We are IntechOpen, the world's leading publisher of Open Access books Built by scientists, for scientists

6,900

186,000

200M

Download

154
Countries delivered to

Our authors are among the

TOP 1%

most cited scientists

12.2%

Contributors from top 500 universities



WEB OF SCIENCE

Selection of our books indexed in the Book Citation Index in Web of Science™ Core Collection (BKCI)

Interested in publishing with us? Contact book.department@intechopen.com

Numbers displayed above are based on latest data collected.

For more information visit www.intechopen.com



Convergence of the Neumann Series for the Schrödinger Equation and General Volterra Equations in Banach Spaces

Fernando D. Mera and Stephen A. Fulling

Additional information is available at the end of the chapter

http://dx.doi.org/10.5772/52489

1. Introduction

The time-dependent Schrödinger equation, like many other time-evolution equations, can be converted along with its initial data into a linear integral equation of Volterra type (defined below). Such an equation can be solved formally by iteration (the Picard algorithm), which produces a Neumann series whose jth term involves the jth power of an integral operator. The Volterra structure of the integral operator ensures that the time integration in this term is over a j-simplex, so that its size is of the order of 1/j!. One would therefore expect to be able to prove that the series converges, being bounded by an exponential series. The difficulty in implementing this idea is that the integrand usually is itself an operator in an infinite-dimensional vector space (for example, representing integration over the spatial variables of a wave function). If one can prove that this operator is bounded, uniformly in its time variables, with respect to some Banach-space norm, then one obtains a convergence theorem for the Neumann series. This strategy is indeed implemented for the heat equation in the books of the Rubinsteins [1] and Kress [2]. The objective of the thesis [3] was to treat the Schrödinger equation as much as possible in parallel with this standard treatment of the heat equation. This article reports from the thesis a summary of the rigorous framework of the problem, the main theorem, and the most elementary applications of the theorem.

We stress that the situation for time-evolution equations is different (in this respect, nicer) than for the Laplace and Poisson equations, which are the problems studied in most detail in most graduate textbooks on partial differential equations, such as [4]. In that *harmonic potential theory* the problem is similarly reduced to an integral equation, but the integral equation is not of Volterra type and therefore the Neumann series does not converge



automatically. The terms are bounded by a geometric series but not an exponential one, so to prove convergence it is not enough to show that the Banach-space operator has finite norm; the norm would need to be less than unity, whereas in the PDE application it turns out to be exactly unity. Therefore, in the theory of elliptic PDEs the Neumann series is not used to prove existence of a solution; instead, the Fredholm theory is used to prove existence more abstractly. In time-evolution problems the concrete convergence of the series gives rigorous meaning to formal constructions used by physicists, such as path integrals and perturbation series.

The similarities between the Schrödinger equation and the heat equation were used in [3] to create a theoretical framework for representing and studying the solutions to the Schrödinger problem, which is summarized here. 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 equation is a limited one, because the exponential decay of the heat equation's fundamental solution is not available here. Therefore, different formulations and proofs needed to be constructed for the basic representation theorems in section 2, as well as for the main theorem in section 4. For example, the Poisson integral formula (14) with the Schrödinger kernel (11) is shown to hold in the "Abel summable" sense [5, Sec. 1.5][6, Sec. 6.2].

Section 2 is devoted to the basic integral representation of a solution of the Schrödinger equation in terms of prescribed data and the fundamental solution (11). Here, unlike [3], we do not consider boundary-value problems, so the representation consists of two terms, a Poisson integral incorporating the initial data and a source integral. (In a boundary-value problem there is a third term incorporating boundary data.) For the free Schrödinger equation (6) with a known nonhomogeneous term F(x,t), the source integral (10) simply gives the contribution of F to the solution. In the more interesting case of a homogeneous equation including a potential, F involves the unknown function (multiplied by the potential), so the representation theorem yields an integral equation that must be solved. The crucial feature of the integral operator in (10) is that the upper limit of the time integration is t, the time variable of the solution, rather than $+\infty$ or some constant. This is the Volterra structure that causes the iterative solution of the equation to converge exponentially. Thus the initial-value problem for the Schrödinger PDE has been expressed as a Volterra integral equation of the second kind with respect to time. Our main task is to use the Picard-Neumann method of successive approximation to construct the unique solution of this integral equation. The abstract theory of such iterative solutions for linear operators in arbitrary Banach spaces is outlined in section 3.

The main theorem is proved in section 4. It treats a Volterra integral equation for a function of t taking values at each t in some Banach space, \mathcal{B} , such as $L^2(\mathbb{R}^3)$. More precisely, one has bounded operators $A(t,\tau):\mathcal{B}\to\mathcal{B}$, with the bound independent of the time variables, that satisfy the Volterra property that $A(t,\tau)=0$ unless $\tau< t$. It can then be proved inductively that the jth term of the Neumann series has norm proportional to $t^j/j!$. The conclusion is that the series converges in the topology of $L^\infty((0,T);\mathcal{B})$ for t< T. A variant with L^∞ replaced by L^p is also given.

In section 5 the main theorem is applied to some simple and familiar cases. First, we consider classical integral equations, such as one with a kernel that is Hilbert–Schmidt in space and Volterra in time. Then we return to the Schrödinger problem set up in section 2, with a

bounded potential function. In that case the unitarity of the free Schrödinger evolution operator between fixed times is the key to proving boundedness of the integral operator, and the resulting Neumann series is a standard form of time-dependent perturbation theory.

2. The Poisson integral and source integral theorems

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

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

where *H* is the Hamiltonian, given by

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

In the "free" case, V(x,t) = 0, the equation becomes

$$i\hbar\partial_t \Psi(x,t) = -a^2 \Delta_x \Psi(x,t), \quad \forall (x,t) \in \mathbb{R}^n \times \mathbb{R},$$
 (3)

where

$$a^2 = \frac{\hbar^2}{2m} \,. \tag{4}$$

For the differential operator appearing in (3) we introduce the notation

$$L = a^2 \Delta_x + i\hbar \partial_t \,. \tag{5}$$

Unlike the corresponding operator for the heat equation, L is formally self-adjoint with respect to the usual L^2 inner product.

We now consider the more general equation

$$Lu(x,t) \equiv a^2 \Delta_x u(x,t) + i\hbar \partial_t u(x,t) = F(x,t), \tag{6}$$

again in all of space-time. If the source term F(x,t) is prescribed, (6) is a nonhomogeneous version of the free Schrödinger equation. In order to get an integral equation for the homogeneous problem with a potential V(x,t), however, we will later take F(x,t) to be V(x,t)u(x,t). In any case, one imposes the initial condition

$$u(x,0) = f(x), \quad \forall (x,t) = (x,0) \in \mathbb{R}^n \times \{t=0\}$$
 (7)

and usually concentrates attention tacitly on t > 0.

