The Schrödinger Equation as a Volterra Integral Problem

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Outline

- 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.
- We follow the books of the Rubinsteins and Kress to show for the Schrödinger equation similar results to those for the heat equation. This presentation proves that the Schrödinger equation with a source function does indeed have a unique solution.

Introduction

- In this presentation 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.

Introduction

- 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 theorem 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 $n \rightarrow \infty$.
- 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.

Introduction

- 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.
- 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.

Fundamental Solution of the Schrödinger equation

The fundamental solution to the equation Schrödinger equation in $\mathbb{R}^n$ is the free propagator,

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

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:

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

and thus the nonhomogenous kernel can also be expressed by $\tilde{K}(x,t,y,\tau) = \theta(t-\tau)K_f(x,y,t,\tau)$.

Poisson Integral Theorem

Theorem 1:Poisson Integral Theorem

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

$$u(x,t) = K_f * f = \int_{\mathbb{R}^n} K_f(x-y,t)f(y)\,dy \tag{1}$$

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

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

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.

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

$$\eta(x,t) = \lim_{t\to 0}\int_U K_f(x,y,t)f(y)\,dy = \begin{cases} f(x) & \text{if } x \in U,\ \forall t > 0 \\ \frac{f(x)}{2} & \text{if } x \in \partial U,\ \forall t > 0 \\ 0 & \text{if } x \notin \bar{U},\ \forall t > 0 \end{cases} \tag{3}$$

Representation Theorem

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

$$u(x,t) = \Gamma(x,t) + U(x,t) + \Pi(x,t) \tag{4}$$

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:

$$u(x,t) = \Gamma(x,t) + U(x,t) + \Pi(x,t) \tag{5}$$

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

$$\Pi(x,t) = \int_U K_f(x,t;y,t_0)h(y)\,dy \tag{6}$$

$$U(x,t) = i\int_{t_0}^{t}\int_U K_f(x,t;y,\tau)Lu(y,\tau)\,dyd\tau \tag{7}$$

and,

$$\Gamma(x,t) = ia^2\int_{t_0}^{t}\int_{\partial U}\left(K_f(x,t;y,\tau)\partial_{\nu(y)}u(y,\tau) - u(y,\tau)\partial_{\nu(y)}K_f(x,t;y,\tau)\right)ds(y)d\tau \tag{8}$$

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

The following corollary is proved to be true, and its proof depends on the Reciprocity Theorem. The reciprocity of the Green function is given by:

$$G(y,\tau;x,t) = G^*(x,t;y,\tau). \tag{9}$$

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

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

$$u(x,t) = \Gamma(x,t) + U(x,t) + \Pi(x,t) \tag{10}$$

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

$$\Pi(x,t) = \int_U G(x,t;y,t_0)h(y)\,dy \tag{11}$$

$$U(x,t) = i\int_{t_0}^{t}\int_U G(x,t;y,\tau)Lu(y,\tau)\,dyd\tau \tag{12}$$

and,

$$\Gamma(x,t) = ia^2\int_{t_0}^{t}\int_{\partial U}\Big(G(x,t;y,\tau)\partial_{\nu(y)}u(y,\tau) - u(y,\tau)\partial_{\nu(y)}G(x,t;y,\tau)\Big)\,ds(y)d\tau \tag{13}$$

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

Green Functions and Initial Value Problems

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

$$-\Delta_x u(x,t) + V(x,t)u(x,t) = i\partial_t u(x,t) \tag{14}$$

$$u(x,0) = f(x) \qquad \forall x \in \mathbb{R}^n \tag{15}$$

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

$$|V(x,t)| \leq M \qquad \forall (x,t) \in \mathbb{R}^n \times \mathbb{R} \tag{16}$$

Suppose the function $V(x,t)$ is a piecewise continuous and a piecewise smooth function on $\mathbb{R}^n \times \mathbb{R}$.
Then by the Representation Integral Theorem the solution $u(x,t)$ can be written as the following integral equation:

$$\begin{aligned} u(x,t) &= \Pi(x,t) + U(x,t) \equiv \hat{U}f(x) + \hat{Q}u(x,t) \\ &= \int_{\mathbb{R}^n} K_f(x,t;y,0)f(y)\,dy - i\int_0^t \int_{\mathbb{R}^n} K_f(x,t;y,\tau)V(y,\tau)u(y,\tau)\,dyd\tau \end{aligned} \tag{17}$$

