Neumann Series and Green's Functions

Fernando D.Mera

June 24, 2009

Introduction

- Schrödinger Operator and the Fundamental Identity

This presentation will began with the case of the Schrödinger equation with zero potential, and it will use the book *Partial Differential Equations in Classical Mathematical Physics* by Isaak Rubinstein and Lev Rubinstein as a foundation.

Later on the presentation,the problem with boundary conditions for the nonhomogenous Schrödinger equation and a potential function dependent on position will be considered.

In the presentation,the Volterra integral equations and their application to solution of boundary-value problems in quantum mechanics are introduced.

Finally, the Picard method of successive approximations will be used to find an approximate solution to the quantum-mechanical problem of a particle traveling in a multidimensional region.

The Schrödinger operator L_S is

$$L_S u(\mathbf{x},\tau) = -a^2 \Delta u(\mathbf{x},\tau) - i\frac{\partial u(\mathbf{x},\tau)}{\partial \tau} \quad (1)$$

where $a^2 = \frac{\hbar}{2m}$.
The following calculations are motivated by Isaak and Levi Rubenstein's treatment on the heat operator and its adjoint operator.
In this presentation, our case deals with the Shrödinger equation, and we seek to explore what are the differences and similarities between the heat equation and the Schrödinger equation.

Theorem

Let f be a continuous function on $\mathbb{R}^n$ with compact support. Then the Poisson integral is

$$u(x,t) = \int_{-\infty}^{\infty} f(y)K(x-y,t)\,dy \tag{2}$$

is a solution of the equation

$$Lu(x,t) = -a^2\frac{\partial u(x,t)}{\partial x^2} - i\frac{\partial u(x,t)}{\partial t} = 0 \qquad \forall t > 0. \tag{3}$$

The Poisson integral defines an infinitely differentiable solution of the Schrödinger equation with no potential in $\mathbb{R}^n \times (0,\infty)$. This solution can be continuously extended into $\mathbb{R}^n \times [0,\infty]$ with the initial condition $u(x,0) = f(x)$.

Theorem

Let $V = G \times (0, t]$, where $G \subset \mathbb{R}^n$. Consider the following boundary-value problem: Find a function $u(\mathbf{r}, \tau) \in C^{2,1}(V) \bigcap C^{1,0}(\overline{V})$, such that

$$Lu(\mathbf{x}, t) + F(\mathbf{x}, t) = 0 \qquad \forall(\mathbf{x}, t) \in V \qquad (4)$$

$$u(\mathbf{x}, 0) = \varphi(\mathbf{x}) \qquad \forall \mathbf{x} \in G, \qquad (5)$$

$$u(\mathbf{x}, t) = f_1(\mathbf{x}, t) \qquad \forall \mathbf{x} \in \partial\overline{G}, \qquad (6)$$

$$\frac{\partial u(\mathbf{x}, t)}{\partial n} = f_2(\mathbf{x}, t) \qquad \forall \mathbf{x} \in \partial G, \qquad (7)$$

If,

$$\frac{\partial}{\partial t} n_{\mathbf{x}} = 0 \qquad \forall(\mathbf{x}, t) \in \partial V \qquad (8)$$

then, if the solution of problem (4)-(7) exists,it is also unique.

Consider the following boundary-value problem:

$$L_S u(\mathbf{x},t) + F(\mathbf{x},t) = 0, \quad \forall \mathbf{x} \in G \quad \forall t > 0 \tag{9}$$

$$\alpha(\mathbf{x},t)\frac{\partial u(\mathbf{x},t)}{\partial n} + \beta(\mathbf{x},t)u(\mathbf{x},t) = f(\mathbf{x},t) \quad \forall(\mathbf{x},t) \in \partial V \tag{10}$$

$$u(\mathbf{x},0) = \varphi(\mathbf{x}) \quad \forall \mathbf{x} \in V \tag{11}$$

where α, β, f, and F are prescribed functions such that

$$\alpha^2(\mathbf{x},t)+\beta^2(\mathbf{x},t)>0 \quad \mathbf{x}\in\partial\overline{G} \quad \forall t_0<\tau<t \tag{12}$$

$$\alpha(\mathbf{x},t)\equiv 0\rightarrow\beta(\mathbf{x},t)\equiv 1,\beta(\mathbf{x},t)\equiv 0\rightarrow\alpha(\mathbf{x},t)\equiv 1 \tag{13}$$

$$\alpha(\mathbf{x},t)\neq 0,\beta(\mathbf{x},t)\neq 0 \quad \forall(\mathbf{x},t)\in\partial V \quad \forall t_0<\tau<t \tag{14}$$

$$\rightarrow\alpha\equiv 1,\ \beta\equiv h(\mathbf{x},t),\ f(\mathbf{x},t)=h(\mathbf{x},t)\psi(\mathbf{x},t) \tag{15}$$

Then, the solution to the given boundary-value problem is given by:

$$u(\mathbf{x}, t) = \int_G \varphi(\mathbf{r}) g(\mathbf{x}, t, \mathbf{r}, 0)\, dv_{\mathbf{r}} + I(\mathbf{x}, t) \\ \int_0^t d\tau \int_G F(\mathbf{r}, \tau) g(\mathbf{x}, t, \mathbf{r}, \tau)\, dv_{\mathbf{r}} \tag{16}$$

where, I is determined by the type of boundary-value problem.

