the Volterra integral operator in the following way,

$$\hat{Q}\phi(t) = \int_0^t A(t,\tau)\phi(\tau)\,d\tau, \quad \text{(VI.24)}$$

where $\varphi \in \mathcal{B}$. Let $A : \mathcal{B} \to \mathcal{B}$ be a measurable and uniformly bounded operator. Thus there exists a number D such that

$$\|A(t,\tau)\|_{\mathcal{B}\to\mathcal{B}} \le D < \infty \quad \forall (t,\tau) \in \bar{I}^2 \quad \text{(VI.25)}$$

Furthermore, $A(t, \tau) = 0$ when $\tau < t$. Then $A(t, \tau)$ satisfies the hypothesis of the Generalized Young's Inequality with $C = Dt$. Thus, by Theorem 8, we have that $\|A\phi\|_{L^p(I;\mathcal{B})} \leq C\|\phi\|_{L^p(I;\mathcal{B})}$. Therefore, we obtain an estimate of the Volterra operator $\hat{Q}$ acting on ϕ, and by the Generalized Young's inequality, we have

$$\|\hat{Q}\phi\|_{L^p(I;\mathcal{B})} \leq \int_0^t \|A\phi\|_{L^p(I;\mathcal{B})} \, d\tau \leq C\|\phi\|_{L^p(I;\mathcal{B})} \int_0^t d\tau = C\|\phi\|_{L^p(I;\mathcal{B})} t \qquad \text{(VI.26)}$$

We want to show that the series $\psi = \sum_{j=0}^{\infty} \psi_j$ where

$$\psi_j \equiv \hat{Q}^j \phi. \qquad \text{(VI.27)}$$

converges with respect to the norm $\|\cdot\|_{L^p}$. Then, we compute L^p-L^∞ norm estimates for the following equation:

$$\begin{aligned} \|\psi_2\|_{L^p(I;\mathcal{B})} &\leq \int_0^t \|A\psi_1\|_{L^p(I;\mathcal{B})} \, d\tau_1 \leq \int_0^t C\|\psi_1\|_{L^p(I;\mathcal{B})} \, d\tau_1 \\ &\leq C^2\|\phi\|_{L^p(I;\mathcal{B})} \int_0^t \tau_1 \, d\tau_1 = C^2\|\phi\|_{L^p(I;\mathcal{B})} \frac{t^2}{2} \end{aligned} \qquad \text{(VI.28)}$$

Then by mathematical induction: $\psi_n = \hat{Q}\psi_{n-1} = \hat{Q}^n \phi$ implies

$$\|\psi_n\|_{L^p(I;\mathcal{B})} \leq C^n\|\phi\|_{L^p(I;\mathcal{B})} \frac{t^n}{n} \qquad \text{(VI.29)}$$

Thus the series $\sum_{n=0}^{\infty} \psi_n$ is majorized by

$$\|\phi\|_{L^p(I;\mathcal{B})} + \|\phi\|_{L^p(I;\mathcal{B})} \sum_{n=1}^{\infty} C^n \frac{t^n}{n} = \|\phi\|_{L^p(I;\mathcal{B})} e^{Ct} \qquad \text{(VI.30)}$$

Therefore, the Neumann series converges with respect to the topology $L^p(I; \mathcal{B})$. ∎

Next, we give a formal definition of the spectral radius. The following definition of the spectral radius can be found in Chapter III of Kress' book [2].

Definition 6 *Let $A : X \to X$ be a bounded linear operator on a normed space X. A complex number λ is called an eigenvalue of A if there exists an element $\varphi \in X$,*

$\varphi \neq 0$, such that $A\varphi = \lambda\varphi$. The element φ is called an eigenelement of A. A complex number λ is called a regular value of A if $(\lambda I - A)^{-1} : X \to X$ exists and is bounded. The set of all regular values of A is called the resolvent set $\rho(A)$ and $R(\lambda; A) := (\lambda I - A)^{-1}$ is called the resolvent of A. The complement of $\rho(A)$ in $\mathbb{C}$ is called the spectrum $\sigma(A)$ and

$$r(A) := \sup_{\lambda \in \sigma(A)} |\lambda| \tag{VI.31}$$

is called the spectral radius of A.

Now, we can prove that the spectral radius of the Volterra operator is equal to zero.

Theorem 11 *Suppose A is a Volterra integral operator from X to itself, where X is a normed space. If the resolvent $(\lambda I - A)^{-1}$ exists and is bounded, then the spectral radius $r(A)$ is equal to 0.*

Proof: Suppose the Volterra operator $A : X \to X$ is a bounded integral operator, where X is a normed space. Assume that the resolvent $R(\lambda; A)$ exists and is bounded. For the Volterra operator, the resolvent $R(\lambda; A)$ exists and is bounded for all $\lambda \neq 0$. Thus, the resolvent set $\rho(A) = \{\forall \lambda \neq 0 | \lambda$ is a regular value of $A\}$. Then, the spectrum $\sigma(A)$ is the complement of the resolvent set and is given by

$$\sigma(A) = \mathbb{R} \backslash \rho(A) = 0 \tag{VI.32}$$

Then, by the definition of the spectral radius, we have $r(A) = \sup_{\lambda \in \sigma(A)} |\lambda| = 0$. ∎

CHAPTER VII

APPLICATIONS OF THE VOLTERRA THEOREM

In this section, we apply the Volterra and General Volterra Theorems to four different types of kernels, the Hilber-Schmidt kernel, the L^1 and L^∞ kernels, and the Schrödinger kernel. In this section, we will present several different types of applications of theorems 9 and 10. The first three examples are classical and example 4 is the unitary quantum-mechanical example. The closest example to quantum mechanics is example 4 where the spatial operator is a unitary operator. Each example presents two versions, corresponding to the Volterra and General Volterra theorems, respectively.

Let I be an interval in the temporal dimension, and let $L^{n,m}(I; \mathbb{R}^d)$ be the Banach space of $L^m(\mathbb{R}^d)$ functions over I. Thus we will denote the Lebesgue space $L^{n,m}(I; \mathbb{R}^d)$ as the following

$$L^{n,m}(I; \mathbb{R}^d) = \left\{ \phi : \left(\int_I \left[\int_{\mathbb{R}^d} |\phi(y, \tau)|^m \, dy \right]^{n/m} d\tau \right)^{1/n} = \|\phi\|_{L^{n,m}(I;\mathbb{R}^d)} < \infty \right\}.$$

(VII.1)

If m and n are equal, then the Lebesgue space $L^{n,m}(I; \mathbb{R}^d)$ will be written as $L^n(I; \mathbb{R}^d)$.

A. Example 1

Let the Banach space $\mathcal{B}$ be $L^\infty(\mathbb{R}^n)$ and let $K(x, t; y, \tau)$ be a bounded integrable (e.g., continuous) real or complex-valued kernel, satisfying the Volterra condition in (t, τ). Let the Lebesgue space L^p in time be $L^\infty(I)$. Define the Volterra kernel acting on ϕ by

$$A(t, \tau)\phi(t) = \int_{\mathbb{R}^n} K(x, t; y, \tau)\phi(y, \tau) \, dy$$

(VII.2)

where $\phi(x,t) \in L^\infty(I; \mathbb{R}^n)$. Then

$$
\begin{aligned}
|A(t,\tau)\phi(t)| &\leq \int_{\mathbb{R}^n} |K(x,t;y,\tau)||\phi(y,\tau)|\, dy \\
&\leq \|\phi\|_{L^\infty(I;\mathbb{R}^n)} \int_{\mathbb{R}^n} |K(x,t;y,\tau)|\, dy
\end{aligned}
\tag{VII.3}
$$

and by the Generalized Young's Inequality theorem, we obtain the following result:

$$
\|A(t,\tau)\phi(t)\|_{L^\infty(\mathbb{R}^n)} \leq C\|\phi\|_{L^\infty(I;\mathbb{R}^n)}
\tag{VII.4}
$$

where

$$
\int_{\mathbb{R}^n} |K(x,t;y,\tau)|\, dy \leq C
\tag{VII.5}
$$

and hence,

$$
\|\psi\|_{L^\infty(I;\mathbb{R}^n)} \leq C\|\phi\|_{L^\infty(I;\mathbb{R}^n)} t
\tag{VII.6}
$$

Thus we have verified all the hypothesis of Theorem 9, and we conclude that that the solution φ is given by the Neumann series $\varphi = \sum_{n=0}^{\infty} \psi_n$. Hence by the Volterra Theorem, the Volterra integral equation with a linear bounded operator $A(t,\tau)$ and with a bounded integrable kernel $K(x,t;y,\tau)$ can be solved by successive approximations.

Let the Banach space $\mathcal{B}$ be $L^\infty(\mathbb{R}^n)$ and let $K(x,t;y,\tau)$ be a bounded integrable (e.g., continuous) real or complex-valued kernel, satisfying the Volterra condition in (t,τ). Suppose the Lebesgue space L^p in time is taken to be $L^1(I)$. Define Volterra kernel acting on ϕ by

$$
A(t,\tau)\phi(t) = \int_{\mathbb{R}^n} K(x,t;y,\tau)\phi(y,\tau)\, dy
\tag{VII.7}
$$

where $\phi(x,t) \in L^{1,\infty}(I;\mathbb{R}^n)$. Then

$$
\begin{aligned}
|A(t,\tau)\phi(t)| &\leq \int_{\mathbb{R}^n} |K(x,t;y,\tau)||\phi(y,\tau)|\, dy \\
&\leq \|\phi\|_{L^\infty(I;\mathbb{R}^n)} \int_{\mathbb{R}^n} |K(x,t;y,\tau)|\, dy
\end{aligned}
\tag{VII.8}
$$

and by the Generalized Young's Inequality theorem, we obtain the following result:

$$\|A(t,\tau)\phi(t)\|_{L^\infty(\mathbb{R}^n)} \leq C\|\phi(\tau)\|_{L^\infty(\mathbb{R}^n)} \tag{VII.9}$$

where

$$\int_{\mathbb{R}^n} |K(x,t;y,\tau)|\, dy \leq C \tag{VII.10}$$

and hence,

$$\|A\phi\|_{L^{1,\infty}(\mathbb{R}^n)} \leq C\|\phi\|_{L^{1,\infty}(\mathbb{R}^n)} \tag{VII.11}$$

Hence by the General Volterra Theorem, the Volterra integral equation with a linear bounded operator $A(t,\tau)$ and with a bounded integrable kernel $K(x,t;y,\tau)$ can be solved by successive approximations.

B.   Example 2

Let the Banach space $\mathcal{B}$ be $L^1(\mathbb{R}^n)$ and let $K(x,t;y,\tau)$ be a bounded integrable (e.g., continuous) real or complex-valued kernel, satisfying the Volterra condition in (t,τ). Define the Volterra operator $\hat{Q}$ acting on ϕ by

$$\psi(t) = \hat{Q}\phi(t) = \int_0^t \int_{\mathbb{R}^n} K(x,t;y,\tau)\phi(y,\tau)\, dy d\tau, \tag{VII.12}$$

where $\phi(x,t) \in L^{\infty,1}(I;\mathbb{R}^n)$. Then the bounded operator $A(t,\tau)$, acting on $\phi \in L^1(\mathbb{R}^n)$, is defined by

$$A(t,\tau)\phi(t) = \int_{\mathbb{R}^n} K(x,t;y,\tau)\phi(y,\tau)\, dy \tag{VII.13}$$

Then, we take the absolute value of the linear operator $A(t,\tau)$ operating on the function ϕ, and this gives

$$|A(t,\tau)\phi(t)| \leq \int_{\mathbb{R}^n} |K(x,t;y,\tau)||\phi(y,\tau)|\, dy \tag{VII.14}$$

and by the Generalized Young's Inequality Theorem, we obtain the following norm estimate

$$\|A(t,\tau)\phi(t)\|_{L^1(\mathbb{R}^n)} \leq C\|\phi(\tau)\|_{L^1(\mathbb{R}^n)} \qquad \text{(VII.15)}$$

where,

$$\int_{\mathbb{R}^n} |K(x,t;y,\tau)|\,dx \leq C \qquad \text{(VII.16)}$$

Therefore by the General Volterra Theorem, the Volterra integral equation with a linear bounded operator $A(t,\tau)$ and with a bounded integrable kernel $K(x,t;y,\tau)$ can be solved by successive approximations.