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,

$$u(x,t) + iSVu(x,t) = \hat{U}f(x) \tag{18}$$

and where

$$\hat{Q}u(x,t) = -iSVu(x,t) = -i\int_0^t \hat{U}(t-\tau)V(\tau)u(\tau)\,d\tau \tag{19}$$

In more detail, we can express equation (18) as

$$u(x,t) + i\int_0^t \hat{U}(t-\tau)V(\tau)u(\tau)\,d\tau = \hat{U}f(x) \tag{20}$$

where,

$$\hat{U}(t-\tau)V(\tau)u(\tau) = \int_{\mathbb{R}^n} K_f(x,t;y,\tau)V(y,\tau)u(y,\tau)\,dy \tag{21}$$

Therefore, equation (17) is a Volterra integral equation of the second kind with respect to time.

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 4 and 5 are from Rainer Kress' book [8].

Theorem 4

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

$$(\lambda I - A)^{-1} = \sum_{k=0}^{\infty} \lambda^{-k-1} A^k \tag{22}$$

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

Theorem 5

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

$$\varphi_{n+1} = \hat{V}\varphi_n + f, \quad n = 0, 1, 2, \ldots \tag{23}$$

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

Theorem 6:Volterra Theorem

Let the kernel $A(t,\tau)$ be a uniformly bounded linear integral 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 $t < \tau$. The Volterra integral operator, $\hat{Q} : L^\infty(I;\mathcal{B}) \to L^\infty(I;\mathcal{B})$, is defined by

$$\hat{Q}\varphi(t) = \int_0^T A(t,\tau)\varphi(\tau)\,d\tau = \int_0^t A(t,\tau)\varphi(\tau)\,d\tau, \tag{24}$$

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 $L^\infty(I;\mathcal{B})$.

Theorem 7:General Volterra Theorem

Let the kernel $A(t,\tau)$ be a uniformly bounded linear integral 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 $t < \tau$. The Volterra integral operator, $\hat{Q} : L^p(I;\mathcal{B}) \to L^p(I;\mathcal{B})$, is defined by

$$\hat{Q}\varphi(t) = \int_0^T A(t,\tau)\varphi(\tau)\,d\tau = \int_0^t A(t,\tau)\varphi(\tau)\,d\tau, \tag{25}$$

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 $L^p(I;\mathcal{B})$.

Application of the Volterra Theorem

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 $K_f(x,t;y,0) = (4\pi i t)^{-n/2} e^{i|x-y|^2/4t}$, is the solution of the free Schrödinger equation with initial data $u(x,0) = h(x)$ in $L^2(\mathbb{R}^n)$.
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 (20) or,

$$u(x,t) + i\int_0^t \hat{U}(t-\tau)V(\tau)u(\tau)\,d\tau = \hat{U}h(x) \tag{26}$$

Because of the structure of equation (26), the operator is effectively Volterra. Hence, the Volterra theorem applies.
In theorem 6, we take $\mathcal{B} = \mathcal{H}$, and $A = UV$ as defined in equation (21):

$$\hat{U}(t-\tau)V(\tau)u(\tau) = \int_{\mathbb{R}^n} K_f(x,t;y,\tau)V(y,\tau)u(y,\tau)\,dy \tag{27}$$

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

$$\|V(\tau)f(\tau)\|^2_{L^2(\mathbb{R}^n)} = \int_{\mathbb{R}^n} |V(y,\tau)f(y,\tau)|^2\,dy \leq C^2 \int_{\mathbb{R}^n} |f(y,\tau)|^2\,dy = C^2\|f(\tau)\|^2_{L^2(\mathbb{R}^n)}. \tag{28}$$

Therefore,

$$\|V(\tau)f(\tau)\|_{L^2(\mathbb{R}^n)} \leq C\|f(\tau)\|_{L^2(\mathbb{R}^n)} \quad \forall f \in \mathcal{H}. \tag{29}$$