The initial-value problem for (6) with the nonhomogeneous initial condition (7) can be reduced to the analogous problem with homogeneous initial condition by decomposing the solution u into two integral representations:

$$u(x,t) = \Phi(x,t) + \Pi(x,t), \tag{8}$$

where $\Phi(x,t)$, called the source term, contains the effects of F and has null initial data, while $\Pi(x,t)$, the Poisson integral term, solves the homogeneous equation (3) with the data (7). We shall show (Theorem 2) that

$$\Pi(x,t) = e^{-itH_0/\hbar} f(x) = \int_{\mathbb{R}^n} K_f(x,y,t) f(y) \, dy \tag{9}$$

and

$$\Phi(x,t) = \int_0^t e^{-itH_0/\hbar} e^{i\tau H_0/\hbar} F(\cdot,\tau) \, d\tau = -\frac{i}{\hbar} \int_0^t \int_{\mathbb{R}^n} K_f(x,y,t-\tau) F(y,\tau) \, dy \, d\tau. \tag{10}$$

Here $K_f(x, y, t)$ is the fundamental solution (free propagator) to the Schrödinger equation (3) in \mathbb{R}^n , which is given by

$$K_{\rm f}(x,y,t) \equiv K_{\rm f}(x-y,t) = \left(\frac{m}{2\pi\hbar it}\right)^{n/2} e^{im|x-y|^2/2\hbar t}, \quad \forall x,y \in \mathbb{R}^n, t \neq 0.$$
 (11)

The formula (9) is equivalent to the statement that $K_f(x, y, t)$ as a function of (x, t) satisfies the homogeneous free Schrödinger equation and the initial condition

$$K_{\mathbf{f}}(x,y,0) = \lim_{t \downarrow \tau} K_{\mathbf{f}}(x,y,t-\tau) = \delta(x-y). \tag{12}$$

Thus $K_f(x,y,t)$ vanishes as a distribution as $t \to 0$ in the region $x \neq y$, even though as a function it does not approach pointwise limits there. The formula (10) is equivalent to the alternative characterization that K_f is the causal solution of the nonhomogeneous equation

$$LK_{\rm f}(x,y,t-\tau) = \delta(x-y)\delta(t-\tau), \tag{13}$$

where *L* acts on the (x, t) variables.

The following theorem introduces the Poisson integral, which gives the solution of the initial-value problem for the free Schrödinger equation. Our discussion of the Poisson integral is somewhat more detailed than that of Evans [7], especially concerning the role of Abel summability.

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

$$u(x,t) = K_{f} * f = \int_{\mathbb{R}^{n}} K_{f}(x - y, t) f(y) \, dy \tag{14}$$

exists and is a solution of the equation

$$Lu(x,t) = a^2 \Delta_x u(x,t) + i\hbar \partial_t u(x,t) = 0, \quad \forall (x,t) \in \mathbb{R}^n \times \mathbb{R},$$
 (15)

and it satisfies the initial condition (7) in the sense of Abel summability. The Poisson integral defines a solution of the free Schrödinger equation in $\mathbb{R}^n \times \{t \neq 0\}$ (including negative t). This solution is extended into $\mathbb{R}^n \times \mathbb{R}$ by the initial condition u(x,0) = f(x) at 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 (15), (14) can be interchanged to verify that the Poisson integral solves the Schrödinger equation. This hypothesis is obtained from [7, Chapter IV].

The harder part is verifying the initial value. Assuming t > 0, let $y = x + \gamma z$, where $\gamma^2 =$ $2\hbar t/m$; then we can rewrite the Poisson integral as

$$u(x,t) = \left(\frac{1}{\pi i}\right)^{n/2} \int_{\mathbb{R}^n} e^{i|z|^2} f(x+\gamma z) dz$$
 (16)

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

$$(\pi i)^{n/2}u(x,t) = \int_{\mathbb{R}^n} e^{i|z|^2} f(x+\gamma z) dz = I_1 + I_2 + I_3,$$
(17)

where

$$I_{1} = \int_{|z| \le \epsilon} e^{i|z|^{2}} \{ f(x + \gamma z) - f(x) \} dz,$$

$$I_{2} = \int_{|z| \ge \epsilon} e^{i|z|^{2}} f(x + \gamma z) dz,$$
(18)

$$I_2 = \int_{|z| \ge \epsilon} e^{i|z|^2} f(x + \gamma z) \, dz,\tag{19}$$

$$I_3 = \int_{|z| < \epsilon} e^{i|z|^2} f(x) dz. \tag{20}$$

To dispose of I_1 , let x be a point in \mathbb{R}^n where f is continuous: $\forall \eta > 0 \ \exists \delta > 0$ such that $\forall y \in \mathbb{R}^n \text{ with } |y-x| < \delta \text{ one has } |f(y)-f(x)| < \eta. \text{ Given } \epsilon \text{ (however large) and } \eta \text{ (however large)}$ small), choose t (hence γ) so small that $\gamma \epsilon < \delta$; then $|f(x + \gamma z) - f(x)| < \eta$ for all z such that $|z| \leq \epsilon$. Therefore,

$$|I_1| \le \eta \int_{|z| \le \epsilon} dz,\tag{21}$$

which can be made arbitrarily small in the limit $t \to 0$.

On the other hand, since $f \in L^1(\mathbb{R}^n)$,

$$|I_2| \le \int_{|z| \ge \epsilon} |f(x + \gamma z)| \, dz \to 0 \tag{22}$$

(not necessarily uniformly in x) as $\epsilon \to \infty$. Thus the initial value $u(x,0^+)$ comes entirely from I_3 .

To evaluate I_3 we use the Fresnel integral formula

$$\int_{\mathbb{R}^n} e^{i|z|^2} dz = (\pi i)^{n/2}.$$
 (23)

A proof of (23) with n=1, which converges classically, appears in [8, pp. 82–83]. The one-dimensional formula appears to imply the product version by

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

Therefore, we have

$$\lim_{\epsilon \to \infty} I_3 = (\pi i)^{n/2} f(x), \tag{24}$$

which is what we want to prove.

However, the integral on the left side of (23) is rather questionable when n > 1, so we reconsider it in polar coordinates:

$$\int_{\mathbb{R}^n} e^{i|z|^2} dz = \int_0^\infty \int_{S^{n-1}} e^{i\rho^2} \rho^{n-1} d\rho d\Omega \equiv \omega_n \int_0^\infty \rho^{n-1} e^{i\rho^2} d\rho.$$

The surface area of the unit *n*-sphere is

$$\omega_n = 2\pi^{n/2}/\Gamma\left(\frac{n}{2}\right). \tag{25}$$

With the substitutions $t = \rho^2$, m = (n-2)/2, we obtain

$$\int_{\mathbb{R}^n} e^{i|z|^2} dz = \frac{\omega_n}{2} \int_0^\infty t^m e^{it} dt, \tag{26}$$

which technically is not convergent. Therefore. we insert the Abel factor $e^{-\alpha t}$ ($\alpha > 0$) into (26) to get

$$A(\alpha) \equiv \frac{\omega_n}{2} \int_0^\infty e^{-\alpha t} t^m e^{it} dt.$$
 (27)

This integral is convergent, and it can be transformed as

$$\frac{2A(\alpha)}{\omega_n} = \lim_{r \to \infty} \int_0^r e^{-\alpha t} t^m e^{it} dt = \lim_{r \to \infty} i \int_0^{ir} e^{-i\alpha z} (iz)^m e^{-z} dz.$$

The path of integration can be moved back to the positive real axis, because the integral over the arc of radius *r* tends to 0. Thus

$$\frac{2A(\alpha)}{\omega_n} = i^{n/2} \int_0^\infty e^{-i\alpha z} z^{(n/2)-1} e^{-z} \, dz,$$

and in the limit

$$A(0) = \frac{1}{2}\omega_n i^{n/2} \Gamma\left(\frac{n}{2}\right) = (\pi i)^{n/2}.$$
 (28)

This analysis confirms (23) in an alternative way and gives it a rigorous meaning.