Green's Functions and Boundary-Value Problems

In the previous slides, the solutions for the free-particle case were shown to be unique. In this section, the Green's function will be determined for, the Schrödinger equation. Let us consider the following linear boundary-value problem:

$$L_S\psi(\mathbf{x},t) + V(\mathbf{x})\psi(\mathbf{x},t) = 0 \qquad \forall(\mathbf{x},t) \in V, t > 0 \tag{17}$$

with the initial and boundary conditions

$$u(\mathbf{x},0) = f(\mathbf{x}), \mathbf{x} \in G, \quad \alpha(\mathbf{x},t)\psi(\mathbf{x},t)+\beta(\mathbf{x},t)\frac{\partial\psi(\mathbf{x},t)}{\partial n}\bigg|_{\partial G} = h(\mathbf{x},t) \quad \forall t > 0. \tag{18}$$

Definition

Define $G(\mathbf{x}, t; \mathbf{r}, \tau)$ $\forall \mathbf{x}, \mathbf{r} \in G$, and $t \in (0, t]$,and $\tau \in (0, t]$ by $G(\mathbf{x}, t; \mathbf{r}, \tau) = K(\mathbf{x}, \mathbf{r}, (t - \tau)) - \widetilde{G}(\mathbf{x}, t; \mathbf{r}, \tau)$, where the function $G(\mathbf{x}, t; \mathbf{r}, \tau)$ can satisfy the Dirichlet, Neumann, or Robin boundary conditions. In the above definition of the Green's function, $K(\mathbf{x}, \mathbf{r}, (t - \tau))$ is the quantum free propagator.

Then, we assume that, $L_S \widetilde{G}(\mathbf{x}, t; \mathbf{r}, \tau) = 0$ $\forall (\mathbf{r}, \tau) \in V$,where $(\mathbf{x}, t)$ is a fixed point, and $G(\mathbf{x}, t; \mathbf{r}, \tau)$ can be solution to the Dirichlet, Neumann or Robin boundary condtions.

Definition

$$\widetilde{G}(\mathbf{x}, t; \mathbf{r}, \tau) = 0 \quad \forall (\mathbf{r}, \tau) \in V \tag{19}$$

(Dirichlet boundary value condition)

$$\widetilde{G}(\mathbf{x}, t; \mathbf{r}, \tau) = K(\mathbf{x}, \mathbf{r}, (t - \tau)) \quad \forall (\mathbf{r}, \tau) \in \partial V \tag{20}$$

(Neumann boundary value conditions)

$$\frac{\partial}{\partial n_{\mathbf{r}}} \widetilde{G}(\mathbf{x}, t; \mathbf{r}, \tau) = \frac{\partial}{\partial n_{\mathbf{r}}} K(\mathbf{x}, \mathbf{r}, (t - \tau)) \qquad \forall (\mathbf{r}, \tau) \in \partial V \tag{21}$$

(Robin boundary value conditions)

$$\begin{aligned} &\left[\frac{\partial}{\partial n_{\mathbf{r}}} + \left(\beta(\mathbf{r}, t) - \frac{1}{\alpha^2} \frac{\partial}{\partial \tau} n_{\mathbf{r}}\right)\right] \widetilde{G} = \\ &\quad \left(\frac{\partial}{\partial n_{\mathbf{r}}} + \left(\beta(\mathbf{x}, t) - \frac{1}{\alpha^2} \frac{\partial}{\partial \tau} n_{\mathbf{r}}\right)\right) K \quad \forall (\mathbf{r}, \tau) \in \partial V \end{aligned} \tag{22}$$