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,

$$\|U(t,\tau)V(\tau)f(\tau)\|_{L^2(\mathbb{R}^n)} \leq C\|f(\tau)\|_{L^2(\mathbb{R}^n)}. \tag{30}$$

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

$$A(t,\tau)f(\tau) = \int_{\mathbb{R}^n} K(x,t;y,\tau)f(y,\tau)\,dy = \int_{\mathbb{R}^n} K_f(x,t;y,\tau)V(y,\tau)f(y,\tau)\,dy \tag{31}$$

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

$$\|\psi\|_{L^{\infty,2}(I;\mathbb{R}^n)} = \|SVf\|_{L^{\infty,2}(I;\mathbb{R}^n)} \leq C\|f\|_{L^{\infty,2}(I;\mathbb{R}^n)}T \tag{32}$$

where,

$$\psi(t) = SVf(t) = \int_0^t U(t,\tau)V(\tau)f(\tau)\,d\tau \tag{33}$$

Thus we have verified all the hypotheses of Theorem 6, 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.

Hamilton-Jacobi Equation and Classical Paths

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 $G_{scl}(x, y, E)$ [1]. They looked only at the energy-domain (time-independent) Green function in semiclassical approximation. In this presentation we will deal with the semiclassical propagator $G_{scl}(x, t; y, \tau)$ which is a time-dependent Green function.
First let us define the Volterra kernel $\hat{Q}$ by the following equations,

$$(-i\hbar\partial_t + H)G_{scl}(x, t; y, \tau) = \delta(x - y)\delta(t - \tau) - Q(x, t; y, \tau) \tag{34}$$

or,

$$G_{scl}(x, t; y, \tau)(-i\hbar\partial_t + H) = \delta(x - y)\delta(t - \tau) - Q(x, t; y, \tau) \tag{35}$$

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

$$(-i\hbar\partial_t + H)\hat{G}_{scl} = I - \hat{Q}. \tag{36}$$

or,

$$\hat{G}_{scl}(-i\hbar\partial_t + H) = I - \hat{Q}. \tag{37}$$

where $\hat{Q}$ is a Volterra operator.

Then we obtain the Green function for the initial value problem from equation (36) and this equation is rewritten as

$$\hat{G}^{-1}\hat{G}_{scl} = I - \hat{Q}. \tag{38}$$

or,

$$\hat{G}_{scl} = \hat{G}(I - \hat{Q}) = \hat{G} - \hat{G}\hat{Q} \tag{39}$$

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:

$$\hat{G} = \hat{G}_{scl}(I - \hat{Q})^{-1} \tag{40}$$

where

$$\hat{Q}\phi(t) = \int_0^t \Lambda(t,\tau)\phi(\tau)\,d\tau \tag{41}$$

and,

$$[\Lambda(t,\tau)\varphi(\tau)](x) = \int_{\mathbb{R}^n} Q(x,t;y,\tau)\varphi(y,\tau)\,dy \tag{42}$$

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

$$\hat{G}_{scl}\phi(t) = \int_0^t \Gamma(t,\tau)\phi(\tau)\,d\tau \tag{43}$$

where,

$$[\Gamma(t,\tau)\phi(\tau)](x) = \int_{\mathbb{R}^n} G_{scl}(x,t;y,\tau)\phi(y,\tau)\,d\tau \tag{44}$$

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'

$$\hat{G} = \hat{G}_{scl} + \hat{G}_{scl}\hat{Q} + \hat{G}_{scl}\hat{Q}^2 + \cdots . \tag{45}$$

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

$$G(x,t;y,\tau) = G_{scl}(x,t;y,\tau) + \int_0^t \Gamma(t,\tau_1)\Lambda(\tau_1,\tau)\,d\tau_1 + \int_0^t \int_0^{\tau_1} \Gamma(t,\tau_2)\Lambda(\tau_2,\tau_1)\Lambda(\tau_1,\tau)\,d\tau_2 d\tau_1 + \cdots \tag{46}$$

Theorem 8

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.