This completes the proof that the Poisson integral has the initial value u(x,0) = f(x) at all points x where f is continuous.

Theorem 2 establishes formula (10) rigorously. Our proof is partly based on [9], which considers the nonhomogeneous Schrödinger equation (6) in the more abstract form

$$i\hbar \frac{\partial u(t)}{\partial t} = H_0 u(t) + F(t). \tag{29}$$

Here and later, I will denote the time interval (0,T), where T is a positive constant. In Theorem 2 we deal with the space $L^{\infty}(I;\mathcal{B})$ of functions u(t) taking values in the Banach space \mathcal{B} , equipped with the norm (cf. Definition 5)

$$||u||_{L^{\infty}(I;\mathcal{B})} = \inf\{M \ge 0 : ||u(t)||_{\mathcal{B}} \le M \text{ for almost all } t \in [0,T]\}.$$
 (30)

Theorem 2. Let f(x) belong to some Banach space \mathcal{B} of functions on \mathbb{R}^n that includes those for which $(1+|y|^2)f(y) \in L^1(\mathbb{R}^n)$. Furthermore, suppose that the source term F(x,t) is continuous in t and satisfies the condition

$$||F(\cdot,t)||_{L^1(\mathbb{R}^n)} \le \xi(t), \qquad ||\xi||_{L^\infty(I)} \le M$$
 (31)

for some positive constant M. The solution of the initial-value problem for the nonhomogeneous Schrödinger equation (6) can be represented in the form $u = \Pi + \Phi$ of (8), where the initial term is

$$\Pi(x,t) = \int_{\mathbb{R}^n} K_f(x,y,t) f(y) \, dy \tag{32}$$

and the source term is

$$\Phi(x,t) = -\frac{i}{\hbar} \int_0^t \int_{\mathbb{R}^n} K_f(x,y,t-\tau) F(y,\tau) \, dy \, d\tau. \tag{33}$$

Here $K_f(x,y,t)$ is the fundamental solution (11) and u(x,0) = f(x). The solution u belongs to the Banach space $L^{\infty}(I;\mathcal{B})$.

Proof. Theorem 1 shows that the Poisson integral Π solves the initial-value problem for the homogeneous Schrödinger equation. We claim that the solution of the full problem has the Volterra integral representation

$$u(x,t) = \int_{\mathbb{R}^n} K_f(x,y,t) f(y) \, dy - \frac{i}{\hbar} \int_0^t \int_{\mathbb{R}^n} K_f(x,y,t-\tau) F(y,\tau) \, dy \, d\tau$$

$$\equiv \Pi(x,t) + \Phi(x,t). \tag{34}$$

By applying the Schrödinger operator (5) to u(t), we have

$$Lu = L\Pi + L\Phi = a^{2}\Delta_{x}\Phi + i\hbar\frac{\partial\Phi}{\partial t}$$

$$= a^{2}\left(-\frac{i}{\hbar}\right)\Delta_{x}\int_{\mathbb{R}^{n}}K_{f}(x,y,t-\tau)F(y,\tau)\,dy\,d\tau$$

$$+ i\hbar\frac{\partial}{\partial t}\left(-\frac{i}{\hbar}\int_{0}^{t}\int_{\mathbb{R}^{n}}K_{f}(x,y,t-\tau)F(y,\tau)\,dy\,d\tau\right)$$

$$= \int_{0}^{t}\int_{\mathbb{R}^{n}}LK_{f}(x,y,t-\tau)F(y,\tau)\,dy\,d\tau$$

$$+ \lim_{t\downarrow\tau}\int_{\mathbb{R}^{n}}K_{f}(x,y,t-\tau)F(y,\tau)dy.$$
(35)

But $LK_f(x, y, t - \tau) = 0$ for all $t > \tau$, and Theorem 1 shows that $K_f(x, y, t - \tau) \to \delta(x - y)$. Therefore, we have

$$L\Phi = F(x, t). \tag{36}$$

Furthermore, it is clear that F(x,0) = 0. Therfore, by linearity the sum $u = \Pi + \Phi$ solves the problem.

Another way to express (34) is via unitary operators:

$$u(t) = e^{-itH_0/\hbar} f(x) - \frac{i}{\hbar} \int_0^t e^{-itH_0/\hbar} e^{i\tau H_0/\hbar} F(\tau) d\tau.$$
 (37)

Consider the integral

$$-i\hbar^{-1} \int_{0}^{t} e^{i\tau H_{0}/\hbar} Lu(\tau) d\tau = -i\hbar^{-1} \int_{0}^{t} e^{i\tau H_{+}0/\hbar} \left(-a\Delta u(\tau) + i\hbar \frac{\partial u(\tau)}{\partial \tau} \right) d\tau$$

$$= -i\hbar^{-1} \int_{0}^{t} e^{i\tau H_{0}/\hbar} \left(-H_{0}u(\tau) + i\hbar \frac{\partial u}{\partial \tau} \right) d\tau$$

$$= \int_{0}^{t} \frac{\partial}{\partial \tau} \left(e^{i\tau H_{0}/\hbar} u(\tau) \right) d\tau$$

$$= e^{itH_{0}/\hbar} u(t) - u(0).$$
(38)

This calculation implies that

$$u(t) = e^{-itH_0/\hbar}u(0) - i\hbar^{-1}e^{-itH_0/\hbar} \int_0^t e^{i\tau H_0/\hbar} Lu(\tau) d\tau, \tag{39}$$

which is equivalent to (37) and to the Volterra integral formula (34). The expression $u(t)-e^{-itH_0/\hbar}u(0)$ is simply the source term $\Phi(x,t)$. Taking its Banach space norm and using the unitarity of the evolution operator $e^{-itH_0/\hbar}$ and the fundamental theorem of calculus, we have

$$\|\Phi(t)\| = \left\| i\hbar^{-1}e^{-itH_{0}/\hbar} \int_{0}^{t} e^{i\tau H_{0}/\hbar} Lu(\tau) d\tau \right\|$$

$$\leq \frac{1}{\hbar} \int_{0}^{t} \|Lu\| d\tau \leq \frac{1}{\hbar} \int_{0}^{t} \xi(\tau) d\tau \leq \frac{Mt}{\hbar} ,$$
(40)

because of (31). Therefore, $\Phi \to 0$ when $t \to 0$. Since $e^{-itH_0/\hbar}u(0)$ is another way of writing $\Pi(x,t)$, we have again established that (8) is the desired solution.

Remark 3. The L^1 condition of Theorem 1 has not been used in the second, more abstract proof of Theorem 2, because the limits $(t \downarrow 0)$ are being taken in the topology of the quantum Hilbert space $L^2(\mathbb{R}^n)$, not pointwise.

Corollary 4. The homogeneous Schrödinger initial-value problem,

$$i\hbar\partial_t\Psi(x,t) = -a^2\Delta\Psi(x,t) + V(x,t)\Psi(x,t), \qquad \Psi(x,0) = f(x), \tag{41}$$

is equivalent to a nonhomogeneous Volterra integral equation of the second kind,

$$\Psi(x,t) = \int_{\mathbb{R}^n} K_f(x,y,t) f(y) \, dy - \frac{i}{\hbar} \int_0^t \int_{\mathbb{R}^n} K_f(x,y,t-\tau) V(y,\tau) \Psi(y,\tau) \, dy \, d\tau. \tag{42}$$

Proof. (42) is (34) with the source F in (6) identified with $V\Psi$.