Let the Banach space $\mathcal{B}$ be $L^1(\mathbb{R}^n)$ and let $K(x,t;y,\tau)$ be a bounded integrable (e.g., continuous) real or complex-valued kernel, satisfying the Volterra condition in (t,τ). Let the Lebesgue space L^p be $L^1(I)$. Define the function ψ as

$$\psi(t) = \hat{Q}\phi(t) = \int_0^t \int_{\mathbb{R}^n} K(x,t;y,\tau)\phi(y,\tau)\,dy d\tau, \qquad \text{(VII.17)}$$

where $\phi(x,t) \in L^1(I;\mathbb{R}^n)$. Then the bounded operator $A(t,\tau)$, acting on $\phi \in L^1(\mathbb{R}^n)$, is defined by

$$A(t,\tau)\phi(t) = \int_{\mathbb{R}^n} K(x,t;y,\tau)\phi(y,\tau)\,dy \qquad \text{(VII.18)}$$

Then, we take the absolute value of the linear operator $A(t,\tau)$ operating on the function ϕ, and this gives

$$|A(t,\tau)\phi(t)| \leq \int_{\mathbb{R}^n} |K(x,t;y,\tau)||\phi(y,\tau)|\,dy \qquad \text{(VII.19)}$$

and by the Generalized Young's Inequality Theorem, we obtain the following norm estimate

$$\|A(t,\tau)\phi(t)\|_{L^1(\mathbb{R}^n)} \leq C\|\phi(\tau)\|_{L^1(\mathbb{R}^n)} \qquad \text{(VII.20)}$$

where,

$$\int_{\mathbb{R}^n} |K(x,t;y,\tau)|\, dx \leq C \tag{VII.21}$$

Then we take the L^1 with respect to time of inequality (VII.20) and we obtain

$$\|A\phi\|_{L^1(I;\mathbb{R}^n)} \leq C\|\phi\|_{L^1(I;\mathbb{R}^n)} \tag{VII.22}$$

Thus we have verified all the hypotheses of the General Volterra Theorem, and we conclude that that the solution φ is given by the Neumann series $\varphi = \sum_{n=0}^{\infty} \psi_n$.

C.   Example 3

Let the Banach space $\mathcal{B}$ be $L^2(\mathbb{R}^n)$ and consider a bounded integrable (e.g., continuous) real or complex-valued kernel $A(t,\tau)$, satisfying the Volterra condition in (t,τ). The Hilbert-Schmidt kernel is a function $K : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{F}$ on the space variables, where $\mathbb{F} = \{\mathbb{C}, \mathbb{R}\}$. The norm of the Hilbert-Schmidt kernel is given by

$$\left(\int_{\mathbb{R}^n \times \mathbb{R}^n} |K(x,t;y,\tau)|^2\, dxdy\right)^{1/2} = \|K(t,\tau)\|_{L^2(\mathbb{R}^{2n})} \leq N < \infty \tag{VII.23}$$

The linear operator $A(t,\tau)$ is defined on $L^\infty(I^2)$, and $A(t,\tau)$ is a Hilbert-Schmidt operator. Then the Hilbert- Schmidt operator $A(t,\tau) : L^2(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$ is given by

$$A(t,\tau)\phi(t) = \int_{\mathbb{R}^n} K(x,t;y,\tau)\phi(y,\tau)\, dy \quad \forall \phi \in L^{\infty,2}(I;\mathbb{R}^n) \tag{VII.24}$$

It follows that the operator $A(t,\tau)$ is bounded. The function $K(x,t;y,\tau)$ belongs to $L^{\infty,2}(I^2;\mathbb{R}^{2n})$. Then we take the absolute values of $A(t,\tau)\phi(t)$ and we obtain

$$\begin{aligned}
|A(t,\tau)\phi(t)| &\leq \int_{\mathbb{R}^n} |K(x,t;y,\tau)||\phi(y,\tau)|dy \\
&\leq \left(\int_{\mathbb{R}^n} |K(x,t;y,\tau)|^2 dy\right)^{1/2} \left(\int_{\mathbb{R}^n} |\phi(y,\tau)|^2 dy\right)^{1/2}
\end{aligned} \tag{VII.25}$$

and hence,

$$\|A(t,\tau)\phi(t)\|_{L^2(\mathbb{R}^n)} \leq \|K(t,\tau)\|_{L^2(\mathbb{R}^{2n})}\|\phi(\tau)\|_{L^2(\mathbb{R}^n)} \leq N\|\phi(\tau)\|_{L^2(\mathbb{R}^n)} \qquad \text{(VII.26)}$$

and where,

$$N \equiv \|K\|_{L^{\infty,2}(I^2;\mathbb{R}^{2n})} \qquad \text{(VII.27)}$$

Therefore by the General Volterra Theorem, the Volterra integral equation with a Hilbert-Schmidt kernel $K(x,t;y,\tau) \in L^{\infty,2}(I^2;\mathbb{R}^n)$ can be solved by successive approximations.

Let $\mathcal{H}$ be $L^2(\mathbb{R}^n)$ and consider a bounded integrable (e.g., continuous) real or complex-valued kernel $K(x,t;y,\tau)$, satisfying the Volterra condition in (t,τ). Suppose the Lebesgue space in time is $L^2(I)$. The linear operator $K(x,t;y,\tau)$ is defined on $L^2(\mathbb{R}^{2n})$, and A is a Hilbert-Schmidt operator on the (x,y) variables. Then the Hilbert- Schmidt operator $A(t,\tau)$ is given by

$$A(t,\tau)\phi(t) = \int_{\mathbb{R}^n} K(x,t;y,\tau)\phi(y,\tau)\,dy \quad \forall \phi \in L^2(I;\mathbb{R}^n) \qquad \text{(VII.28)}$$

It follows that the operator $A(t,\tau)$ is bounded. The Hilbert-Schmidt kernel is a function $K : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{F}$ with an L^2 norm in the (x,y) variables defined as

$$\left(\int_{\mathbb{R}^n}\int_{\mathbb{R}^n} |K(x,t;y,\tau)|^2\,dy dx\right)^{1/2} = \|K(t,\tau)\|_{L^2(\mathbb{R}^{2n})} \qquad \text{(VII.29)}$$

Therefore, the function $K(x,t;y,\tau)\phi(x,t)$ belongs to $L^2(\mathbb{R}^{2n})$. Hence,

$$\begin{aligned} |A(t,\tau)\phi(t)| &\leq \int_{\mathbb{R}^n} |K(x,t;y,\tau)||\phi(y,\tau)|\,dy \\ &\leq \left(\int_{\mathbb{R}^n} |K(x,t;y,\tau)|^2\,dy\right)^{1/2}\left(\int_{\mathbb{R}^n} |\phi(y,\tau)|^2\,dy\right)^{1/2} \end{aligned} \qquad \text{(VII.30)}$$

or,

$$|A(t,\tau)\phi(t)|^2 \leq \left(\int_{\mathbb{R}^n} |K(x,t;y,\tau)|^2 \, dy\right)\left(\int_{\mathbb{R}^n} |\phi(y,\tau)|^2 \, dy\right) \qquad \text{(VII.31)}$$

and hence,

$$\|A(t,\tau)\phi(t)\|_{L^2(\mathbb{R}^n)}^2 \leq \left(\int_{\mathbb{R}^n}\int_{\mathbb{R}^n} |K(x,t;y,\tau)|^2 \, dydx\right)\left(\int_{\mathbb{R}^n} |\phi(y,\tau)|^2 \, dy\right)$$
$$= \|K(t,\tau)\|_{L^2(\mathbb{R}^{2n})}^2 \|\phi(\tau)\|_{L^2(\mathbb{R}^n)}^2 \qquad \text{(VII.32)}$$

Thus,

$$\|A(t,\tau)\phi(t)\|_{L^2(\mathbb{R}^n)} \leq \|K\|_{L^{\infty,2}(I^2;\mathbb{R}^{2n})}\|\phi(\tau)\|_{L^2(\mathbb{R}^n)} \qquad \text{(VII.33)}$$

and hence,

$$\|A\phi\|_{L^2(I;\mathbb{R}^n)} \leq \|K\|_{L^{\infty,2}(I^2;\mathbb{R}^{2n})}\|\phi\|_{L^2(I;\mathbb{R}^n)} \qquad \text{(VII.34)}$$

Thus, we have shown that the norm of $A(t,\tau)\phi(t)$ is bounded, and hence

$$\|\psi\|_{L^2(I;\mathbb{R}^n)} \leq \|K\|_{L^{\infty,2}(I^2;\mathbb{R}^{2n})}\|\phi\|_{L^2(I;\mathbb{R}^n)}t \qquad \text{(VII.35)}$$

Therefore by the General Volterra Theorem, the Volterra integral equation with a Hilbert-Schmidt kernel in space and a uniformly bounded kernel in time can be solved by successive approximations.

D. Example 4

Let $V(x,t)$ be a bounded potential, and $x \in \mathbb{R}^n$. The potential V may be time-dependent, but in that case its bound should be independent of t (i.e., $V \in L^\infty(I;\mathbb{R}^n)$, with $\|V\|_{L^\infty(I;\mathbb{R}^n)} \equiv C$). Let the Banach space $\mathcal{B}$ be the Hilbert space $L^2(\mathbb{R}^n)$. Recall that $u(t) \equiv U_f(t,\tau)h = K_f * h$, where $K_f(x,t;y,0) = (4\pi it)^{-n/2}e^{i|x-y|^2/4t}$, is the solution of the free Schrödinger equation with initial data $u(x,0) = h(x)$ in $L^2(\mathbb{R}^n)$.

Remark: A unitary operator is a linear transformation $U : \mathcal{H}_1 \to \mathcal{H}_2$ that is a surjective isometry. In other words a unitary operator is an isomorphism whose

range coincides with its domain. Also, a unitary operator between metric spaces is a map that preserves the norm. The following is a modified definition from John B. Conway's book *A Course in Functional Analysis* [4].

Definition 7 *If $\mathcal{H}_1$ and $\mathcal{H}_2$ are Hilbert spaces, an isomorphism between $\mathcal{H}_1$ and $\mathcal{H}_2$ is a linear surjection $U : \mathcal{H}_1 \to \mathcal{H}_2$ such that*

$$\langle Uh, Ug \rangle = \langle h, g \rangle \tag{VII.36}$$

$\forall h, g \in \mathcal{H}_1$. *In this case $\mathcal{H}_1$ and $\mathcal{H}_2$ are said to be isomorphic.*

It is well known that $U_f(t, \tau)$ is a unitary operator, and hence the norm of U_f as an operator from $\mathcal{H}$ to itself is $\|U_f(t, \tau)\|_{L^2(\mathbb{R}^{2n})} = 1$. A proof that the operator $U_f(t, \tau)$ is a unitary operator can be found on Chapter 4 of Evans's book [5]. We wish to solve the Schödinger equation with the potential V by iteration. The equivalent integral equation is equation (V.8). However, the kernel is not of the type studied in Example 2 (or 1). Because of the structure of equation (V.8), the operator is effectively Volterra. Hence, the Volterra theorem applies.

In theorem 9, take $\mathcal{B} = \mathcal{H}$, $A = UV$ as defined in equation (V.9). It remains to check that UV is a bounded operator on $\mathcal{H}$ with bound independent of t and τ. Here $V(\tau)$ is the operator from $\mathcal{H}$ to $\mathcal{H}$ defined by multiplication of $f(y, \tau)$ by $V(y, \tau)$, and $\|V(\tau)\|$ is its norm. But

$$\|V(\tau)f(\tau)\|_{L^2(\mathbb{R}^n)}^2 = \int_{\mathbb{R}^n} |V(y, \tau)f(y, \tau)|^2 \, dy \leq C^2 \int_{\mathbb{R}^n} |f(y, \tau)|^2 \, dy = C^2 \|f(\tau)\|_{L^2(\mathbb{R}^n)}^2. \tag{VII.37}$$

Therefore,

$$\|V(\tau)f(\tau)\|_{L^2(\mathbb{R}^n)} \leq C \|f(\tau)\|_{L^2(\mathbb{R}^n)} \quad \forall f \in \mathcal{H}. \tag{VII.38}$$

In other words $\|V\|_{L^\infty(I;\mathbb{R}^n)}$, the norm of the operator $V(\tau) \leq C \equiv \|V\|_{L^\infty(I;\mathbb{R}^n)}$, is the

uniform norm of the function $V(x,t)$. Therefore,

$$\|U(t,\tau)V(\tau)f(\tau)\|_{L^2(\mathbb{R}^n)} \leq C\|f(\tau)\|_{L^2(\mathbb{R}^n)}. \tag{VII.39}$$

and the operator norm of $A = UV$ is bounded by $\|U(t,\tau)V(\tau)\|_{L^2(\mathbb{R}^n)} \leq C$. Then,

$$A(t,\tau)f(\tau) = \int_{\mathbb{R}^n} K(x,t;y,\tau)f(y,\tau)\,dy = \int_{\mathbb{R}^n} K_f(x,t;y,\tau)V(y,\tau)f(y,\tau)\,dy \tag{VII.40}$$

Therefore, we obtain the following $L^{2,\infty}$ norm estimates for $\hat{Q}f = SVf$

$$\|\psi\|_{L^{\infty,2}(I;\mathbb{R}^n)} = \|SVf\|_{L^{\infty,2}(I;\mathbb{R}^n)} \leq C\|f\|_{L^{\infty,2}(I;\mathbb{R}^n)}T \tag{VII.41}$$

where,

$$\psi(t) = SVf(t) = \int_0^t U(t,\tau)V(\tau)f(\tau)\,d\tau \tag{VII.42}$$

Thus we have verified all the hypotheses of Theorem 9, and we conclude that the solution of the Schrödinger equation with potential V is the series $\varphi = \sum_{n=0}^{\infty} \psi_n$, where $\psi_0(t) = f(t) = \hat{U}(t,\tau)h(x)$, and where $h(x)$ is the initial data.