Theorem

*(**The Reciprocity of Green's Functions**) Let $(\mathbf{r}, \tau)$ be considered as a variable point and $(\mathbf{x}, t) \in V$ as a fixed one. Then,*

$$L_S \widetilde{G}(\mathbf{r}, \tau; \mathbf{x}, t) = 0 \qquad (\mathbf{r}, \tau) \in G \times (\tau, t] \tag{23}$$

$$\widetilde{G}(\mathbf{r}, \tau; \mathbf{x}, t) = 0 \tag{24}$$

$$\widetilde{G}(\mathbf{r}, \tau; \mathbf{x}, t) = K(\mathbf{r}, \mathbf{x}, (t-\tau)) \quad \forall (\mathbf{x}, t) \in \partial V \tag{25}$$

$$\left(\frac{\partial}{\partial n_{\mathbf{r}}} + \beta(\mathbf{r}, \tau)\right) \widetilde{G}(\mathbf{r}, \tau; \mathbf{x}, t) = \left(\frac{\partial}{\partial n_{\mathbf{r}}} + \beta(\mathbf{r}, \tau)\right) K(\mathbf{r}, \mathbf{x}, (t-\tau)) \quad \forall (\mathbf{r}, \tau) \in \partial V \tag{26}$$

so that $G(\mathbf{r}, \tau; \mathbf{x}, t)$ being considered as a function of the first pair of variables, is a solution of the Schrödinger equation satisfying boundary conditions of Dirchlet, Neumann, or Robin boundary value problem respectively. Therefore, we obtain the reciprocity of Green's functions, i.e.,

$$G(\mathbf{x}, t; \mathbf{r}, \tau) = G^*(\mathbf{r}, \tau; \mathbf{x}, t). \tag{27}$$

Potential Theory

- Potential Theory and Green's functions

Theorem

The double-layer potential with continuous density ϕ can be continuously extended from $G \times (0, t]$ into $\overline{G} \times (0, t]$ with the conditions that $x \in \partial G$ and $t \in (0, t]$. Thus, the surface potential of double layer is

$$W(\mathbf{x}, t) = \int_0^t \int_{\partial G} \phi(\mathbf{x}, t) \frac{\partial K(\mathbf{x}, \mathbf{r}, t - \tau)}{\partial n} \, ds d\tau \qquad (28)$$

and the solution to the problem is

$$u(\mathbf{x}, t) = \int_0^t \int_{\partial G} \phi(\mathbf{x}, t) \frac{\partial K(\mathbf{x}, \mathbf{r}, t - \tau)}{\partial n} \, ds d\tau - \frac{1}{2}\phi(\mathbf{x}, t) \qquad (29)$$

where the time integral exists as an improper integral.

Theorem

The single-layer potential with continuous density ϕ can be continuously extended from $G \times (0, t]$ into $\overline{G} \times (0, t]$ with the conditions that $x \in \partial G$ and $t \in (0, t]$. Thus, the surface potential of single layer is

$$H(\mathbf{x}, t) = \int_0^t \int_{\partial G} \phi(\mathbf{x}, t) K(\mathbf{x}, \mathbf{r}, t - \tau)\, ds d\tau \tag{30}$$

Since the density ϕ is assumed to be continuous, it is also bounded, and therefore H is continuous everywhere in Ω^{3+1} and

$$LH(\mathbf{x}, t) = 0 \quad \forall \mathbf{x} \in \partial V. \tag{31}$$

In this case the time integral exists as an improper integral. Therefore, there exist $\frac{\partial u(\mathbf{x},t)}{\partial n}$ such that

$$\frac{\partial u(\mathbf{x}, t)}{\partial n} = \frac{\partial H(\mathbf{x}, t)}{\partial n} - \frac{1}{2}\phi(\mathbf{x}, t). \tag{32}$$

Integral Equations

- Integral Equations and Normed Spaces

It is assumed that the lateral boundary of the compact region G is static. In operator notation, the Volterra integral equation of the second kind is written in the following manner:

$$\psi - A\psi = f \tag{33}$$

in an appropriate normed space, which in our case is the L^2-space. Obviously, the existence and uniqueness of a solution to an integral operator equation can be found via the inverse operator.

Theorem

Let $G \subset \mathbb{R}$ be a nonempty compact and Jordan measurable set that coincides with the closure of its interior. Let $K : G \times G \to \mathbb{C}$ be a continuous function. Then the linear operator $A : C(G) \to C(G)$ defined by

$$(A\varphi)(x) := \int_G K(x,y)\varphi(y)\, dy, \qquad x \in G, \tag{34}$$

is called an integral operator with continuous kernel K. It is bounded operator with

$$\|A\|_\infty = \max_{x\in G} \int_G |K(x,y)| dy. \tag{35}$$

Then, $u_m(x,t)$ is converging to the solution $u(x,t)$ if the following conditions are satisfied:
1) the infinite series is uniformly convergent,
2) the kernel K and the function f belong to the L^2 space,
3) and finally,the integral operators are bounded linear operators on L^2.

If these three conditions are satisfied, then it is possible to use the Neumann series to approximate the solution to the original problem, which is the initial boundary value problem of the Shrödinger equation with a potential term V(x).