3. Integral equations and Neumann series

In this section we introduce integral operators in arbitrary Banach spaces in order to set up a framework for constructing solutions to the Schrödinger equation. This section is a preliminary to the general Volterra theorems that are proved in section 4. It uses as a foundation Kress's treatment of linear integral equations [2].

In operator notation, an integral equation of the second kind has the structure

$$\phi - \hat{Q}\phi = f,\tag{43}$$

where \hat{Q} is a bounded linear operator from a Banach space \mathcal{W} to itself, and ϕ and f are in \mathcal{W} . A solution ϕ exists and is unique for each f if and only if the inverse operator $(1-\hat{Q})^{-1}$ exists (where 1 indicates the identity operator). For Volterra operators, the focus of our attention, the existence of the inverse operator will become clear below. Equivalently, the theorems of the next section will prove that the spectral radius of a Volterra operator is zero. For these purposes we need to work in Lebesgue spaces $\mathcal{W} = L^p(I;\mathcal{B})$ (including, especially, $p = \infty$) of functions of t to obtain useful estimates.

Definition 5. Let (Ω, Σ, μ) be a measure space and \mathcal{B} be a Banach space. The collection of all essentially bounded measurable functions on Ω taking values in \mathcal{B} is denoted $L^{\infty}(\Omega, \mu; \mathcal{B})$, the reference to μ being omitted when there is no danger of confusion. The essential supremum of a function $\varphi \colon \Omega \to \mathcal{B}$ is given by

$$\|\varphi\|_{L^{\infty}(\Omega;\mathcal{B})} = \inf\{M \ge 0 : \|\varphi(x)\|_{\mathcal{B}} \le M \text{ for almost all } x\}. \tag{44}$$

Definition 6. Let \mathcal{B}_1 and \mathcal{B}_2 be Banach spaces and Ω be some measurable space. For each $(x,y) \in \Omega \times \Omega \equiv \Omega^2$ let $A(x,y) : \mathcal{B}_1 \to \mathcal{B}_2$ be a bounded linear operator, and suppose that the function $A(\cdot,\cdot)$ is measurable. At each (x,y) define its norm

$$||A(x,y)||_{\mathcal{B}_1 \to \mathcal{B}_2} = \inf\{M \ge 0 : ||A(x,y)\phi|| \le M||\phi||, \quad \forall \phi \in \mathcal{B}_1\}.$$
 (45)

If $\mathcal{B}_1 = \mathcal{B}_2 = \mathcal{B}$, then one abbreviates $||A(x,y)||_{\mathcal{B}_1 \to \mathcal{B}_2}$ as $||A(x,y)||_{\mathcal{B}}$ or even ||A(x,y)||. Now define the uniform norm

$$||A||_{L^{\infty}(\Omega^{2};\mathcal{B}_{1}\to\mathcal{B}_{2})} \equiv \inf\{M \geq 0 : ||A(x,y)|| \leq M \text{ for almost all } (x,y) \in \Omega^{2}\}$$

$$\equiv \operatorname{ess sup}_{(x,y)\in\Omega^{2}} ||A(x,y)||_{\mathcal{B}_{1}\to\mathcal{B}_{2}}$$

$$(46)$$

and call $A(\cdot, \cdot)$ a uniformly bounded operator kernel if $||A||_{L^{\infty}(\Omega^2; \mathcal{B}_1 \to \mathcal{B}_2)}$ is finite.

Definition 7. In Definition 6 let $\Omega = I = (0, T)$. If A is a uniformly bounded operator kernel, the operator \hat{Q} defined by

$$\hat{Q}f(t) = \int_0^t A(t,\tau)f(\tau) d\tau \tag{47}$$

is called a bounded Volterra operator on $L^{\infty}(I;\mathcal{B})$ with kernel A.

Remark 8. In (47) one may write the integration as $\int_0^T \cdots d\tau$ if one has defined $A(t,\tau)$ to be 0 whenever $\tau > t$. In that case A is called a Volterra kernel.

In Corollary 4 we have reformulated the Schrödinger equation as an integral equation of the second kind. The existence and uniqueness of its solution can be found by analysis of the Neumann series. The successive approximations (Picard's algorithm)

$$\phi_N = \hat{Q}\phi_{N-1} + f = \sum_{j=0}^{N} \hat{Q}^j f$$
 (48)

converge to the exact solution of the integral equation (43), if some technical conditions are satisfied. In the terminology of an arbitrary Banach space, one must establish that

- 1. the function $\phi_0 \equiv f$ belongs to a Banach space \mathcal{B} ,
- 2. the integral operator \hat{Q} is a bounded Volterra operator on $L^{\infty}(I;\mathcal{B})$, and
- 3. the infinite (Neumann) series $\phi = \sum_{j=0}^{\infty} \hat{Q}^{j} f$ is a convergent series with respect to the topology of $L^{\infty}(I; \mathcal{B})$.

If these three conditions are satisfied, then the Neumann series provides the exact solution to the integral equation (43). In the Schrödinger case, therefore, it solves the original initial-value problem for the Schrödinger equation. This program will be implemented in detail in the next two sections.

4. Volterra kernels and successive approximations

In this section we implement the method of successive approximations set forth in section 3. The Volterra operator has a nice property, known as the simplex structure, which makes its infinite Neumann series converge. This claim is made precise in our main theorems.

It follows from the convergence of the Neumann series that the spectral radius of the Volterra integral operator of the second kind is zero. In Kress's treatment of the heat equation [2] the logic runs in the other direction — convergence follows from a theorem on spectral radius. For the Schrödinger equation we find it more convenient to prove convergence directly.

Hypotheses

- \mathcal{B} is a Banach space, and I = (0, T) is an interval, with closure \overline{I} .
- For all $(t,\tau) \in \overline{I}^2$, $A(t,\tau)$ is a linear operator from \mathcal{B} to \mathcal{B} .
- the operator kernel $A(t,\tau)$ is measurable and uniformly bounded, in the sense of Definition 6, with bound $\|A\|_{L^{\infty}(I^2;\mathcal{B}\to\mathcal{B})}=D$.
- $A(t,\tau)$ satisfies the Volterra condition, $A(t,\tau)=0$ if $\tau>t$.

Our primary theorem, like the definitions in section 3, deals with the space $L^{\infty}(I;\mathcal{B})$. We also provide variants of the theorem and the key lemma for other Lebesgue spaces, $L^1(I;\mathcal{B})$ and $L^p(I;\mathcal{B})$. In each case, the space \mathcal{B} is likely, in applications, to be itself a Lebesgue space of functions of a spatial variable, $L^m(\mathbb{R}^n)$, with no connection between m and p.

The first step of the proof is a fundamental lemma establishing a bound on the Volterra operator that fully exploits its simplex structure. This argument inductively establishes the norm of each term in the Neumann series, from which the convergence quickly follows. In the lemmas, j (the future summation index) is understood to be an arbitrary nonnegative integer (or even a real positive number).