Let $V(x,t)$ be a bounded potential, and $x \in \mathbb{R}^n$. The potential V may be time-dependent, but in that case its bound should be independent of t(i.e., $V \in L^\infty(I;\mathbb{R}^n)$, with $\|V\|_{L^\infty(I;\mathbb{R}^n)} \equiv C$). Let the Banach space $\mathcal{B}$ be the Hilbert space $L^2(\mathbb{R}^n)$. Suppose the Lebesgue space in time is also the Hilbert space $L^2(I)$. In the first example in Example 4, the norm of the potential function V and f is shown to be bounded and the inequality is given by

$$\|V(\tau)f(\tau)\|_{L^2(\mathbb{R}^n)} \leq C\|f(\tau)\|_{L^2(\mathbb{R}^n)} \quad \forall f \in \mathcal{H}. \tag{VII.43}$$

Then, we take the L^2 norm with respect to the time variable and we obtain

$$\|Vf\|_{L^2(I;\mathbb{R}^n)} \leq C\|f\|_{L^2(I;\mathbb{R}^n)} \tag{VII.44}$$

Also, the operator $A = UV$ is shown to be bounded by $\|UV\|_{L^2(\mathbb{R}^n)} \leq C$. Thus, we have shown that the norm of Vf is bounded, and hence

$$\|\psi\|_{L^2(I;\mathbb{R}^n)} \leq C\|f\|_{L^2(I;\mathbb{R}^n)}t \qquad \text{(VII.45)}$$

Therefore by the General Volterra Theorem, the Volterra integral equation with a unitary operator in space can be solved by successive approximations.

CHAPTER VIII

HAMILTON-JACOBI EQUATION AND CLASSICAL PATHS

In this chapter, the semiclassical Neumann series will be shown to have norm convergence. In other words, a semiclassical propagator $G_{scl}(x, t; y, \tau)$ will be used to construct the full quantum Green function. Then, we use the results from section V and VI to conclude that the successive method of approximations can used to obtain a solution to the semiclassical Volterra integral equation.

Let us consider the case of a quantum particle subject to a bounded potential $V(x, t)$. Then the wave function of the particle can be written as

$$\psi(x, t) = A(x, t) e^{\frac{i}{\hbar} S(x,t)} \tag{VIII.1}$$

where $A(x, t)$ and $S(x, t)$ are the amplitude and the action of $\psi(x, t)$, respectively. Then, we substitute equation (VIII.1) into the time-dependent Schrödinger equation, and we obtain the following partial-differential equation,

$$0 = A\left[\frac{\partial S}{\partial t} + \frac{1}{2m}(\nabla S)^2 + V\right] - i\hbar\left[\frac{\partial A}{\partial t} + \frac{1}{m}(\nabla A \cdot \nabla S) + \frac{1}{2m}A\Delta S\right] - \frac{\hbar^2}{2m}\Delta A \tag{VIII.2}$$

where Δ is the Laplacian operator. The classical limit is obtained by taking the limit $\hbar \to 0$. Then, we separate the real and imaginary parts of the above equation, and we get

$$\frac{\partial S}{\partial t} + \frac{1}{2m}(\nabla S)^2 + V = \frac{\hbar^2}{2m}\frac{\Delta A}{A} \tag{VIII.3}$$

and,

$$m\frac{\partial A}{\partial t} + (\nabla A \cdot \nabla S) + \frac{1}{2}A\Delta S = 0 \tag{VIII.4}$$

Then, if we take the limit of $\hbar \to 0$, equation (VIII.3) becomes

$$\frac{\partial S}{\partial t} + \frac{1}{2m}(\nabla S)^2 + V(x, t) = 0 \tag{VIII.5}$$

and this equation is the Hamilton-Jacobi equation. In this case, the phase $S(x,t)$ is interpreted as the classical action. Another assumption we make is that there exists a local curve $x(t)$ which satisfies the following equations

$$\frac{dx(t)}{dt} = \frac{\partial H}{\partial p} = \frac{1}{m}\nabla S(x(t),t) \tag{VIII.6}$$

and,

$$\frac{dp(t)}{dt} = -\frac{\partial H}{\partial x} \tag{VIII.7}$$

or,

$$p(t) = m\frac{dx(t)}{dt} = \nabla S(x(t),t). \tag{VIII.8}$$

and where $H(x,\nabla S,t)$ is the classical Hamiltonian function. The classical Hamiltonian function is defined by $H(x,p,t) = \frac{p^2}{2} + V(x,t)$. Equation (VIII.6) enables one to construct the action $S(x,t)$ from a knowledge of the classical solutions $x(t)$. Then, we take the total time derivative of the action, and we obtain

$$\frac{dS}{dt} = \frac{\partial S}{\partial t} + \dot{x} \cdot \nabla S = -H + \dot{x} \cdot p \equiv L(x(t), \dot{x}(t)) \tag{VIII.9}$$

This equation implies that we can get solutions of the Hamilton-Jacobi equation by integrating the Lagrangian L along the trajectories. Thus, the action S can be defined by

$$S(x,y,t) = \int_0^t L(x(u), \dot{x}(u)) \, du + S_0 \tag{VIII.10}$$

where S_0 is initial data, and then $S(x,y,t)$ solves the Hamilton-Jacobi equation. Also if there exists a local solution of the Hamilton-Jacobi equation, then it will satisfy the following partial differential equation

$$\frac{\partial S}{\partial t} + H(x, \nabla S(x,t), t) = 0 \tag{VIII.11}$$

In the following calculations we make use of the semiclassical Green's function by using

some results from *Semiclassical Phyiscs* by Matthias Brack and Rajat K. Bhaduri [10]. It is in a similar fashion that we present the convergence of the semiclassical approximation. An interesting property of the quantum propagator $G(x, t; y, 0)$ is that it satisfies the following equation

$$G(x, t; y, 0) = \int_{\mathbb{R}^3} G(x, t; r, \tau) G(r, \tau; y, 0) \, dr \qquad \text{(VIII.12)}$$

In other words the quantum propagator describes the motion of a quantum-mechanical particle travelling from the space-time point $(y, 0)$ to (x, t) and can be interpreted as passing through all possible intermediate points (r, τ). The Green function $G(x, t; y, 0)$ satisfies the homogeneous Schrödinger equation in the variables (x, t), except at the source point $(y, 0)$. In this article we are considering a potential $V(x, t) \in C^\infty(\mathbb{R}^3 \times \mathbb{R})$, and thus in a local space-time region the particle evolves under the semiclassical propagator between encounters with $\frac{\Delta A}{A}$. It is this basic concept which underlies the theory of this semiclassical approximation. The free propagator $K_f(x, t; y, 0)$ in the space-time $\mathbb{R}^n \times \mathbb{R}^+$ is the following function,

$$K_f(x, t; y, 0) = \left(\frac{m}{2\pi i \hbar t}\right)^{n/2} e^{im|x-y|^2/2\hbar t} \qquad \text{(VIII.13)}$$

The exponent in $K_f(x, y, t)$ is basically the action $S_0(x, y, t)$ times $\frac{i}{\hbar}$ for a free particle. Then the determinant of the negative second partial derivatives of $S_0(x, y, t)$ is

$$\det\left(-\frac{\partial^2 S_0}{\partial x_i \partial y_j}\right) = \left(\frac{m}{t}\right)^n \qquad \text{(VIII.14)}$$

Then the quantum free propagator in $\mathbb{R}^n \times \mathbb{R}^+$ can be written in the following manner:

$$K_f(x, t; y, 0) = A_0(t) e^{\frac{i}{\hbar} S_0(x, y, t)} = \left(\frac{1}{2\pi i \hbar}\right)^{n/2} \sqrt{\det\left(-\frac{\partial^2 S_0}{\partial x_i \partial y_j}\right)} \exp\left\{\frac{i}{\hbar} S_0(x, y, t)\right\}$$
$$\text{(VIII.15)}$$

Similarly, we can write a semiclassical propagator $G_{scl}(x, t; y, 0)$ in the following man-

ner:

$$G_{scl}(x, t; y, 0) = (2\pi i\hbar)^{-n/2}\sqrt{\det C}\, e^{iS/\hbar} \qquad\qquad \text{(VIII.16)}$$

where C is an $n \times n$ matrix, and its elements are $C_{ij} = -\frac{\partial^2 S}{\partial x_i \partial y_j}$. Also, $\sqrt{\det C}\, e^{iS/\hbar}$ arises as the solution of the transport equation (VIII.4), with a normalization that gives the correct initial value to $G(x, t; y, 0)$ on the surface $t = 0$. Alternatively, if one thinks of $G(x, t; y, 0)$ as a solution of the nonhomogeneous Schrödinger equation in all space-time, it gives the correct delta-function singularity at $(x, t) = (y, 0)$.

Recall that to solve the Schrödinger equation through order $\hbar$ we need to solve

$$\frac{\partial A}{\partial t} + \frac{1}{m}\nabla A \cdot \nabla S + \frac{1}{2m}A\Delta S = 0 \qquad\qquad \text{(VIII.17)}$$

but S solves the Hamilton-Jacobi equation, and we obtain

$$\nabla S = p \doteq m\dot{x} \qquad\qquad \text{(VIII.18)}$$

Therefore, we obtain the following partial differential equation

$$-\frac{1}{2m}A\Delta S = \left(\frac{\partial}{\partial t} + \frac{1}{m}\nabla S \cdot \nabla\right)A = \left(\frac{\partial}{\partial t} + \dot{x} \cdot \nabla\right)A = \frac{dA}{dt} \qquad \text{(VIII.19)}$$

Then we can solve for $\ln A$ by integrating the classical trajectories and hence

$$A(x, t) = \exp\left[-\frac{1}{2m}\int_0^t \Delta S(x(u), u)\, du\right] \qquad\qquad \text{(VIII.20)}$$

However, the amplitude function can be expressed in an alternative way:

$$A(x, t) = (2\pi i\hbar)^{-n/2}\sqrt{\det C} \qquad\qquad \text{(VIII.21)}$$

where $C = \nabla_x\nabla_y S$, and $\det C$ is known as the Van Vleck determinant. In this section, we assume that the amplitude function is a twice differentiable function, i.e, $A \in C^2(\mathbb{R}^n)$. The fact that the determinant factor is a solution is well known but

very nontrivial [10]. The normalization issue is very similar to the case of the free propagator back in Chapters II and III. The classical action S also depends on (y, s) and we have set $\tau = 0$ without loss of generality, but can restore it by replacing t by $t - \tau$. This will become important on the next few pages, and we will need to start writing S and A as functions of all four arguments.