Then, we have,

$$(I - A)\psi = f, \tag{36}$$

and the formal solutions is

$$\psi = (I - A)^{-1} f \tag{37}$$

with the following Neumann series,

$$\psi = f + Af + A^2 f + \cdots . \tag{38}$$

Therefore, we obtain the partial sums,

$$\psi_m = \sum_{k=0}^{m} A^k f \tag{39}$$

of the Neumann series which satisfy the recurrence relation $\psi_{n+1} = A\psi_n + f$, $\forall n \geq 0$. Finally, in our case, we have, $f(x,t) = \Pi(x,t)$, and

$$(Af)(x,t) = \int_0^t \int_G V(x) f(x,t) K_f(x-y, t-\tau)\, dyd\tau, \tag{40}$$

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

$$\psi_1 = f(x,t) + U_1(x,t) = f(x,t) + \int_0^t \int_G V(x) f(x,t) K_f(x-y, t-\tau)\, dyd\tau. \tag{41}$$

Volterra Kernels

- Volterra Kernels and Successive Approximations

In this section we will revisit the method of successive approximations. In this case, we assume that A is a bounded linear operator in a Banach space X. Physicists are more interested in the special case of Hilbert spaces because this has applications in quantum mechanics. If the spectral radius of the integral operator $r(A) < 1$, then we are guaranteed that the Neumann series converges in the operator norm.The following theorems are from Rainer Kress(Page 171).

Theorem

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

$$(\lambda I - A)^{-1} = \sum_{k=0}^{\infty} \lambda^{-k-1} A^k \tag{42}$$

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

Theorem

Let $A : X \to X$ be a bounded linear operator in a Banach space X with spectral radius $r(A) < 1$. Then the successive approximations

$$\varphi_{n+1} = A\varphi_n + f, n = 0, 1, 2, ...,\tag{43}$$

converge for each $f \in X$ and each $\varphi_0 \in X$ to the unique solution of $\varphi - A\varphi = f$.

Green's functions and Unbounded Regions

- Green's functions and Unbounded Regions

Now, we are ready to tackle the two-dimensional boundary value problem with unbounded regions. Consider the Schrödinger equation, with the following initial conditions:

$$\frac{\partial^2 u(x,t)}{\partial x^2} + V(x)u(x,t) = -i\frac{\partial u(x,t)}{\partial t} \tag{44}$$

$$u(x,0) = h(x), \qquad x \in (-\infty, \infty) \tag{45}$$

The solution to this problem can be found by applying the integral fundamental relation, and assuming that $G = K_f$. Therefore, $u(x,t)$ must be a solution of the integrodifferential equation

$$u(x,t) = \int_0^t d\tau \int_{-\infty}^{\infty} V(\xi)u(\xi,t)K_f d\xi + \int_{-\infty}^{\infty} h(\xi)K_f d\xi \tag{46}$$

Then, the sequence u_n is converging to the solution $u(x, t)$ if the following conditions are satisfied:
1) the infinite series is uniformly convergent,
2) the kernel K and the function f belong to the L^2 space,
3) and finally, the integral operators are bounded linear operators on L^2.

If these three conditions are satisfied, then it is possible to use the Neumann series to approximate the solution to the Dirichlet problem on the real line. Once again, we want to solve the Volterra integral equation $u - V_k u = f$, and we just have initially, a u_0 approximating $u(x, t)$. Then, we have, the partial sums,

$$u_m = \sum_{n=0}^{m} V_k^n f \tag{47}$$

of the Neumann series which satisfy the recurrence relation $u_{n+1} = V_k u_n + f$, $\forall n \geq 0$.

Finally, in our case, we have, $f(x,t) = \Pi(x,t)$, and

$$(V_k f)(x,t) = \int_0^t \int_{\mathbb{R}} V(x) f(x,t) K_f(x-y, t-\tau)\, dy d\tau, \tag{48}$$

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

$$u_1 = f(x,t) + U_1(x,t) = f(x,t) + \int_0^t \int_{\mathbb{R}} V(x) f(x,t) K_f(x-y, t-\tau)\, dy d\tau, \tag{49}$$

where $K_f(x-\xi, t-\tau)$is the quantum free propagator, and

$$f(x,t) = \Pi(x,t) = \int_{-\infty}^{\infty} h(\xi) K_f(x-\xi, t-\tau) d\xi \tag{50}$$

($f(x,t)$ is a function belonging to the L^2 space). In this problem, the kernel K is assumed to belong the L^2 space.

Conclusion

Conclusion

In this presentation, the Schrödinger operator was introduced, and it was shown that a solution $u(x, t)$ can be found by the method of Green's functions. The next step will be to generalize the previous cases to the second and third order boundary value problem for bounded and unbounded regions.

The method of successive approximations was used to approximate the exact solution. However, the method of successive approximations has two drawbacks.

First, the Neumann series ensures existence of solutions to integral equations of the second kind only for sufficiently small kernels, and second,in general the series cannot be summed in closed form.