Lemma 9. Let the Volterra integral operator, $\hat{Q}: L^{\infty}(I; \mathcal{B}) \to L^{\infty}(I; \mathcal{B})$, be defined by

$$\hat{Q}\phi(t) = \int_0^T A(t,\tau)\phi(\tau) d\tau = \int_0^t A(t,\tau)\phi(\tau) d\tau. \tag{49}$$

Let $\phi \in L^{\infty}(I;\mathcal{B})$ and assume that $\exists C > 0$ such that for each subinterval J_t of the form (0,t), we have $\|\phi\|_{L^{\infty}(J_t;\mathcal{B})} \equiv \operatorname{ess\,sup}_{0<\tau< t} \|\phi(\tau)\|_{\mathcal{B}} \leq Ct^j$. Assume that the Hypotheses are satisfied. Then it follows that

$$\|\hat{Q}\phi\|_{L^{\infty}(J_t,\mathcal{B})} \le \frac{DC}{j+1} t^{j+1}. \tag{50}$$

Proof. Recall that D is defined so that $||A(t,\tau)|| \leq D < \infty$ for all $(t,\tau) \in \overline{I}^2$. The $L^{\infty}(J_t;\mathcal{B})$ norm of the function $\hat{Q}\phi(\cdot)$ is

$$\|\hat{Q}\phi\|_{L^{\infty}(J_{t};\mathcal{B})} = \sup_{t_{1} \leq t} \left\| \int_{0}^{t_{1}} A(t,\tau)\phi(\tau) d\tau \right\| \leq \sup_{t_{1} \leq t} \int_{0}^{t_{1}} \|A(t,\tau)\phi(\tau)\| d\tau$$

$$\leq \sup_{t_{1} \leq t} \int_{0}^{t_{1}} \|A(t,\tau)\| \|\phi(\tau)\| d\tau \leq \sup_{t_{1} \leq t} \int_{0}^{t_{1}} DC\tau^{j} d\tau$$

$$= \sup_{t_{1} \leq t} DC \frac{t_{1}^{j+1}}{j+1} = \frac{DCt^{j+1}}{j+1}. \qquad \Box$$
(51)

Lemma 10. Let the Volterra integral operator, $\hat{Q}: L^1(I;\mathcal{B}) \to L^1(I;\mathcal{B})$, be defined by (49). Let $\phi \in L^1(I;\mathcal{B})$, and assume that $\exists C > 0$ such that for each subinterval $J_t = (0,t)$, we have

$$\|\phi\|_{L^1(J_t;\mathcal{B})} \equiv \int_0^t \|\phi(\tau)\| d\tau \le Ct^j.$$
 (52)

Assume that the Hypotheses are satisfied. Then it follows that

$$\|\hat{Q}\phi\|_{L^1(J_t,\mathcal{B})} \le \frac{DC}{j+1}t^{j+1}.$$
 (53)

Proof. The argument is the same as before, except that the $L^1(J_t; \mathcal{B})$ norm of $\hat{Q}\phi(\cdot)$ is

$$\|\hat{Q}\phi\|_{L^{1}(J_{t};\mathcal{B})} = \int_{0}^{t} \left\| \int_{0}^{t_{1}} A(t,\tau)\phi(\tau) d\tau \right\| dt_{1} \leq \int_{0}^{t} \int_{0}^{t_{1}} \|A(t,\tau)\| \|\phi(\tau)\| d\tau$$

$$\leq \int_{0}^{t} D \int_{0}^{t_{1}} \|\phi(\tau)\| d\tau dt_{1} \leq \int_{0}^{t} D \|\phi\|_{L^{1}(J_{t_{1}};\mathcal{B})} dt_{1}$$

$$\leq \int_{0}^{t} DCt_{1}^{j} dt_{1} = \frac{DCt^{j+1}}{j+1}. \qquad \Box$$

$$(54)$$

Corollary 11. Let the Volterra integral operator, $\hat{Q}: L^p(I;\mathcal{B}) \to L^p(I;\mathcal{B})$, where $1 , be defined by (49). Let <math>\phi \in L^p(I;\mathcal{B})$ and assume that $\exists C > 0$ such that for each subinterval $J_t = (0,t)$, we have

$$\|\phi\|_{L^p(J_t;\mathcal{B})} \equiv \left(\int_0^t \|\phi(\tau)\|_{\mathcal{B}}^p d\tau\right)^{1/p} \le Ct^n.$$
 (55)

Assume that the Hypotheses are satisfied. Then it follows that

$$\|\hat{Q}\phi\|_{L^p(J_t,\mathcal{B})} \le \frac{DC}{j+1} t^{j+1}.$$
 (56)

Proof. This follows from Lemmas 9 and 10 by the Riesz–Thorin theorem [10, pp. 27–28].

It may be of some interest to see how the L^p theorem can be proved directly. The proof of the needed lemma uses Folland's proof of Young's inequality [4] as a model.

Lemma 12. Let the Volterra integral operator, $\hat{Q}: L^p(I;\mathcal{B}) \to L^p(I;\mathcal{B})$, where $1 , be defined by (49). Let <math>\phi \in L^p(I;\mathcal{B})$ and assume that $\exists C > 0$ such that for each subinterval $J_t = (0,t)$, we have

$$\|\phi\|_{L^p(J_t;\mathcal{B})} \equiv \left(\int_0^t \|\phi(\tau)\|_{\mathcal{B}}^p d\tau\right)^{1/p} \le Ct^n.$$
 (57)

Assume that the Hypotheses are satisfied. Then it follows that

$$\|\hat{Q}\phi\|_{L^p(J_t,\mathcal{B})} \le \frac{DCt^{j+1}}{[p(j+1)]^{1/p}}.$$
 (58)

Proof. Let q be the conjugate exponent $(p^{-1}+q^{-1}=1)$. The Banach-space norm of $\hat{Q}\phi(t)$ satisfies

$$\|\hat{Q}\phi(t_{1})\|_{\mathcal{B}} \leq \left(\int_{0}^{t_{1}} \|A(t_{1},\tau)\| d\tau\right)^{1/q} \left(\int_{0}^{t_{1}} \|A(t_{1},\tau)\| \|\phi(\tau)\|^{p} d\tau\right)^{1/p}$$

$$\leq D^{1/q} \left(\int_{0}^{t_{1}} d\tau\right)^{1/q} \left(\int_{0}^{t_{1}} D\|\phi(\tau)\|^{p} d\tau\right)^{1/p}$$

$$\leq D^{1/q} D^{1/p} t_{1}^{1/q} \left(\int_{0}^{t_{1}} \|\phi(\tau)\|^{p} d\tau\right)^{1/p}$$

$$\leq D t_{1}^{1/q} \left(\int_{0}^{t_{1}} \|\phi(\tau)\|^{p} d\tau\right)^{1/p}.$$
(59)

Then we must raise both sides to the *p*th power and integrate, seeing by Fubini's theorem that

$$\int_{0}^{t_{1}} \|\hat{Q}\phi(t_{1})\|^{p} dt_{1} \leq \int_{0}^{t} D^{p} t_{1}^{p/q} \int_{0}^{t_{1}} \|\phi(\tau)\|^{p} d\tau dt_{1} \leq \int_{0}^{t} D^{p} \int_{0}^{t} t_{1}^{p/q} \|\phi\|_{L^{p}(J_{t_{1}};\mathcal{B})}^{p} dt_{1}
\leq D^{p} \int_{0}^{t} C^{p} t_{1}^{np+p/q} dt_{1} \leq D^{p} C^{p} \frac{t^{np+p/q+1}}{np+\frac{p}{q}+1} = D^{p} C^{p} \frac{t^{(j+1)p}}{jp+p},$$
(60)

since $1 + \frac{p}{q} = p$. Now take the *p*th root, getting

$$\|\hat{Q}\phi\|_{L^p(J_t;\mathcal{B})} \le DC \, \frac{t^{j+1}}{[p(j+1)]^{1/p}} \,. \qquad \Box$$
 (61)

The following theorem is the main theorem of [3]; its proof is corrected here.