The solution of the Schrödinger equation is given in terms of classical paths. The Green function of the Schrödinger equation may be written as a sum of terms, each of which can linked with a classical path. In the 1974 Balian and Bloch paper, a semiclassical propagator is used to obtain the multiple scattering expansion of $G_{scl}(x, t; y, 0)$ [3]. First let us define a Volterra kernel $\hat{Q}$ by one of the following equations,

$$(-i\hbar\partial_t + H)G_{scl}(x, t; y, \tau) = \delta(x - y)\delta(t - \tau) - Q_R(x, t; y, \tau) \qquad \text{(VIII.22)}$$

or,

$$G_{scl}(x, t; y, \tau)(-i\hbar\partial_t + H) = \delta(x - y)\delta(t - \tau) - Q_L(x, t; y, \tau) \qquad \text{(VIII.23)}$$

Thus the operator version of the above two equations, for instance, is given by

$$(-i\hbar\partial_t + H)\hat{G}_{scl} = I - \hat{Q}_R \qquad \text{(VIII.24)}$$

or,

$$\hat{G}_{scl}(-i\hbar\partial_t + H) = I - \hat{Q}_L \qquad \text{(VIII.25)}$$

where $\hat{Q}_R$ and $\hat{Q}_L$ are Volterra operators. Then we obtain the Green function for the initial value problem from equation (VIII.24) and this equation is rewritten as

$$\hat{G}^{-1}\hat{G}_{scl} = I - \hat{Q}_R \qquad \text{(VIII.26)}$$

or,

$$\hat{G}_{scl} = \hat{G}(I - \hat{Q}) = \hat{G} - \hat{G}\hat{Q}_R \qquad \text{(VIII.27)}$$

where $\hat{G}^{-1} = (-i\hbar\partial_t + H)$ and $G_{scl} = A(x,t)e^{iS(x,t)/\hbar}$ is a semiclassical propagator. Therefore we can write the formal solution in operator notation:

$$\hat{G} = \hat{G}_{scl}(I - \hat{Q}_R)^{-1} \qquad \text{(VIII.28)}$$

where

$$\hat{Q}_R\phi(t) = \int_0^t \Lambda(t,\tau)\phi(\tau)\,d\tau \qquad \text{(VIII.29)}$$

and,

$$[\Lambda(t,\tau)\varphi(\tau)](x) = \int_{\mathbb{R}^n} Q_R(x,t;y,\tau)\varphi(y,\tau)\,dy \qquad \text{(VIII.30)}$$

The space operator $\hat{G}_{scl}$ is defined by

$$\hat{G}_{scl}\phi(t) = \int_0^t \Gamma(t,\tau)\phi(\tau)\,d\tau \qquad \text{(VIII.31)}$$

where,

$$[\Gamma(t,\tau)\phi(\tau)](x) = \int_{\mathbb{R}^n} G_{scl}(x,t;y,\tau)\phi(y,\tau)\,d\tau \qquad \text{(VIII.32)}$$

The above formal solution is analogous to that of the nonhomogeneous Volterra integral equation of the second kind. The initial approximation in this case will be a semiclassical propagator $G_{scl} = A(x,t;y,\tau)e^{iS(x,t;y,\tau)}$. The kernel Q is given by $Q(x,y,t,\tau) = -(L+V)G_{scl}(x,t;y,\tau) + \delta^n(x-y)\delta(t-\tau) = [\Delta A(x,t;y,\tau)]e^{iS(x,t;y,\tau)/\hbar}$. The perturbation expansion of the exact solution of the Schrödinger equation is

$$\hat{G} = \hat{G}_{scl} + \hat{G}_{scl}\hat{Q}_R + \hat{G}_{scl}\hat{Q}_R^2 + \cdots . \qquad \text{(VIII.33)}$$

Then, we can rewrite the above operator equation in the following manner:

$$G(x, t; y, \tau) = G_{scl}(x, t; y, \tau) + \int_0^t \Gamma(t, \tau_1)\Lambda(\tau_1, \tau) \, d\tau_1$$

$$+ \int_0^t \int_0^{\tau_1} \Gamma(t, \tau_2)\Lambda(\tau_2, \tau_1)\Lambda(\tau_1, \tau) \, d\tau_2 d\tau_1 + \cdots$$

(VIII.34)

Then, we can rewrite the above operator equation in the following manner:

$$G(x, t; y, \tau) = G_{scl}(x, t; y, \tau) + \int_0^t \int_{\mathbb{R}^n} G_{scl}(x, t; y_1, \tau_1)\left\{\frac{\Delta_{y_1} A(y_1, \tau_1; y, \tau)}{A(y_1, \tau_1; y, \tau)}\right\}$$

$$\times G_{scl}(y_1, \tau_1; y, \tau) \, dy_1 d\tau_1 + \int_0^t \int_0^{\tau_1} \int_{\mathbb{R}^n} \int_{\mathbb{R}^n} G_{scl}(x, t; y_2, \tau_2)\left\{\frac{\Delta_{y_2} A(y_2, \tau_2; y_1, \tau_1)}{A(y_2, \tau_2; y_1, \tau_1)}\right\}$$

$$\times G_{scl}(y_2, \tau_2; y_1, \tau_1)\left\{\frac{\Delta_{y_1} A(y_1, \tau_1; y, \tau)}{A(y_1, \tau_1; y, \tau)}\right\} G_{scl}(y_1, \tau_1; y, \tau) \, dy_2 dy_1 d\tau_2 d\tau_1 + \cdots$$

(VIII.35)

and the Laplacian operator Δ acts upon the first space variable of the amplitude function $A(x, t; y, \tau)$.

A closer connection to Volterra integral equations is used by considering the other way of deriving the Volterra integral of the second kind. In other words, use equation (VIII.25) and solve for the exact Green operator $\hat{G}$. Hence, we obtain the following operator equation

$$\hat{G}_{scl}\hat{G}^{-1} = I - \hat{Q}_L$$

(VIII.36)

or,

$$\hat{G}_{scl} = (I - \hat{Q}_L)\hat{G}$$

(VIII.37)

If we apply equation (VIII.37) to ϕ to get a Volterra integral equation, and this gives the Volterra structure:

$$\psi - \hat{Q}_L\psi = f$$

(VIII.38)

and where, $\psi = \hat{G}\phi$, and $f = \hat{G}_{scl}\phi$. Therefore we can write the formal solution in

operator notation:

$$\hat{G} = (I - \hat{Q}_L)^{-1}\hat{G}_{scl} \qquad \text{(VIII.39)}$$

where $\hat{Q}_L\phi(t) = \int_0^t \Lambda(t,\tau)\phi(\tau)\,d\tau$ and $\Lambda(t,\tau)\phi(\tau) = \int_{\mathbb{R}^n} Q_L(x,t;y,\tau)\phi(y,\tau)\,dy$. The perturbation expansion of the exact solution of the Schrödinger equation is

$$\hat{G} = \hat{G}_{scl} + \hat{Q}_L\hat{G}_{scl} + \hat{Q}_L^2\hat{G}_{scl} + \cdots . \qquad \text{(VIII.40)}$$

Then, we can rewrite the above operator equation in the following manner:

$$\begin{aligned}
G(x,t;y,\tau) = G_{scl}(x,t;y,\tau) &+ \int_0^t \Lambda(t,\tau_1)\Gamma(\tau_1,\tau)\,d\tau_1 \\
&+ \int_0^t \int_0^{\tau_1} \Lambda(t,\tau_2)\Lambda(\tau_2,\tau_1)\Gamma(\tau_1,\tau)\,d\tau_2 d\tau_1 + \cdots
\end{aligned} \qquad \text{(VIII.41)}$$

Then, we can rewrite the above operator equation in the following manner:

$$\begin{aligned}
G(x,t;y,\tau) = G_{scl}(x,t;y,\tau) &+ \int_0^t \int_{\mathbb{R}^n} [\Delta_{y_1} A(x,t;y_1,\tau_1)]e^{iS(x,t;y_1,\tau_1)/\hbar} \\
\times\, G_{scl}(y_1,\tau_1;y,\tau)\,dy_1 d\tau_1 &+ \int_0^t \int_0^{\tau_1} \int_{\mathbb{R}^n} \int_{\mathbb{R}^n} [\Delta_{y_2} A(x,t;y_2,\tau_2)]e^{iS(x,t;y_2,\tau_2)/\hbar} \\
\times\, [\Delta_{y_1} A(y_2,\tau_2;y_1,\tau_1)]&e^{iS(y_2,\tau_2;y_1,\tau_1)/\hbar}G_{scl}(y_1,\tau_1;y,\tau)\,dy_2 dy_1 d\tau_2 d\tau_1 + \cdots
\end{aligned}$$

$$\text{(VIII.42)}$$

and the Laplacian operator Δ acts upon the second space variable of the amplitude function $A(x,t;y,\tau)$.

In the following theorem, we will use the operator notation where $\hat{G}_{scl}$ is on the left-hand side of the Volterra operator $\hat{Q}_R$. In this chapter, we only consider the Volterra operator $\hat{Q}_R$. From now on until the end of this chapter, the Volterra operator $\hat{Q}_R$ will be written simply as $\hat{Q}$. Thus the Volterra integral operator $\hat{Q}$ will act on some function φ which belongs to the Lebesgue space $L^{\infty,2}(I;\mathbb{R}^n)$.

Remark: In the case of the free propagator, the space operator is given by

$$U_0(t, \tau)\phi(\tau) = \int_{\mathbb{R}^n} K_f(x, t; y, \tau)\phi(y, \tau) \, dy \qquad \text{(VIII.43)}$$

and hence,

$$\|U_0(t, \tau)\phi(\tau)\|_{L^2(\mathbb{R}^n)} = \|\phi(\tau)\|_{L^2(\mathbb{R}^n)}. \qquad \text{(VIII.44)}$$

In the case of the semiclassical propagator, we lose the unitarity of the space operator, and we obtain only an inequality for the L^2 norm of Λ:

$$\|\Lambda(t, \tau)\phi(\tau)\|_{L^2(\mathbb{R}^n)} \leq M\|\phi(\tau)\|_{L^2(\mathbb{R}^n)} \qquad \text{(VIII.45)}$$

and the smallest number M is the operator norm of $\|\Lambda\|_{op}$ of $\Lambda(t, \tau)$. Once again, the uniform norm of the semiclassical Green function G_{scl} is not finite because the uniform norm of $A(x, t)$ is not finite either, i.e, $\|G_{scl}\|_{L^{\infty,2}(I^2;\mathbb{R}^{2n})} = \|A\|_{L^{\infty,2}(I^2;\mathbb{R}^{2n})} = \infty$.

Theorem 12 *Let $\Lambda(t, \tau)$ be a semiclassical kernel, and suppose the following two hypotheses hold:*

i.) $\|\frac{\Delta A}{A}\|_{L^{\infty}(I^2;\mathbb{R}^{2n})} < \infty$

ii.) Γ *is a bounded operator from $L^2(\mathbb{R}^n)$ to itself.*

Then the semiclassical operator is a bounded linear integral operator such that $\Lambda : L^2(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$. It follows that, the Volterra integral equation in the space $L^{\infty,2}(I; \mathbb{R}^n)$ with the semiclassical kernel $Q(x, t; y, \tau)$ can be solved by successive approximations.