An application of this theorem will be presented by Krishna Thapa in his presentation "WKB Approximation of a Power Wall."

Potential Theory and Green Functions

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 in the next few slides. At this point, an informal preview of the Representation Theorem will be shown, and the representation formulas and jump-discontinuity will be proved later in this presentation. Then, we are interested in the homogeneous boundary-value problem,

$$Lu(x,t) = 0 \tag{47}$$

$$u(x,t) = g(x,t) \quad \text{on } \partial U \times \mathbb{R}^+ \tag{48}$$

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

$$u(x,t) = \Pi(x,t) + U(x,t) + \Gamma(x,t) \tag{49}$$

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

$$u(x,t) = \Gamma_D(x,t) = \int_0^t \int_{\partial U} \partial_{\nu(y)} K_f(x,t;y,\tau)\varphi(y,\tau)\, d\sigma(y) d\tau \tag{50}$$

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

$$Lu(x,t) = 0 \tag{51}$$

$$\partial_{\nu(x)} u(x,t) = g(x,t) \quad \text{on } \partial U \times \mathbb{R}^+ \tag{52}$$

Then the solution is given by the single-layer potential

$$u(x,t) = \Gamma_N(x,t) = \int_0^t \int_{\partial U} K_f(x,t;y,\tau)\mu(y,\tau)\, d\sigma(y)d\tau \tag{53}$$

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

$$W_{\pm}(x,t) = W(x,t) \mp \frac{1}{2}\varphi(x,t), \qquad \forall x \in \partial U \tag{54}$$

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,

$$\left(\Delta + i\partial_t\right)u(x,t) = 0, \qquad \forall (x,t) \in U \times \mathbb{R}^+ \tag{55}$$

$$u(x,0) = 0, \quad \forall x \in U \tag{56}$$

$$u(x,t) = g(x,t), \quad \forall (x,t) \in \partial U \times \mathbb{R}^+ \tag{57}$$

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

$$u(x,t) = g(x,t) = W_+(x,t) = W(x,t) - \frac{1}{2}\mu(x,t), \qquad \forall (x,t) \in \partial U \times \mathbb{R}^+ \tag{58}$$

or,

$$-\frac{1}{2}\mu(x,t) + W(x,t) = g(x,t), \forall (x,t) \in \partial U \times \mathbb{R}^+ \tag{59}$$

or,

$$\mu(x,t) - 2\int_0^t \int_{\partial U} \partial_{\nu(y)} K_f(x,t;y,\tau)\mu(y,\tau)\, d\sigma(y)d\tau = -2g(x,t), \qquad \forall x,y \in \partial U, \forall t \in \mathbb{R}^+ \tag{60}$$

Theorem 9

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

$$v_{\pm}(x,t) = \int_0^t \int_{\partial U} \varphi(y,\tau)\partial_{\nu(y)} K_f(x,t;y,\tau)\, d\sigma(y) \mp \frac{1}{2}\varphi(x,t), \quad x \in \partial U, t \in (0,T], \tag{61}$$

and where the integral exists as an improper integral.

Theorem 10

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

$$\partial_{\nu(x)} u_{\pm}(x,t) = \int_0^t \int_{\partial U} \phi(y,\tau)\partial_{\nu(y)} K_f(x,t;y,\tau)\, d\sigma(y) d\tau \pm \frac{1}{2}\phi(x,t), \tag{62}$$

$\forall x, y \in \partial U$,and $t \in (0, T]$. In this case the integral exists as an improper integral.

Next, we will show some corollaries which are one of the main points of this presentation. 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

$$Lu(x,t) = 0 \tag{63}$$

$$u(x,t) = f(x,t) \qquad \text{on } \partial U \times (0,T] \tag{64}$$

and the homogeneous Neumann boundary value problem is

$$Lu(x,t) = 0 \tag{65}$$

$$\partial_{\nu(x)} u(x,t) = g(x,t) \qquad \text{on } \partial U \times (0,T] \tag{66}$$

where f and g satisfies the Dirichlet and Neumann boundary conditions respectively. These two functions functions also satisfy the initial condition