Theorem 13. (L^{∞} **Volterra Theorem)** Let the Hypotheses be satisfied, and let \hat{Q} be defined by (49). Let f belong to $L^{\infty}(I;\mathcal{B})$. Then the Volterra integral equation

$$\phi = \hat{Q}\phi + f \tag{62}$$

can be solved by successive approximations. That is, the Neumann series for ϕ ,

$$\phi = \sum_{j=0}^{\infty} \hat{Q}^j f,\tag{63}$$

converges in the topology of $L^{\infty}(I; \mathcal{B})$.

Proof. Let $||f||_{L^{\infty}(I;\mathcal{B})} = C_0$. Of course, $||f||_{L^{\infty}(J_t;\mathcal{B})} \leq C_0$ on a smaller interval, $J_t = (0,t)$, so by Lemma 9 with j = 0,

$$\|\hat{Q}^1 f\|_{L^{\infty}(I_t;\mathcal{B})} \le DC_0 t.$$
 (64)

Then by inductively applying Lemma 9 with $C = D^{j-1}C_0/(j-1)!$, we see that the *j*th term of the Neumann series, $\hat{Q}^j f$, has, because of its simplex structure, the bound

$$\|\hat{Q}^j f\|_{L^{\infty}(J_t;\mathcal{B})} \le D^j C_0 \frac{t^j}{j!}. \tag{65}$$

Therefore, the series (63) is majorized by

$$C_0 \sum_{n=0}^{\infty} \frac{D^j t^j}{j!} = \|f\|_{L^{\infty}(I;\mathcal{B})} e^{Dt}$$
(66)

for all $t \in (0, T]$. Therefore, the Neumann series converges in the topology of $L^{\infty}(I; \mathcal{B})$.

The L^{∞} norm on the time behavior is the most natural and likely one to apply to solutions of a time-evolution equation (especially for the Schrödinger equation with \mathcal{B} a Hilbert space, because of the unitary of the evolution). However, the other L^p norms may prove to be useful, and it is easy to generalize the theorem to them. Note that the appropriate condition on $A(t,\tau)$ is still the uniform boundedness of Definition 6.

Theorem 14. (L^1 **Volterra Theorem)** Let the Hypotheses be satisfied, and let \hat{Q} be defined by (49). Let f belong to $L^1(I;\mathcal{B})$. Then the Volterra integral equation $\phi = \hat{Q}\phi + f$ can be solved by successive approximations. That is, the Neumann series for ϕ , (63), converges in the topology of $L^1(I;\mathcal{B})$.

Proof. Let $||f||_{L^1(I;\mathcal{B})} = C_0$ and argue as before, except that Lemma 10 is used to bound all the terms $||\hat{Q}^j f||_{L^1(I_t;\mathcal{B})}$.

Theorem 15. (L^p **Volterra Theorem)** Let the Hypotheses be satisfied, and let \hat{Q} be defined by (49). Let f belong to $L^p(I;\mathcal{B})$. Then the Volterra integral equation $\phi = \hat{Q}\phi + f$ can be solved by successive approximations. That is, the Neumann series converges in the topology of $L^p(I;\mathcal{B})$.

Proof. The proof based on the Riesz–Thorin theorem goes exactly like the previous two, using Corollary 11. To prove the theorem directly, let $||f||_{L^p(I;\mathcal{B})} = C_0$ and use Lemma 12 inductively to show

$$\|\hat{Q}^{j}f\|_{L^{p}(J_{t};\mathcal{B})} \leq \frac{D^{j}}{p^{j/p}} \|f\|_{L^{p}(I;\mathcal{B})} \frac{t^{j}}{(j!)^{1/p}}.$$
(67)

To see whether the series

$$\sum_{j=0}^{\infty} \|\hat{Q}^{j} f\|_{L^{p}(I;\mathcal{B})} = \|f\|_{L^{p}(I;\mathcal{B})} \sum_{j=0}^{\infty} \frac{D^{j}}{p^{j/p}} \frac{t^{j}}{(j!)^{1/p}}$$
(68)

is convergent, we use the ratio test. Let

$$L = \lim_{j \to \infty} \left| \frac{a_{j+1}}{a_j} \right|, \qquad a_j = \|\hat{Q}^j f\|_{L^p(I;\mathcal{B})}. \tag{69}$$

Let $M(p) = Dp^{-1/p}$. Then

$$L = \lim_{n \to \infty} \frac{\|f\|_{L^{p}(I;\mathcal{B})} M(p)^{j+1} t^{j+1}}{[(j+1)!]^{1/p}} \cdot \frac{(j!)^{1/p}}{\|f\|_{L^{p}(I;\mathcal{B})} M(p)^{j} t^{j}}$$

$$= M(p) t \lim_{j \to \infty} (j+1)^{-1/p} = 0,$$
(70)

Thus L < 1, and by the ratio-test and series-majorization theorems, the Neumann series converges absolutely in the topology of $L^p(I; \mathcal{B})$.

5. Applications of the Volterra theorem

In this section we present some quick applications of the general Volterra theorem of section 4. The conclusions are already well known, or are obvious generalizations of those that are, so these examples just show how they fit into the general framework. More serious applications are delayed to later papers. The first set of examples comprises some of the standard elementary types of Volterra integral equations [11–13], generalized to vector-valued functions and functions of additional variables. The second application is to the Schrödinger problem set up in section 2; the result is essentially what is known in textbooks of quantum mechanics as "time-dependent perturbation theory".

Although we use the L^{∞} version of the theorem, Theorem 13, one could easily apply Theorems 14 and 15 as well. Thus a general setting for many examples is the generic double Lebesgue space defined as follows. As usual, let I=(0,T) be the maximal time interval considered. In the role of \mathcal{B} , consider the Lebesgue space $L^m(\mathbb{R}^n)$ of functions of an n-dimensional spatial variable. Then $L^{p,m}(I;\mathbb{R}^n)$ is the Banach space of functions on I taking values in $L^m(\mathbb{R}^n)$ and subjected to the L^p norm as functions of t. Thus

$$L^{p,m}(I;\mathbb{R}^n) = \left\{ \phi : \left(\int_I \left[\int_{\mathbb{R}^n} |\phi(y,\tau)|^m \, dy \right]^{p/m} d\tau \right)^{1/p} \equiv \|\phi\|_{L^{p,m}(I;\mathbb{R}^n)} < \infty \right\}. \tag{71}$$

When either p or m is ∞ , the Lebesgue norm is replaced by the essential supremum in the obvious way.

5.1. Classical integral equations

5.1.1. Spatial variables

For x and y in \mathbb{R}^n , let $K(x,t;y,\tau)$ be a uniformly bounded complex-valued function, satisfying the Volterra condition in (t,τ) . The Volterra operator kernel $A(t,\tau):L^m(\mathbb{R}^n)\to$

 $L^m(\mathbb{R}^n)$ is defined by

$$A(t,\tau)\phi(x) = \int_{\mathbb{R}^n} K(x,t;y,\tau)\phi(y) \, dy,\tag{72}$$

for $\phi \in L^m(\mathbb{R}^n)$. (We shall be using this equation for functions ϕ that depend on τ as well as y, so that $A(t,\tau)\phi$ is a function of (x,t,τ) .) To assure that $A(t,\tau)$ is a bounded Banach-space operator, we need to impose an additional technical condition on the kernel function K. The simplest possibility is to exploit the generalized Young inequality [4, Theorem (0.10)].