Proof: First of all we want to prove that the Neumann series converges. We want to show that $G = \sum_{j=0}^{\infty}(\hat{G}_{scl}\hat{Q})^j\varphi$ is a convergent series. Suppose, we make the assumption on the amplitude function $A(x, t)$, and $\Delta A(x, t)$ that $\|\frac{\Delta A}{A}\|_{L^{\infty}(I^2;\mathbb{R}^{2n})} < \infty$. Let the Banach space $\mathcal{B}$ be the Hilbert space $L^2(\mathbb{R}^n)$. Then we would like to prove that the semiclassical Green operator $\hat{G}_{scl}$ is a linear bounded operator from $L^2(\mathbb{R}^n)$

to itself. The Volterra operator is defined in the following way,

$$
\begin{aligned}
[\hat{G}_{scl}\hat{Q}\varphi(t)](x) &\equiv \int_0^t \Gamma(t,\tau_1)\Lambda(\tau_1,\tau)\varphi(\tau)\,d\tau \\
&= \int_0^t \int_{\mathbb{R}^n} G_{scl}(x,t;y_1,\tau_1)Q(y_1,\tau_1;y,\tau)\varphi(y,\tau)\,dyd\tau
\end{aligned}
\tag{VIII.46}
$$

Thus, the first term of the Neumann series is given by

$$
\psi_1(t) \equiv \hat{G}_{scl}\hat{Q}\varphi(t) = \int_0^t \Gamma(t,\tau_1)\Lambda(\tau_1,\tau)\varphi(\tau)\,d\tau,
\tag{VIII.47}
$$

and where the space operator $\Lambda(t,\tau)$ is given by

$$
\begin{aligned}
\Lambda(t,\tau)\varphi(\tau) &= \int_{\mathbb{R}^n} \Delta A(x,t;y,\tau)e^{iS(x,t;y,\tau)/\hbar}\varphi(y,\tau)\,dy \\
&= \int_{\mathbb{R}^n} \frac{\Delta A(x,t;y,\tau)}{A(x,t;y,\tau)}G_{scl}(x,t;y,\tau)\varphi(y,\tau)\,dy
\end{aligned}
\tag{VIII.48}
$$

and the space operator $\Gamma(t,\tau)$ is given by

$$
\Gamma(t,\tau)\varphi(\tau) = \int_{\mathbb{R}^n} G_{scl}(x,t;y,\tau)\varphi(y,\tau)\,dy
\tag{VIII.49}
$$

and where $\Gamma(t,\tau)$ is a bounded operator from $L^2(\mathbb{R}^n)$ to itself. Since the space operator $\Gamma(t,\tau)$ is bounded operator, this implies the following inequality:

$$
\begin{aligned}
\int_{\mathbb{R}^n} |\Gamma(t,\tau)\varphi(\tau)|^2\,dx &\leq \int_{\mathbb{R}^n}\left(\int_{\mathbb{R}^n}|G_{scl}(x,t;y,\tau)\varphi(y,\tau)|\,dy\right)^2 dx \\
&\leq M^2\|\varphi(\tau)\|_{L^2(\mathbb{R}^n)}^2
\end{aligned}
\tag{VIII.50}
$$

and hence,

$$
\|\Gamma(t,\tau)\varphi(\tau)\|_{L^2(\mathbb{R}^n)} \leq \left(\int_{\mathbb{R}^n}\left(\int_{\mathbb{R}^n}|G_{scl}(x,t;y,\tau)\varphi(y,\tau)|\,dy\right)^2 dx\right)^{1/2} \leq M\|\varphi(\tau)\|_{L^2(\mathbb{R}^n)}
\tag{VIII.51}
$$

where M is independent of t,τ. The semiclassical amplitude $A(x,t;y,\tau)$ is not uniform with respect to time, and this can clearly be seen in the free propagator and

harmonic propagator cases. In order to have an estimate we have to keep the t variable fixed. A way to have a bounded norm estimate is to notice that the kernel Q can be expressed as $Q(x, t; y, \tau) = \Delta A e^{iS/\hbar} = \frac{\Delta A}{A} G_{scl}$. Another assumption that we will make will be assume that $\frac{\Delta A}{A}$ is L^∞ in the space variables, and in the time variables. Thus, we can obtain the bounded estimates for $\Lambda(t, \tau)\varphi(t)$ in the following way

$$|\Lambda(t, \tau)\varphi(\tau)| \leq \left\|\frac{\Delta A}{A}\right\|_{L^\infty(I^2;\mathbb{R}^{2n})} \int_{\mathbb{R}^n} |G_{scl}(x, y, t, \tau)\varphi(y, \tau)|\, dy \qquad \text{(VIII.52)}$$

and hence,

$$\int_{\mathbb{R}^n} |\Lambda(t, \tau)\varphi(\tau)|^2\, dx \leq \left\|\frac{\Delta A}{A}\right\|^2_{L^\infty(I^2;\mathbb{R}^{2n})} \int_{\mathbb{R}^n} \left(\int_{\mathbb{R}^n} |G_{scl}(x, y, t, \tau)\varphi(y, \tau)|\, dy\right)^2$$

$$\text{(VIII.53)}$$

Then we can express the above inequality in the following manner,

$$\|\Lambda(t, \tau)\varphi(\tau)\|_{L^2(\mathbb{R}^n)} \leq \left\|\frac{\Delta A}{A}\right\|_{L^\infty(I^2;\mathbb{R}^{2n})} \left(\int_{\mathbb{R}^n} \left(\int_{\mathbb{R}^n} |G_{scl}(x, t; y, \tau)\varphi(y, \tau)|\, dy\right)^2 dx\right)^{1/2}$$

$$\leq M\|T\|_{L^\infty(I^2;\mathbb{R}^{2n})} \|\varphi(\tau)\|_{L^2(\mathbb{R}^n)}$$

$$\text{(VIII.54)}$$

and where, $T = \frac{\Delta A}{A}$, and $C \equiv \|T\|_{L^\infty(I^2,\mathbb{R}^{2n})}$. Then we obtain an estimate on the function ψ_1 which is given by:

$$\|\psi_1(t)\|_{L^2(\mathbb{R}^n)} \leq N\|\varphi(\tau)\|_{L^2(\mathbb{R}^{2n})} t \qquad \text{(VIII.55)}$$

The above inequality has the Volterra structure, namely that the first term is proportional to t. The second term of the Neumann series is given by

$$\psi_2(t) = \int_0^t \Gamma(t, \tau)\phi(\tau)\, d\tau = \int_0^t \Gamma(t, \tau)\Lambda(t, \tau)\psi_1(\tau)\, d\tau \qquad \text{(VIII.56)}$$

where $\phi(\tau) = \Lambda(t, \tau)\psi_1(\tau)$. Then we take the L^2 norm of the second term of the

Neumann series and hence we obtain

$$\|\psi_2(t)\|_{L^2(\mathbb{R}^n)} \leq \int_0^t \|\Gamma(t,\tau)\phi(\tau)\|_{L^2(\mathbb{R}^n)} d\tau \leq \int_0^t N\|\phi(\tau)\|_{L^2(\mathbb{R}^n)}\tau d\tau \qquad \text{(VIII.57)}$$

or,

$$\begin{aligned}
\|\psi_2(t)\|_{L^2(\mathbb{R}^n)} &\leq N \int_0^t M\|\psi_1(\tau)\|_{L^2(\mathbb{R}^n)} \, d\tau \leq D \int_0^t \|\psi_1(\tau)\|_{L^2(\mathbb{R}^n)} \, d\tau \\
&\leq D \int_0^t \|\varphi(\tau)\|_{L^2(\mathbb{R}^n)}\tau \, d\tau \leq D\|\varphi\|_{L^{\infty,2}(I;\mathbb{R}^n)}\frac{t^2}{2}
\end{aligned} \qquad \text{(VIII.58)}$$

Therefore, the norm estimate of the second Neumann series is given by

$$\|\psi_2\|_{L^{\infty,2}(I;\mathbb{R}^n)} \leq D\|\varphi\|_{L^{\infty,2}(I;\mathbb{R}^n)}\frac{T^2}{2} \qquad \text{(VIII.59)}$$

The second term of the Neumann series ψ_2 is an example of the simplex structure for the general term ψ_n. Since the above hypothesis holds for fixed t, then the solution $\varphi = \sum_{n=0}^{\infty} \psi_n$ is bounded by a convergent infinite series. In analogy with the Volterra theorem, the Volterra integral equation with the semiclassical propagator $G_{scl}(x,t;y,\tau)$ can be solved by successive approximations. ∎

CHAPTER IX

POTENTIAL THEORY AND GREEN FUNCTIONS

A. Introduction to Surface Potentials

In this chapter we seek to show the advantages of using the Schrödinger potentials when constructing the integral equations for the Schrödinger kernel in the case of domains with smooth boundaries. The Schrödinger potentials give an integral equation for the Green function in a bounded and open region in $\mathbb{R}^n$. First, we formulate the classical potential theory by studying the Laplace equation in $\mathbb{R}^n$. The potential theory treatment of the Schrödinger operator is similar to that of the heat operator. Thus, we use the article by Irina Pirozhenko et al in order to draw a parallel between the two partial differential operators [11]. Thus, we assume that the surface of the bounded domain $U \subset \mathbb{R}^n$ is a smooth boundary. The fundamental solution for the Laplace equation is

$$\Phi(x,y) = \begin{cases} \frac{1}{2\pi} \ln \frac{1}{|x-y|} & \text{if } n = 2 \\ \frac{1}{4\pi} \frac{1}{|x-y|} & \text{if } n = 3 \\ \frac{1}{(2n-4)\pi^{n/2}} \frac{\Gamma(\frac{n}{2})}{|x-y|^{n-2}} & \text{if } n \geq 3 \end{cases} \tag{IX.1}$$

The harmonic potentials for the Laplace equation are created by using the fundamental solution $\Phi(x,y)$. The volume potential $V(x)$ is given by

$$V(x) = \int_U \Phi(x,y) Lu(y)\,dy = \int_U \Phi(x,y)\psi(y)\,dy \tag{IX.2}$$

where $\psi(x)$ is a continuous source term function. Similarly, the single-layer potential is given by

$$\Gamma_N(x) = \int_{\partial U} \Phi(x,y)\mu(y)\,dy \tag{IX.3}$$

where $\mu(x)$ is a continuous surface density function. The double-layer potential is expressed in the following manner

$$\Gamma_D(x) = \int_{\partial U} \partial_{\nu(y)} \Phi(x, y) \varphi(y) \, dy \tag{IX.4}$$

and $\varphi(x)$ is a continuous surface density function. These potentials are also solutions of the Laplace equation. In Chapter II, we took care of the initial condition through the Poisson integral. In order to handle the boundary data similarly, the surface Schrödinger potentials are introduced. These surface potentials are continuous on $\partial U \times (0, T]$. The time integrals in both surface Schrödinger potentials are improper integrals with respect to the upper limit. In *Linear Integral Equations*, Kress introduces and proves the existence of the surface heat potentials [2]. It is a well-known fact that the surface heat potentials have a jump discontinuity at the boundary ∂U. This section attempts to prove the existence of the surface Schrödinger potentials. In theorem 15, the jump-relations are proved for the double-layer Schrödinger potential. The fundamental solution of the Schrödinger equation is

$$K_f(x, t; y, \tau) = (4\pi i(t - \tau))^{-n/2} \exp\left(\frac{i|x - y|^2}{4(t - \tau)}\right) \tag{IX.5}$$

where $m = \frac{1}{2}$, and $\hbar = 1$. The free propagator $K_f(x, t; y, \tau)$ satisfies the nonhomogeneous initial condition

$$K_f(x, \tau; y, \tau) = \lim_{t \to \tau+} K_f(x, t; y, \tau) = \delta(x - y) \tag{IX.6}$$

The above nonhomogeneous initial condition allows the construction to the Cauchy problem for the nonhomogeneous Schrödinger initial value problem

$$Lu(x, t) = \Delta_x u(x, t) + i\partial_t u(x, t) = f(x, t) \tag{IX.7}$$

$$u(x, 0) = h(x) \tag{IX.8}$$

where $f(x,t) = V(x,t)u(x,t)$ and $V(x,t)$ is the time-dependent potential. Thus, we can write the solution $u(x,t)$ in terms of integral equations by using the Integral Representation Theorem. Hence,

$$u(x,t) = \Pi(x,t) + U(x,t) \qquad \text{(IX.9)}$$

or,

$$u(x,t) = \int_{\mathbb{R}^n} K_f(x,t;y,0)h(y)\,dy + \int_0^t \int_U K_f(x,t;y,\tau)V(y,\tau)u(y,\tau)\,dyd\tau \quad \text{(IX.10)}$$

From now on, we are going to set the background for the solution to the boundary-value problem. The following formulas for the solution of the Dirichlet and Neumann problems will be shown to exist until the second section of this chapter. At this point, an informal preview of the Representation Theorem will be shown in this section, and the representation formulas and jump-discontinuity will be proved in section 6.2. In this section, we are interested in the homogeneous boundary-value problem,

$$Lu(x,t) = 0 \qquad \text{(IX.11)}$$

$$u(x,t) = g(x,t) \quad \text{on } \partial U \times \mathbb{R}^+ \qquad \text{(IX.12)}$$

where L is the Schrödinger operator. Then by the representation formula

$$u(x,t) = \Pi(x,t) + U(x,t) + \Gamma(x,t) \qquad \text{(IX.13)}$$

where $\Pi(x,t) = 0$ and $U(x,t) = 0$. In this chapter we show that the solution for the Dirichlet boundary value problem is given by the double-layer potential

$$u(x,t) = \Gamma_D(x,t) = \int_0^t \int_{\partial U} \partial_{\nu(y)} K_f(x,t;y,\tau)\varphi(y,\tau)\,d\sigma(y)d\tau \qquad \text{(IX.14)}$$

and where $\mu(x,t)$ is a continuous surface density. Let us also consider the homogeneous Neumann boundary-value problem,

$$Lu(x,t) = 0 \tag{IX.15}$$

$$\partial_{\nu(x)}u(x,t) = g(x,t) \quad \text{on } \partial U \times \mathbb{R}^+ \tag{IX.16}$$