$$f(\cdot,0) = 0 \quad \text{on } \partial U \tag{67}$$

and

$$g(\cdot,0) = 0 \quad \text{on } \partial U \tag{68}$$

Corollary

The double-layer Schrödinger potential

$$u(x,t) = \int_0^t \int_{\partial U} \varphi(y,\tau)\partial_{\nu(y)} K_f(x,t;y,\tau)\, d\sigma(y)d\tau, \qquad x,y \in \partial U, t \in (0,T] \tag{69}$$

with continuous density φ is a solution to the interior Dirichlet problem provided that φ is a solution of the integral equation

$$\varphi(x,t) - 2\int_0^t \int_{\partial U} \varphi(y,\tau)\partial_{\nu(y)} K_f(x,t;y,\tau)\, d\sigma(y)d\tau = -2f(x,t), \qquad x,y \in \partial U, t \in (0,T] \tag{70}$$

Proof.

This proof follows from theorem 9. □

Corollary

The double-layer Schrödinger potential

$$u(x,t) = \int_0^t \int_{\partial U} \varphi(y,\tau)\partial_{\nu(y)} K_f(x,t;y,\tau)\, d\sigma(y)d\tau, \qquad x,y \in \partial U, t \in (0,T] \tag{71}$$

with continuous density φ is a solution to the exterior Dirichlet problem provided that φ is a solution of the integral equation

$$\varphi(x,t) + 2\int_0^t \int_{\partial U} \varphi(y,\tau)\partial_{\nu(y)} K_f(x,t;y,\tau)\, d\sigma(y)d\tau = 2f(x,t), \qquad x,y \in \partial U, t \in (0,T] \tag{72}$$

Proof.

This proof follows from theorem 9. □

Corollary

The single-layer Schrödinger potential

$$u(x,t) = \int_0^t \int_{\partial U} \psi(y,\tau) K_f(x,t;y,\tau)\, d\sigma(y) d\tau, \qquad x,y \in \partial U, t \in (0,T] \tag{73}$$

with continuous density ψ is a solution to the interior Neumann problem provided that ψ is a solution of the integral equation

$$\psi(x,t) + 2\int_0^t \int_{\partial U} \psi(y,\tau) K_f(x,t;y,\tau)\, d\sigma(y) d\tau = 2g(x,t), \qquad x,y \in \partial U, t \in (0,T] \tag{74}$$

Proof.

This proof follows from theorem 10. □

Corollary

The single-layer Schrödinger potential

$$u(x,t) = \int_0^t \int_{\partial U} \psi(y,\tau) K_f(x,t;y,\tau)\, d\sigma(y) d\tau, \qquad x,y \in \partial U, t \in (0,T] \tag{75}$$

with continuous density ψ is a solution to the exterior Neumann problem provided that φ is a solution of the integral equation

$$\varphi(x,t) - 2\int_0^t \int_{\partial U} \psi(y,\tau) K_f(x,t;y,\tau)\, d\sigma(y) d\tau = -2g(x,t), \qquad x,y \in \partial U, t \in (0,T] \tag{76}$$

Proof.

This proof follows from theorem 10. □

The equations (70), (72), (74), and (76) 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

$$\varphi \pm 2\hat{S}\varphi = \pm 2f \tag{77}$$

and

$$\psi \mp 2\hat{S}\psi = \mp 2g \tag{78}$$

where

$$\hat{S}\varphi(x,t) = \int_0^t \int_{\partial U} \partial_{\nu(y)} K_f(x,t;y,\tau)\varphi(y,\tau)\, d\sigma(y) d\tau \tag{79}$$

and 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 11

Let us consider the interior Dirichlet problem only. Suppose that φ is a solution of the integral equation

$$\varphi - 2\hat{S}\varphi = -2f \tag{80}$$

where $\hat{S}$ is the Volterra operator defined on equation (79) 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 $L^\infty(I;\partial U)$.

Summary and 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 $G_{scl} = Ae^{iS/\hbar}$ to the Green function is considered as the building block for the exact Green function [1]. 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 $\partial_{\nu} K_f$ with respect to the topology of $L^{\infty}(I;\partial U)$.

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