Suppose that we wish to treat functions $\phi(y,\tau) \in L^{\infty,\infty}(I;\mathbb{R}^n)$. Then (72) leads to

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

$$\leq ||\phi||_{L^{\infty,\infty}(I;\mathbb{R}^n)} \int_{\mathbb{R}^n} |K(x,t;y,\tau)| \, dy.$$
(73)

Therefore, if

$$\int_{\mathbb{R}^n} |K(x,t;y,\tau)| \, dy \le D \tag{74}$$

uniformly in (x, t, τ) , then

$$||A(t,\tau)\phi||_{L^{\infty,\infty}(I;\mathbb{R}^n)} \le D||\phi||_{L^{\infty,\infty}(I;\mathbb{R}^n)}. \tag{75}$$

That is,

$$||A||_{L^{\infty}(I^2:\mathcal{B}\to\mathcal{B})} \le D,\tag{76}$$

and Lemma 9 applies. Theorem 13 therefore proves that the Volterra integral equation $\phi = \hat{Q}\phi + f$ can be solved by iteration within $L^{\infty,\infty}(I;\mathbb{R}^n)$.

Now suppose instead that we want to work in $L^{\infty,1}(I;\mathbb{R}^n)$. In place of (73) we have

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

$$\leq \|\phi\|_{L^{\infty,1}(I;\mathbb{R}^n)} \sup_{y} |K(x,t;y,\tau)|. \tag{77}$$

This time we need the condition that

$$\int_{\mathbb{R}^n} |K(x,t;y,\tau)| \, dx \le D \tag{78}$$

uniformly in (y, t, τ) ; then

$$||A(t,\tau)\phi||_{L^{\infty,1}(I;\mathbb{R}^n)} \le D||\phi||_{L^{\infty,1}(I;\mathbb{R}^n)}$$
(79)

in place of (75). The argument concludes as before, using Lemma 10 and Theorem 14.

For $L^{\infty,p}(I;\mathbb{R}^n)$, the generalized Young inequality [4] assumes both (74) and (78) and assures that

$$||A(t,\tau)\phi||_{L^{\infty,p}(I;\mathbb{R}^n)} \le D||\phi||_{L^{\infty,p}(I;\mathbb{R}^n)}.$$
(80)

The argument concludes as before, using Lemma 12 and Theorem 15, proving convergence of the Neumann series within $L^{\infty,p}(I;\mathbb{R}^n)$.

5.1.2. Vector-valued functions

A similar but simpler situation is where \mathcal{B} is finite-dimensional, say \mathbb{C}^n . Then $A(t,\tau)$ is an $n \times n$ matrix. Boundedness of A as an operator is automatic, but uniformity in the time variables is still a nontrivial condition. The theorem then gives a vectorial generalization of the usual Neumann series for a scalar Volterra equation.

5.1.3. Hilbert–Schmidt operators

Although the generalized Young approach yields a theorem for $\mathcal{B} = L^2(\mathbb{R}^n)$, the boundedness of operators on that space is often proved from a stronger condition on their kernels. In our context a Hilbert–Schmidt kernel is a function $K : \mathbb{R}^n \times \mathbb{R} \times \mathbb{R}^n \times \mathbb{R} \to \mathbb{C}$ for which

$$\left(\int_{\mathbb{R}^{n}\times\mathbb{R}^{n}}|K(x,t;y,\tau)|^{2}\,dx\,dy\right)^{1/2}\equiv\|K(t,\tau)\|_{L^{2}(\mathbb{R}^{2n})}\leq D<\infty,\tag{81}$$

and, of course, we also want it to be Volterra in (t,τ) . In other words, $K(x,t;y,\tau)$ belongs to $L^{\infty,2}(I^2;\mathbb{R}^{2n})$ and vanishes (or is ignored in the integrals) when $\tau > t$. Then $A(t,\tau):L^2(\mathbb{R}^n)\to L^2(\mathbb{R}^n)$ defined by (72) is a Hilbert–Schmidt operator, which under our assumptions is uniformly bounded with norm at most D.

In parallel with (73) or (77) one has

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

$$\leq \left(\int_{\mathbb{R}^n} |K(x,t;y,\tau)|^2 dy\right)^{1/2} \left(\int_{\mathbb{R}^n} |\phi(y,\tau)|^2 dy\right)^{1/2}$$
(82)

and hence

$$||A(t,\tau)\phi(\cdot)||_{L^{2}(\mathbb{R}^{n})} \leq ||K(t,\tau)||_{L^{2}(\mathbb{R}^{2n})} ||\phi(\tau)||_{L^{2}(\mathbb{R}^{n})} \leq ||K||_{L^{\infty,2}(I^{2}:\mathbb{R}^{2n})} ||\phi(\tau)||_{L^{2}(\mathbb{R}^{n})}. \tag{83}$$

Therefore,

$$||A||_{L^{\infty}(I^2:\mathcal{B}\to\mathcal{B})} \le D,\tag{84}$$

and hence Lemma 9 and Theorem 13 apply as usual, establishing convergence of the Picard solution of $\phi = \hat{Q}\phi + f$ in the topology of $L^{\infty,2}(I,\mathbb{R}^n)$.

5.2. Perturbation theory for the Schrödinger equation

In Corollary 4 we converted the time-dependent Schrödinger problem to a Volterra integral equation, (42), wherein $K_f(x,y,t) = (4\pi i t)^{-n/2} e^{i|x-y|^2/4t}$. The solution of that equation by iteration (successive approximations, Picard algorithm, Neumann series) is effectively a power series in the potential V, so it is the same thing as a perturbation calculation with respect to a coupling constant multiplying V.

In this problem the Banach space \mathcal{B} is the Hilbert space $L^2(\mathbb{R}^n)$. (To assure pointwise convergence to the initial data, according to Theorem 2 and Remark 3, we should also take the intersection with $L^1(\mathbb{R}^n;(1+|x|^2)^{-1}\,dx)$.) In order for our method to work simply, we must assume that V(x,t) is a bounded potential. It may be time-dependent, but in that case its bound should be independent of t. That is, we assume

$$V \in L^{\infty}(\mathbb{R}^n \times I); \qquad |V(y,t)| \le D \text{ (almost everywhere)}.$$
 (85)

Note that the role of f in the abstract Volterra equation (62) is played by the entire first integral term in (42), $\int K_f(x, y, t) f(y) dy$.