Then the solution is given by the single-layer potential

$$u(x,t) = \Gamma_N(x,t) = \int_0^t \int_{\partial U} K_f(x,t;y,\tau)\mu(y,\tau)\,d\sigma(y)d\tau \tag{IX.17}$$

where $\varphi(x,t)$ is a continuous surface density. Also the single-layer potential and double-layer potential satisfy the initial condition $u(x,0) = 0$. Furthermore, the double-layer potential is discontinuous on passing through ∂U. Namely, the solution is given by

$$W_\pm(x,t) = W(x,t) \mp \frac{1}{2}\varphi(x,t), \qquad \forall x \in \partial U \tag{IX.18}$$

where $W_+(x,t)$ is the potential when x approaches the surface ∂U from the interior of U. Similarly, $W_-(x,t)$ is the double-layer potential when x approaches $y \in \partial U$ from the exterior of U. Then we consider the Dirichlet problem for the Schrödinger equation in an open and bounded domain U. Thus,

$$\left(\Delta + i\partial_t\right)u(x,t) = 0, \qquad \forall(x,t) \in U \times \mathbb{R}^+ \tag{IX.19}$$

$$u(x,0) = 0, \quad \forall x \in U \tag{IX.20}$$

$$u(x,t) = g(x,t), \quad \forall(x,t) \in \partial U \times \mathbb{R}^+ \tag{IX.21}$$

Therefore, the solution $u(x,t)$ for the interior Dirichlet problem reduces on the boundary to

$$u(x,t) = g(x,t) = W_+(x,t) = W(x,t) - \frac{1}{2}\mu(x,t), \qquad \forall(x,t) \in \partial U \times \mathbb{R}^+ \tag{IX.22}$$

or,

$$-\frac{1}{2}\mu(x,t) + W(x,t) = g(x,t), \forall (x,t) \in \partial U \times \mathbb{R}^+ \tag{IX.23}$$

or,

$$\mu(x,t) - 2\int_0^t \int_{\partial U} \partial_{\nu(y)} K_f(x,t;y,\tau)\mu(y,\tau)\,d\sigma(y)d\tau = -2g(x,t), \qquad \forall x,y \in \partial U, \forall t \in \mathbb{R}^+ \tag{IX.24}$$

B. Surface Potentials and Volterra integral problem

In the previous subsection, the interior Dirichlet problem was transformed into a Volterra integral equation of the second kind. The following theorems and lemmas attempt to construct a formalism which proves that the Schrödinger surface potentials do in fact exist. However, the boundary ∂U is considered to be of class C^2. Lemma 4 , definition 8 and theorem 13 are from the book *Linear Integral Equations* [2].

Lemma 4 *Let ∂U be of class C^2. Then there exists a positive constant L and a normal vector $\nu(x)$ such that*

$$|\nu(x) \cdot (x - y)| \leq L|x - y|^2 \tag{IX.25}$$

and

$$|\nu(x) - \nu(y)| \leq L|x - y| \tag{IX.26}$$

$\forall x, y \in \partial U$.

Definition 8 *A weakly singular kernel is a kernel K which is continuous for all $x, y \in \partial U$, $x \neq y$, and there exist $M > 0$ and $\alpha \in (0, n]$ such that*

$$|K(x,y)| \leq M|x - y|^{\alpha - n}. \tag{IX.27}$$

where, n is the dimension of the Euclidean space $\mathbb{R}^n$.

Theorem 13 *The integral operator with continuous or weakly singular kernel is a compact operator on $C(\partial U)$ if ∂U is of class C^1.*

The following theorem is a more generalized version of Theorem 6.17 from Rainer Kress' book [2]. In this theorem we allow the harmonic density to depend on the variables x and y and the parameter t. This theorem will be used in theorem 15 to prove that the double-layer Schrödinger potential exists with uniform convergence on ∂U and on compact subintervals of $(0, T]$. The proof of the generalized version of Theorem 6.17 is based upon the proof of Theorem 6.17, but the theorem is extended to include the temporal parameter t, as suggested by Kress.

Theorem 14 *Let ∂U be of class C^2. The double-layer harmonic potential v with continuous density ψ can be continuously extended to $\partial U \times (0, T]$ with limiting values*

$$v_{\pm}(x, t) = \int_{\partial U} \psi(x, y, t) \partial_{\nu(y)} \Phi(x, y) \, d\sigma(y) \mp \frac{1}{2}\psi(x, t), \quad x, y \in \partial U, t \in (0, T], \quad \text{(IX.28)}$$

where t is a parameter, and the integral exists as an improper integral.

Proof: The normal derivative of the fundamental solution of Laplace's equation is bounded, and by lemma 4 we have the estimate

$$|\partial_{\nu(y)} \Phi(x, y)| = \frac{|\nu(y) \cdot (x - y)|}{\omega_n |x - y|^n} \leq \frac{L}{\omega_n |x - y|^{n-2}}, \quad x \neq y \quad \text{(IX.29)}$$

Therefore, the integral in equation (IX.28) has a weakly singular kernel. By Theorem 13 the integral exists for $x \in \partial U$ and $t \in (0, T]$ as an improper integral. Also, the improper integral is a continuous function on $\partial U \times (0, T]$. Let $x \in \partial U$ be represented in the form $x = z + h\nu(z)$, where $z \in \partial U$ and $h \in [-h_0, h_0]$ for some $h_0 > 0$. Therefore, the double-layer harmonic potential v can be expressed in the form

$$v(x, t) = \psi(z, t)w(x) + u(x, t), \quad x = z + h\nu(z) \in D \setminus \partial U, \quad \text{(IX.30)}$$

where

$$w(x) = \int_U \partial_{\nu(y)} \Phi(x, y) \, d\sigma(y) \tag{IX.31}$$

and

$$u(x, t) = \int_U [\psi(y, t) - \psi(z, t)] \partial_{\nu(y)} \Phi(x, y) \, d\sigma(y) \tag{IX.32}$$

If $x \in \partial U$, then the integral in equation is also an improper integral. The function $w(x)$ is basically the double-layer potential with constant density. Thus,

$$w(x) = \int_{\partial U} \partial_{\nu(y)} \Phi(x, y) \, d\sigma(y) = \begin{cases} -1, & \text{if } x \in U \\ -\frac{1}{2}, & \text{if } x \in \partial U \\ 0, & \text{if } x \in \mathbb{R}^n \setminus \bar{U} \end{cases} \tag{IX.33}$$

and, in order to prove the theorem the function $u(x, t)$ has to be continuous on the boundary ∂U. In other words, we need to prove that the limit

$$\lim_{h \to 0} u(z + h\nu(z), t) = u(z, t), \quad z \in \partial U, t \in (0, T] \tag{IX.34}$$

is uniformly continuous on $\partial U \times (0, T]$. The following inequality is obtained from lemma 1,

$$\frac{1}{2}[|z - y|^2 + |x - z|^2] \le |x - y|^2 \tag{IX.35}$$

for $x = z + h\nu(z)$ and $h \in [-h_0, h_0]$. Thus, the normal derivative of the harmonic potential can be expressed in the following form

$$\partial_{\nu(y)} \Phi(x, y) = \frac{\nu(y) \cdot (z - y)}{\omega_n |x - y|^n} + \frac{\nu(y) \cdot (x - z)}{\omega_n |x - y|^n} \tag{IX.36}$$

Thus, using equation (4.26), the normal derivative of $\Phi(x, y)$ can be estimated by

$$\left| \frac{\partial \Phi(x, y)}{\partial \nu(y)} \right| \le \left| \frac{\nu(y) \cdot (z - y)}{\omega_n |x - y|^n} \right| + \left| \frac{\nu(y) \cdot (x - z)}{\omega_n |x - y|^n} \right| \tag{IX.37}$$

or,

$$\left|\frac{\partial\Phi(x,y)}{\partial\nu(y)}\right| \le \frac{L_1|z-y|^2}{\omega_n|x-y|^n} + \frac{L_2|x-z|^2}{\omega_n|x-y|^n} \le \frac{L_1}{\omega_n|x-y|^{n-2}} + \frac{L_2|x-z|}{\omega_n|x-y|^n} \qquad \text{(IX.38)}$$

where, $x - z = h\nu(z)$, and $|x - z| = |h||\nu(z)| < 1$. Thus, $|x - z|^2 \le |x - z| < 1$, and we have

$$\begin{aligned}\left|\frac{\partial\Phi(x,y)}{\partial\nu(y)}\right| &\le \frac{C_1}{|x-y|^{n-2}} + \frac{C_2|x-z|}{[|z-y|^2 + |x-z|^2]^{n/2}} \\ &\le M\left[\frac{1}{|x-y|^{n-2}} + \frac{|x-z|}{[|z-y|^2 + |x-z|^2]^{n/2}}\right]\end{aligned} \qquad \text{(IX.39)}$$

for some constants $C_1, C_2 > 0$ and $M > 0$. Then, we project onto the tangent plane, and we obtain the following estimate

$$\int_{\partial U(z,r)} |\partial_{\nu(y)}\Phi(x,y)|\, d\sigma(y) \le M \int_{\partial U(z,r)} \left[\frac{1}{|x-y|^{n-2}} + \frac{|x-z|}{[|z-y|^2 + |x-z|^2]^{n/2}}\right] d\sigma(y) \tag{IX.40}$$

where, $\partial U(z,r) = \partial U \cap B(z,r)$. Since the surface ∂U is of class C^1, the normal vector ν is continuous on ∂U. Then, there exists $\delta \in (0,1]$ such that

$$\nu(x) \cdot \nu(y) \ge \frac{1}{2}, \qquad \forall x, y \in \partial U \tag{IX.41}$$

and $|x - y| \le \delta$. Since $|x - y| \ge \rho$, then the differential surface element becomes

$$d\sigma(y) = \frac{\rho^{n-2}d\rho d\Omega}{\nu(x) \cdot \nu(y)} \le 2\rho^{n-2}d\rho d\Omega \tag{IX.42}$$

Therefore, if $\nu(x) \cdot \nu(y) \geq \frac{1}{2}$, the surface integral estimate becomes

$$
\begin{aligned}
&\leq 2M \int_{\partial U(z,r)} \left[\frac{1}{\rho^{n-2}} + \frac{|x-z|}{[|z-y|^2 + |x-z|^2]^{n/2}} \right] \rho^{n-2} d\rho d\Omega \\
&\leq 2M \int_{\partial U(z,r)} d\rho d\Omega + 2M \int_{\partial U(z,r)} \frac{|x-z|}{[\rho^2 + |x-z|^2]^{n/2}} \rho^{n-2} d\rho \int d\Omega \\
&\leq C \left[\int_0^r d\rho + \int_0^r \frac{|x-z|}{[\rho^2 + |x-z|^2]^{n/2}} \rho^{n-2} d\rho \right] \\
&\leq C \left[r + \int_0^\infty \frac{\xi^{n-2}}{[\xi^2 + 1]^{n/2}} d\xi \right]
\end{aligned}
\tag{IX.43}
$$

Therefore, the function $w(x)$ is bounded and continuous on ∂U. Then,

$$
\begin{aligned}
\left| \frac{\partial \Phi(x,y)}{\partial \nu(y)} - \frac{\partial \Phi(z,y)}{\partial \nu(y)} \right| &= \left| \frac{\nu(y) \cdot (z-y)}{\omega_n |x-y|^n} + \frac{\nu(y) \cdot (x-z)}{\omega_n |x-y|^n} - \frac{\nu(y) \cdot (z-y)}{\omega_n |x-y|^n} \right| \\
&= \left| \frac{\nu(y) \cdot (x-z)}{\omega_n |x-y|^n} \right| \leq C \frac{|x-z|}{|x-y|^n} \leq C \frac{|x-z|}{|z-y|^n}
\end{aligned}
\tag{IX.44}
$$

for some constant $C > 0$. Thus, the difference between the two functions $w(x)$ and $w(z)$ can be estimated as follows

$$
\left| \int_{\partial U \setminus \partial U(z,r)} \partial_{\nu(y)} \Phi(x,y) - \partial_{\nu(y)} \Phi(z,y) \, d\sigma(y) \right| \leq
$$

$$
\int_{\partial U \setminus \partial U(z,r)} |\partial_{\nu(y)} \Phi(x,y) - \partial_{\nu(y)} \Phi(z,y)| \, d\sigma(y)
\tag{IX.45}
$$

$$
\leq \int_{\partial U \setminus \partial U(z,r)} C \frac{|x-z|}{|z-y|^n} \, d\sigma(y)
$$

If $2|x-z| \leq r$, and $2|x-z| \leq |z-y|$, then $\frac{1}{|z-y|} \leq \frac{1}{r}$. Thus the above estimate becomes

$$
\int_{\partial U \setminus \partial U(z,r)} C \frac{|x-z|}{r^n} \, d\sigma(y) \leq D \frac{|x-z|}{r^n}
\tag{IX.46}
$$

for some constant $D > 0$. Then, a bounded estimate can be given for the function $u(x, t)$, i.e,

$$
\begin{aligned}
|u(x,t) - u(z,t)| &= \left| \int_{\partial U \backslash \partial U(z,r)} [\psi(y,t) - \psi(z,t)][\partial_{\nu(y)}\Phi(x,y) - \partial_{\nu(y)}\Phi(z,y)] \, d\sigma(y) \right| \\
&\leq \int_{\partial U \backslash \partial U(z,r)} |\psi(y,t) - \psi(z,t)||\partial_{\nu(y)}\Phi(x,y) - \partial_{\nu(y)}\Phi(z,y)| \, d\sigma(y)
\end{aligned}
$$

$$(\text{IX.47})$$

Since $\psi(x,t)$ is uniformly continuous on $\partial U \times (0,T]$, $\forall \varepsilon > 0$, there exists $r > 0$ such that

$$
\max_{|y-z| \leq r} |\psi(y,t) - \psi(z,t)| \leq \frac{\varepsilon^{1/2}}{D} \tag{IX.48}
$$

Therefore, the bounded estimate for equation (IX.47) becomes

$$
|u(x,t) - u(z,t)| \leq \frac{\varepsilon^{1/2}}{D} \int_{\partial U \backslash \partial U(z,r)} |\partial_{\nu(y)}\Phi(x,y) - \partial_{\nu(y)}\Phi(z,y)| \, d\sigma(y) \leq \frac{\varepsilon^{1/2}}{D} D \frac{|x-z|}{r^n}
$$

$$(\text{IX.49})$$

Let $\delta < \varepsilon^{1/2} r^n$, then $|x - z| < \delta$, we obtain

$$
|u(x,t) - u(z,t)| < \frac{\varepsilon^{1/2}\delta}{r^n} < \varepsilon \tag{IX.50}
$$

Therefore, the double-layer harmonic potential is uniformly continuous on ∂U and on compact subintervals of $(0, T]$. ∎

Theorem 15 will prove the existence of the double-layer Schrödinger potential.

Theorem 15 *Let ∂U be of class C^2. The double-layer Schrödinger potential v with continuous density φ can be extended to $\partial U \times (0,T]$ with limiting values*

$$
v_{\pm}(x,t) = \int_0^t \int_{\partial U} \varphi(y,\tau) \partial_{\nu(y)} K_f(x,t;y,\tau) \, d\sigma(y) \mp \frac{1}{2}\varphi(x,t), \quad x \in \partial U, t \in (0,T],
$$

$$(\text{IX.51})$$

and where the integral exists as an improper integral.

Proof: In this case, we treat the higher-dimensional problem, i.e., when $n \geq 2$. The proof for $n = 1$ will not be provided here but it is similar and simpler to the higher-dimensional case. Let $x \in U$, where a U is a bounded domain such that $U \subset \mathbb{R}^n$. Then it is possible to interchange the order of integrations over ∂U and $(0, T]$ since the integrand term is continuous throughout $\partial U \times (0, T]$. Then, we obtain

$$v(x, t) = \int_{\partial U} \int_0^t \frac{1}{(4\pi i(t - \tau))^n} \frac{i[\nu(y) \cdot (x - y)]}{2(t - \tau)} \exp\left\{i\frac{(x - y)^2}{4(t - \tau)}\right\} \varphi(y, \tau) \, d\tau d\sigma(y) \tag{IX.52}$$

Let

$$s = \frac{|x - y|}{\sqrt{4(t - \tau)}} \tag{IX.53}$$

and substitute the above equation into equation (IX.52). Then, we can separate the spatial components of the integrand in equation (IX.52) outside of the improper time integral, and we obtain

$$v(x, t) = \int_{\partial U} \frac{i[\nu(y) \cdot (x - y)]}{|x - y|^n} \int_{\frac{|x-y|}{\sqrt{4t}}}^\infty s^{n-1} e^{is^2} \varphi\left(y, t - \frac{|x - y|^2}{4s^2}\right) ds d\sigma(y) \tag{IX.54}$$

Then, we take the time integral to represent the function

$$\psi(x, y, t) = \frac{1}{(\pi i)^{n/2}} \int_{\frac{|x-y|}{\sqrt{4t}}}^\infty e^{is^2} \varphi\left(y, t - \frac{|x - y|^2}{4s^2}\right) ds \tag{IX.55}$$

Therefore, we can treat the double-layer Schrödinger potential as a harmonic double-layer potential with the density ψ, which depends on t as a parameter. Therefore, we can rewrite equation in the following manner:

$$v(x, t) = i \int_{\partial U} \partial_{\nu(y)} \Phi(x, y) \psi(x, y, t) \, d\sigma(y) \tag{IX.56}$$

Then, we prove that ψ is continuous on $\mathbb{R}^n \times \partial U \times (0, T]$ with

$$\lim_{x \to y} \psi(x, y, t) = P_n \psi(y, t) \tag{IX.57}$$

for $y \in \partial U$ and $t \in (0, T]$, where

$$P_n = \frac{1}{(\pi i)^{n/2}} \int_0^\infty s^{n-1} e^{is^2} \, ds = \frac{1}{2\pi^{n/2}} \Gamma\left(\frac{n}{2}\right) \tag{IX.58}$$

The limit holds on the boundary ∂U and for compact subintervals of $(0, T)$. The function ψ is continuous for all $x \neq y$ and $t \in (0, T]$. Then, we show that the limit in equation (IX.57) holds, by the following method:

$$\psi(x, y, t) = \frac{1}{(\pi i)^{n/2}} \int_{\frac{|x-y|}{\sqrt{4t}}}^{\sqrt{|x-y|}} s^{n-1} e^{is^2} \varphi\left(y, t - \frac{|x-y|^2}{4s^2}\right) ds + \frac{\varphi(y, t)}{(\pi i)^{n/2}} \int_{\sqrt{|x-y|}}^\infty s^{n-1} e^{is^2} \, ds$$

$$+ \frac{1}{(\pi i)^{n/2}} \int_{\sqrt{|x-y|}}^\infty s^{n-1} e^{is^2} \left[\varphi\left(y, t - \frac{|x-y|^2}{4s^2}\right) - \varphi(y, t)\right] ds = I_1 + I_2 + I_3 \tag{IX.59}$$

Since $\varphi \in L^1(I; \mathbb{R}^n)$, then the limit of $x \to y$ is given by

$$\lim_{x \to y} I_1(x, y, t) = \lim_{x \to y} \frac{1}{(\pi i)^{n/2}} \int_{\frac{|x-y|}{\sqrt{4t}}}^{\sqrt{|x-y|}} s^{n-1} e^{is^2} \varphi\left(y, t - \frac{|x-y|^2}{4s^2}\right) ds = 0 \tag{IX.60}$$

and this limit holds on ∂U and on compact subintervals of $(0, T]$. In order to handle I_2, we use the Fresnel integral formula

$$P_n = \int_0^\infty s^{n-1} e^{is^2} \, ds = \frac{i^{n/2}}{2} \Gamma\left(\frac{n}{2}\right) \tag{IX.61}$$

Then the limit of the second term can be found by using the Fresnel integral formula and hence,

$$\lim_{x \to y} I_2(x, y, t) = \lim_{x \to y} \varphi(y, t) \frac{1}{(\pi i)^{n/2}} \int_{\sqrt{|x-y|}}^\infty s^{n-1} e^{is^2} \, ds \tag{IX.62}$$

or,

$$\lim_{x \to y} I_2(x, y, t) = \varphi(y, t) \frac{1}{(\pi i)^{n/2}} \int_0^\infty s^{n-1} e^{is^2} \, ds = \frac{1}{2\pi^{n/2}} \Gamma\left(\frac{n}{2}\right) \varphi(y, t) \tag{IX.63}$$

Suppose that the double-layer density φ is continuous and that $\varphi \in L^1(I;\mathbb{R})$. Then we make the substitution $r = s^2$ in the third term I_3 and we have

$$I_3(x,y,t) = \frac{1}{2(\pi i)^{n/2}} \int_{|x-y|}^{\infty} r^m e^{ir} \left[\varphi\left(y, t - \frac{|x-y|^2}{4r}\right) - \varphi(y,t) \right] dr \qquad \text{(IX.64)}$$

where, $m = \frac{n-2}{2}$. Then we insert the Abel factor $e^{-\alpha r}$ into equation (IX.64) and this gives

$$I_3(x,y,t) = \frac{1}{2(\pi i)^{n/2}} \int_{|x-y|}^{\infty} e^{-\alpha r} r^m e^{ir} \left[\varphi\left(y, t - \frac{|x-y|^2}{4r}\right) - \varphi(y,t) \right] dr \qquad \text{(IX.65)}$$

Next, we take the absolute value of equation (IX.65) and we have

$$|I_3| \leq \frac{1}{\pi^{n/2}} \int_{|x-y|}^{\infty} r^m e^{-\alpha r} \left| \varphi\left(y, t - \frac{|x-y|^2}{4r}\right) - \varphi(y,t) \right| dr \qquad \text{(IX.66)}$$

Since $|x - y| < r$, this implies that $\frac{|x-y|^2}{r} < |x - y|$. Therefore, we can bound the bracketed factor in equation (IX.65) by taking the absolute value. Since φ is continuous, $\forall \eta > 0 \ \exists \delta > 0$ such that

$$\left| \varphi\left(y, t - \frac{|x-y|^2}{4r}\right) - \varphi(y,t) \right| < \eta \qquad \text{(IX.67)}$$

$\forall y \in \partial U$ and $\forall t, t_1 \in [0,T]$ such that $|t - t_1| < \delta$ and $\frac{|x-y|^2}{r} < |x - y| < \delta$. Since φ is a continuous function, this implies that

$$|I_3| \leq \frac{\eta}{\pi^{n/2}} \int_{|x-y|}^{\infty} r^m e^{-\alpha r} \, dr \to 0 \qquad \text{(IX.68)}$$

as $x \to y$, and this limit holds in the Abel sense. Therefore, ψ is continuous on $\mathbb{R}^n \times \partial U \times (0,T]$.

Since, the function ψ is analogous to the harmonic density, we use theorem 14, and we obtain the following result,

$$v_{\pm}(x,t) = \lim_{h \to 0} v(x \pm h\nu(x), t) = \int_0^t \int_{\partial U} \partial_{\nu(y)} K_f(x,t;y,\tau)\varphi(y,\tau)\, d\sigma(y)d\tau \mp \frac{1}{2}\varphi(x,t)$$

(IX.69)

where $y \in \partial U$. Therefore, the double-layer potential exists and it is Abel summable on ∂U and on compact subintervals of $(0, T]$. ∎

Theorem 16 *Let ∂U be of class C^2. Then the single-layer potential $u(x,t)$ with continuous density ϕ can be extended to $\partial U \times (0, T]$. On the boundary we have*

$$\partial_{\nu(x)} u_{\pm}(x,t) = \int_0^t \int_{\partial U} \phi(y,\tau)\partial_{\nu(y)} K_f(x,t;y,\tau)\, d\sigma(y)d\tau \pm \frac{1}{2}\phi(x,t),$$

(IX.70)

$\forall x, y \in \partial U$, *and* $t \in (0, T]$. *In this case the integral exists as an improper integral.*

Proof: The proof is similar to the proof for theorem 15. The single-layer surface potential is continuous everywhere in $U \times (0, T]$. Since the integrand of the single-layer potential has no singularities outside $U \times (0, T]$ for any $t \in (0, T]$, it is also continuous everywhere in $\mathbb{R}^{n+1} \setminus (U \times (0, T])$ for any $t \in (0, T]$. Therefore, all we have to show is that the jump relation holds. Then, the expressions for the normal derivatives of the surface potential of a single layer is obtained by substituting the double-layer density $\psi(x,t)$ by the density of the single-layer potential $u(x,t)$. The single-layer jump-relation will have $\cos\phi$ instead of $\cos\varphi$, where ϕ is the angle between the normal vector $\nu(x)$ and the vector $r_{xy} = x - y$. Thus, the proof is identical to that of theorem 15. ∎