From the other term of (42) we extract the kernel function

$$K(x,t;y,\tau) = -\frac{i}{\hbar}K_{\rm f}(x,y,t-\tau)V(y,\tau). \tag{86}$$

It satisfies neither the Hilbert–Schmidt condition (81) nor the generalized Young conditions (73) and (77). However, the resulting operator kernel can be factored as

$$A(t,\tau) = -\frac{i}{\hbar} U_{\rm f}(t-\tau) \hat{V}(\tau), \tag{87}$$

where U_f is the free time evolution (9) implemented by the kernel K_f , and \hat{V} is the operator of pointwise multiplication by the potential $V(y,\tau)$. It is well known [7, Chapter 4] that $U_f(t) = e^{-itH_0/\hbar}$ is unitary, and hence its norm as an operator on $L^2(\mathbb{R}^n)$ is 1. On the other hand,

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

$$\leq D^{2} \int_{\mathbb{R}^{n}} |f(y,\tau)|^{2} dy = D^{2} ||f(\tau)||_{L^{2}(\mathbb{R}^{n})}^{2},$$
(88)

so the operator norm of $\hat{V}(\tau)$ is

$$\|\hat{V}(\tau)\| = \|V(\cdot, \tau)\|_{L^{\infty}(\mathbb{R}^n)} \le \|V\|_{L^{\infty}(I \times \mathbb{R}^n)} \le D.$$
(89)

Therefore, the norm of the product operator is

$$||A(t,\tau)|| = ||(i\hbar)^{-1}U_f(t-\tau)\hat{V}(\tau)|| \le D/\hbar.$$
 (90)

Therefore, Lemma 9 and Theorem 13 apply to the integral equation (42), and we reach the desired conclusion:

Theorem 16. If the potential V(x,t) is uniformly bounded, then the time-dependent Schrödinger problem described in Corollary 4 can be solved by iteration. That is, the perturbation (Neumann) series converges in the topology of $L^{\infty}((0,T),L^2(\mathbb{R}^n))$ for any finite, positive T.

6. Concluding remarks

Most mathematical physics literature on the Schrödinger equation (for example, [14]) works in an abstract Hilbert-space framework and concentrates on proving that particular second-order elliptic Hamiltonian operators are self-adjoint, then describing their spectra and other properties. Here we have investigated a different aspect of the subject; we regard the time-dependent Schrödinger equation as a classical partial differential equation analogous to the heat or wave equation and study it by classical analysis.

The similarities between the Schrödinger and heat equations were exploited to create the theoretical framework, and then their technical differences were addressed. In section 2 the structure of solutions in terms of the free propagator K_f was worked out, and thereby the initial-value problem was recast as an integral equation.

The key feature of that equation is its Volterra character: It involves integration only up to the time in question. In this respect it is like the heat equation and unlike, for instance, the Poisson equation. The consequence of the Volterra property is that when the equation is solved by iteration, the jth iterate involves integration over a j-dimensional simplex (not a hypercube). The resulting volume factor of $(j!)^{-1}$ suggests that the series should converge.

The implementation of that idea in any particular case requires some technical work to prove that the operators $A(t,\tau)$ connecting any two times are bounded, and uniformly so. In section 4 we showed, in the setting of any Banach space, that that hypothesis is sufficient to establish the convergence of the Neumann series. In section 5 we verified the hypothesis in several simple examples, including the Schrödinger problem with a bounded potential.

In future work we hope to apply the Volterra theorem in contexts more complicated than the simple examples presented here. Preliminary work on those applications appears in Chapters 8 and 9 of [3]. Chapter 9 and [15] (see also [16]) implement an idea due to Balian and Bloch [17] to use a semiclassical Green function to construct a perturbation expansion for a smooth potential V(x,t). The solution of the Schrödinger equation is approximated in terms of classical paths, and the resulting semiclassical propagator $K_{\rm scl} = Ae^{iS/\hbar}$ is used as the building block for the exact propagator. The result is a series in \hbar , rather than in a

coupling constant as in Theorem 16. The domain of validity of the construction in its simplest form is limited because the caustic structure of $K_{\rm scl}$ can spoil the uniform boundedness; improvements are an open field of research.

Chapter 8 dealt with the application of the Volterra method to boundary-value problems for the Schrödinger equation. Following the heat-equation theory [1, 2, 18], the solutions were formally represented as single-layer and double-layer potentials, giving rise to Volterra integral equations on the boundary. Unfortunately, the proof in [3] of the existence and boundedness of the resulting operators is defective. The problem remains under investigation, and we hope that generalizing the Volterra theorem to a less obvious space (similarly to Theorems 14 and 15) will provide the answer.

Acknowledgements

We are grateful to Ricardo Estrada, Arne Jensen, Peter Kuchment, and Tetsuo Tsuchida for various pieces of helpful advice. The paper [18] originally led us to the mathematical literature [1] on the series solution of the Schrödinger equation. This research was supported by National Science Foundation Grants PHY-0554849 and PHY-0968269.

Author details

Fernando D. Mera and Stephen A. Fulling*

* Address all correspondence to: fulling@math.tamu.edu

Departments of Mathematics and Physics, Texas A&M University, College Station, TX, USA

References

- [1] I. Rubinstein and L. Rubinstein. *Partial Differential Equations in Classical Mathematical Physics*. Cambridge University Press, New York, 1998.
- [2] R. Kress. Linear Integral Equations. Springer-Verlag, New York, second edition, 1999.
- [3] F. D. Mera. The Schrödinger equation as a Volterra problem. Master's thesis, Texas A&M University, College Station, TX, May 2011.
- [4] G. B. Folland. *Introduction to Partial Differential Equations*. Princeton University Press, Princeton, New Jersey, second edition, 1995.
- [5] G. H. Hardy. Divergent Series. Chelsea Publishing Co., New York, second edition, 1991.
- [6] R. R. Estrada and R. P. Kanwal. *A Distributional Approach to Asymptotics: Theory and Applications*. Birkhäuser, Boston, second edition, 2002.
- [7] L.C. Evans. *Partial Differential Equations, Graduate Studies in Mathematics*, volume 19. American Mathematical Society, Providence, RI, second edition, 2010.
- [8] G. F. Carrier, M. Krook, and C. E. Pearson. *Functions of a Complex Variable: Theory and Technique*. Society for Industrial and Applied Mathematics, New York, 1966.

- [9] G. A. Hagedorn and A. Joye. Semiclassical dynamics with exponentially small error estimates. *Commun. Math. Phys.*, 207:439–465, 1999.
- [10] M. Reed and B. Simon. *Methods of Modern Mathematical Physics II: Fourier Analysis, Self-Adjointness.* Academic Press, New York, 1975.
- [11] W. V. Lovitt. *Linear Integral Equation*. Dover Publications, New York, 1950.
- [12] F.G. Tricomi. Integral Equations. Dover Publications, New York, 1985.
- [13] B. L. Moiseiwitsch. Integral Equations. Dover Publications, New York, 2005.
- [14] H. L. Cycon, R. G. Froese, W. Kirsch, and B. Simon. *Schrödinger Operators with Application to Quantum Mechanics and Global Geometry*. Springer, Berlin, 1987.
- [15] F. D. Mera, S. A. Fulling, J. D. Bouas, and K. Thapa. WKB approximation to the power wall. in preparation.
- [16] J. D. Bouas, S. A. Fulling, F. D. Mera, K. Thapa, C. S. Trendafilova, and J. Wagner. Investigating the spectral geometry of a soft wall. In A. Barnett, C. Gordon, P. Perry, and A. Uribe, editors, Spectral Geometry, Proceedings of Symposia in Pure Mathematics, Vol. 84, 2012, pp. 139-154
- [17] R. Balian and C. Bloch. Solution of the Schrödinger equation in terms of classical paths. *Ann. Phys.*, 85:514–545, 1974.
- [18] I. Pirozhenko, V. V. Nesterenko, and M. Bordag. Integral equations for heat kernel in compound media. *J. Math. Phys*, 46:042305, 2005.