Next, we will show some corollaries which are the goal of this section. By using theorem 8 and 9, we can finally solve the main two problems of this section, the Dirichlet and Neumann boundary value problem. The homogeneous Dirichlet

boundary value problem is

$$Lu(x,t) = 0 \qquad\qquad\qquad \text{(IX.71)}$$

$$u(x,t) = f(x,t) \qquad \text{on } \partial U \times (0,T] \qquad\qquad \text{(IX.72)}$$

and the homogeneous Neumann boundary value problem is

$$Lu(x,t) = 0 \qquad\qquad\qquad \text{(IX.73)}$$

$$\partial_{\nu(x)}u(x,t) = g(x,t) \qquad \text{on } \partial U \times (0,T] \qquad\qquad \text{(IX.74)}$$

where f and g satisfies the Dirichlet and Neumann boundary conditions respectively. These two functions functions also satisfy the initial condition

$$f(\cdot,0) = 0 \quad \text{on } \partial U \qquad\qquad \text{(IX.75)}$$

and

$$g(\cdot,0) = 0 \quad \text{on } \partial U \qquad\qquad \text{(IX.76)}$$

Corollary 3 *The double-layer Schrödinger potential*

$$u(x,t) = \int_0^t \int_{\partial U} \varphi(y,\tau)\partial_{\nu(y)}K_f(x,t;y,\tau)\, d\sigma(y)d\tau, \qquad x,y \in \partial U, t \in (0,T] \quad \text{(IX.77)}$$

with continuous density φ is a solution to the interior Dirichlet problem provided that φ is a solution of the integral equation

$$\varphi(x,t) - 2\int_0^t \int_{\partial U} \varphi(y,\tau)\partial_{\nu(y)}K_f(x,t;y,\tau)\, d\sigma(y)d\tau = -2f(x,t), \qquad x,y \in \partial U, t \in (0,T]$$
$$\text{(IX.78)}$$

Proof: This proof follows from theorem 15. ∎

Corollary 4 *The double-layer Schrödinger potential*

$$u(x,t) = \int_0^t \int_{\partial U} \varphi(y,\tau)\partial_{\nu(y)}K_f(x,t;y,\tau)\, d\sigma(y)d\tau, \qquad x,y \in \partial U, t \in (0,T] \quad \text{(IX.79)}$$

with continuous density φ is a solution to the exterior Dirichlet problem provided that φ is a solution of the integral equation

$$\varphi(x,t) + 2\int_0^t \int_{\partial U} \varphi(y,\tau)\partial_{\nu(y)}K_f(x,t;y,\tau)\,d\sigma(y)d\tau = 2f(x,t), \qquad x,y \in \partial U, t \in (0,T]$$

$$\text{(IX.80)}$$

Proof: This proof follows from theorem 15. ∎

Corollary 5 *The single-layer Schrödinger potential*

$$u(x,t) = \int_0^t \int_{\partial U} \psi(y,\tau)K_f(x,t;y,\tau)\,d\sigma(y)d\tau, \qquad x,y \in \partial U, t \in (0,T] \qquad \text{(IX.81)}$$

with continuous density ψ is a solution to the interior Neumann problem provided that ψ is a solution of the integral equation

$$\psi(x,t) + 2\int_0^t \int_{\partial U} \psi(y,\tau)K_f(x,t;y,\tau)\,d\sigma(y)d\tau = 2g(x,t), \qquad x,y \in \partial U, t \in (0,T]$$

$$\text{(IX.82)}$$

Proof: This proof follows from theorem 16. ∎

Corollary 6 *The single-layer Schrödinger potential*

$$u(x,t) = \int_0^t \int_{\partial U} \psi(y,\tau)K_f(x,t;y,\tau)\,d\sigma(y)d\tau, \qquad x,y \in \partial U, t \in (0,T] \qquad \text{(IX.83)}$$

with continuous density ψ is a solution to the exterior Neumann problem provided that φ is a solution of the integral equation

$$\varphi(x,t) - 2\int_0^t \int_{\partial U} \psi(y,\tau)K_f(x,t;y,\tau)\,d\sigma(y)d\tau = -2g(x,t), \qquad x,y \in \partial U, t \in (0,T]$$

$$\text{(IX.84)}$$

Proof: This proof follows from theorem 16. ∎

The equations (IX.78), (IX.80), (IX.82), and (IX.84) are Volterra integral equations of the second kind with respect to time. These four integral equations can be

written in compact operator notation in the following way

$$\varphi \pm 2\hat{S}\varphi = \pm 2f \tag{IX.85}$$

and

$$\psi \mp 2\hat{S}\psi = \mp 2g \tag{IX.86}$$

where the first equation is for the Dirichlet problem, and the second equation is for the Neumann problem. It remains to prove that these Volterra integral equations can be solved by the method of successive approximations. The next problem we tackle is to prove that the surface Volterra integral equations can indeed by solved by the Picard algorithm. The following theorem is an application of the Volterra theorem when the spatial Banach space $\mathcal{B}$ is $L^\infty(\partial U)$.

Theorem 17 *Let us consider the interior Dirichlet problem only. Suppose that $\varphi \in L^\infty(I; \partial U)$ is a solution of the integral equation*

$$\varphi - 2\hat{S}\varphi = -2f \tag{IX.87}$$

where $\hat{S}$ is the Volterra operator defined on equation (IX.89) *and where f is the boundary data. Thus, the Neumann series of the above Volterra equation converges to the exact solution with respect to the topology $L^\infty(I; \partial U)$.*

Proof: Let $\mathcal{H} = L^\infty(I; \mathcal{B})$ be the Banach space with norm $\| \cdot \|_{L^\infty(I;\mathcal{B})}$, where $I = (0, T)$. Suppose that the function $\phi : I \to L^\infty(I; \mathcal{B})$ is a bounded function with norm $\|\varphi\|_{L^\infty(I;\mathcal{B})} = \sup_{\tau \in [0,T]} |\,\|\varphi(\tau)\|\,|$. We shall show that the surface Schrödinger operator is a bounded operator from $L^\infty(I; \partial U)$ to itself. Suppose the continuous density function φ belongs to $L^\infty(I; \partial U)$. Thus there exists a number C such that

$$\forall (t, \tau) \in \bar{I}^2 \wedge \forall \varphi \in L^{\infty,2}(I; \mathbb{R}^n) \implies \|\hat{S}\varphi\|_{L^\infty(\mathbb{R}^n)} \leq C\|\phi\|_{L^\infty(\mathbb{R}^n)} \tag{IX.88}$$

The integral operator $\hat{S} : L^\infty(\partial U) \to L^\infty(\partial U)$ is given by

$$\hat{S}\varphi(x,t) = \int_0^t \int_{\partial U} \partial_{\nu(y)} K_f(x,t;y,\tau)\varphi(y,\tau)\, d\sigma(y)d\tau \tag{IX.89}$$

$\forall x, y \in \partial U$ and $t \in (0, T]$. In this case, the integral is an improper integral with respect to time. Therefore, the normal derivative of the free propagator is

$$\partial_{\nu(y)} K_f(x,t;y,\tau) = \frac{1}{(4\pi i(t-\tau))^{n/2}} \left(\frac{i[\nu(y)\cdot(x-y)]}{2(t-\tau)} \right) \exp\left(\frac{i|x-y|^2}{4(t-\tau)} \right). \tag{IX.90}$$

Namely, by using lemma 4, the normal derivative of $K_f(x,t;y,\tau)$ can be given a bounded estimate, and hence

$$|\partial_{\nu(y)} K_f(x,t;y,\tau)| \le \frac{L|x-y|^2}{|t-\tau|^{n/2}|t-\tau|} \qquad t > \tau, \tag{IX.91}$$

and where L is a positive constant. Then, we define the space operator $\hat{K}(t,\tau)$ in the following way

$$\hat{K}(t,\tau)\varphi(\tau) = \int_{\partial U} \partial_{\nu(y)} K(x,t;y,\tau)\varphi(y,\tau)\, d\sigma(y)$$
$$= \int_{\partial U} \frac{1}{(4\pi i(t-\tau))^{n/2}} \frac{i[\nu(x)\cdot(x-y)]}{2(t-\tau)} \exp\left(\frac{i|x-y|^2}{4(t-\tau)} \right) \varphi(y,\tau)\, d\sigma(y)$$
$$\tag{IX.92}$$

Then we do the change of variables $r = \frac{x-y}{(4(t-\tau))^{1/2}}$ in equation (IX.92) and hence we obtain

$$\hat{K}(t,\tau)\varphi(\tau) = \frac{1}{2(\pi i)^{n/2}} \int_{\partial U(r)} \frac{i[\nu(x)\cdot r]}{(2(t-\tau))^{1/2}} e^{ir^2} \varphi(y,\tau)\, d\sigma(r) \tag{IX.93}$$

Then, we take square of the absolute value of $\hat{K}\varphi$ and we obtain

$$|\hat{K}(t,\tau)\varphi(\tau)| \le \frac{1}{2(\pi)^{n/2}} \int_{\partial U(r)} \frac{|\nu(x)\cdot r|]}{(2(t-\tau))^{1/2}} \varphi(x - 4(t-\tau)^{1/2}r, \tau)\, d\sigma(r)$$
$$\le \frac{D\|\varphi(\tau)\|_{L^\infty(\partial U)}}{(2(t-\tau))^{1/2}} \int_{\partial U(r)} |\nu(x)\cdot r|\, d\sigma(r) \le \frac{M\|\varphi(\tau)\|_{L^\infty(\partial U)}}{(2(t-\tau))^{1/2}}$$
$$\tag{IX.94}$$

Then, we take the uniform norm on the boundary ∂U of the quantum surface operator and we obtain

$$
\begin{aligned}
\|\hat{S}\varphi(\tau)\|_{L^\infty(\partial U)} &\leq \int_0^t \|\hat{K}(t,\tau)\varphi(\tau)\|_{L^\infty(\partial U)}\, d\tau \leq \int_0^t \frac{M\|\varphi(\tau)\|_{L^\infty(\partial U)}}{(2(t-\tau))^{1/2}}\, d\tau \\
&\leq M\|\varphi\|_{L^\infty(I;\partial U)} \int_0^t \frac{1}{(2(t-\tau))^{1/2}}\, d\tau \leq N\|\varphi\|_{L^\infty(I;\partial U)} t^{1/2}
\end{aligned}
\tag{IX.95}
$$

and hence,

$$
\|\hat{S}\varphi\|_{L^\infty(I;\partial U)} \leq N\|\varphi\|_{L^\infty(I;\partial U)} T^{1/2}
\tag{IX.96}
$$

Therefore, the quantum surface operator is a bounded operator from $L^\infty(I;\partial U)$ to itself. The Volterra structure is still present in the inequality (IX.96). The only difference is that the first term of the Neumann series will be proportional to $t^{1/2}$ instead of t. In analogy with the Volterra theorem, the Volterra integral equation with the quantum surface kernel $\partial_{\nu(x)} K_f(x,t;y,\tau)$ can be solved by successive approximations.
∎

CHAPTER X

CONCLUSION

The similarities between the Schrödinger equation and the heat equation were used to create a theoretical framework which will give the solution to the Schrödinger problem. The Volterra theorem proves that Volterra integral equation with a uniform bounded kernel can be solved by successive approximations with respect to the topology $L^\infty(I; \mathcal{B})$. The general Volterra theorem proves the more general case when $L^p(I; \mathcal{B})$, and where $1 \leq p < \infty$. The boundary-value problem is written in terms of Volterra integral equations of the second kind. Furthermore, the single-layer Schrödinger and double-layer Schrödinger potentials with continuous density functions are shown to be extended to $\partial U \times (0, T]$ with some limiting values.

A perturbation expansion is constructed by using the semiclassical propagator and a uniformly bounded potential $V(x, t)$. The solution of the Schrödinger equation is given in terms of classical paths, and the semiclassical propagator $G_{scl} = A e^{iS/\hbar}$ to the Green function is considered as the building block for the exact Green function [3]. The semiclassical Neumann series were found to have norm convergence, and thus the Neumann series converge to the exact Green function under some technical assumptions. Finally, the interior Dirichlet problem is considered, and the double-layer Schrödinger operator is shown to be bounded from $L^\infty(I; \partial U)$ to itself. Thus Neumann series is shown to converge in the case of the quantum surface kernel $\partial_v K_f$ with respect to the topology of $L^\infty(I; \partial U)$.

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2. Under Construction: Article- "WKB Approximation to the Power Wall", based on my M.S. thesis and on the Spectral Geometry Dartmouth paper.

The typist for this thesis was Fernando Daniel Mera.