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A local solution of the Schrödinger equation

Mircea Grigoriu

Professor of Structural Engineering, Cornell University, Ithaca, NY 14853-3501, USA

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Abstract. A local method is developed for solving the Schrödinger equation. The method is local in the sense that it can determine the value of the solution of the Schrödinger equation at an arbitrary point directly rather than extracting this value from the field solution. The method is based on properties of diffusion processes, the Itô formula, and Monte Carlo simulation. Simplicity, accuracy, and generality are the main features of the proposed local solution. The extension of the proposed method to solve the stochastic version of the Schrödinger equation is elementary. Two examples with Dirichlet and Neumann boundary conditions are presented to demonstrate the application and evaluate the accuracy of the proposed local solution.

1. Introduction

Consider the Schrödinger equation

$$\begin{aligned} &\tfrac{1}{2}\Delta\psi(\boldsymbol{x}) + q(\boldsymbol{x})\psi(\boldsymbol{x}) = 0 \qquad \boldsymbol{x} \in D \\ &\psi(\boldsymbol{x}) = g(\boldsymbol{x}) \qquad \boldsymbol{x} \in \partial D \end{aligned} \tag{1}$$

where $D \subset \mathbb{R}^d$ is a bonded set with boundary ∂D, $\Delta = \sum_{i=1}^{d} \partial^2/\partial x_i^2$ denotes the Laplace operator, and g; q are specified functions. Current methods for solving equation (1) include (a) analytical derivations applied successfully to a limited number of relevant cases, (b) classical numerical techniques, such as the finite-difference and finite-element methods, (c) perturbation and Neumann series expansions or related methods [1], and (d) Monte Carlo simulation based on an iteration procedure using the integral form of (1) and samples drawn from the Green function of the operator of this equation [2, 3]. The method can be applied to find the lowest eigenfunction and eigenvalue of (1) and modified forms of this equation.

The current methods of solution of (1) are global in the sense that they give the solution of this equation at all points of D, or a discrete approximation of this domain, even if the value of ψ is needed at only a single point $\boldsymbol{x} \in D$. This paper presents a local solution of (1) that allows the calculation of the value of ψ at an arbitrary point $\boldsymbol{x} \in D$ directly. The proposed solution is based on properties of diffusion and Brownian motion processes, the Itô formula, and Monte Carlo simulation. Simplicity, accuracy, and generality are the essential features of the proposed local solution of (1). The method can be extended to obtain the local solution of (i) the stochastic version of (1) in which the function q is a real-valued random field defined on D and (ii) a generalized version of the Schrödinger operator defining (1) considered later in the paper (equation (18)). Two examples with the Dirichlet boundary conditions of (1) and Neumann boundary conditions are presented to demonstrate the application and evaluate the accuracy of the proposed local solution.

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2. The Itô formula

Let $\{\boldsymbol{X}(t) \in \mathbb{R}^{d+1}, t \geqslant 0\}$ be a diffusion process defined by the stochastic differential equation

$$\mathrm{d}\boldsymbol{X}(t) = \boldsymbol{a}(\boldsymbol{X}(t))\,\mathrm{d}t + \boldsymbol{b}(\boldsymbol{X}(t))\,\mathrm{d}\boldsymbol{B}(t) \tag{2}$$

where the drift $\boldsymbol{a}$ and the diffusion $\boldsymbol{b}$ are $(d+1, 1)$ and $(d+1, d')$ matrices. The driving input $\boldsymbol{B} \in \mathbb{R}^{d'}$ consists of d' independent one-dimensional Brownian motions so that it has stationary independent Gaussian increments $\boldsymbol{B}(t) - \boldsymbol{B}(s)$, $t \geqslant s$, with mean zero and covariance $\boldsymbol{i}(t-s)$, where $\boldsymbol{i}$ denotes the identity matrix. If $\boldsymbol{a}$ and $\boldsymbol{b}$ satisfy the uniform Lipschitz conditions

$$\begin{aligned} &\|\boldsymbol{a}(\boldsymbol{x}) - \boldsymbol{a}(\boldsymbol{x}')\| \leqslant c\|\boldsymbol{x} - \boldsymbol{x}'\| \\ &\|\boldsymbol{b}(\boldsymbol{x}) - \boldsymbol{b}(\boldsymbol{x}')\|_m \leqslant c\|\boldsymbol{x} - \boldsymbol{x}'\| \end{aligned} \tag{3}$$

where c is a constant, $\|\cdot\|$ denotes the Euclidean norm, and $\|\boldsymbol{b}\|_m = (\sum_{i=1}^{d+1}\sum_{j=1}^{d'} b_{i,j}^2)^{1/2}$, then the solution

$$\boldsymbol{X}(t) - \boldsymbol{X}(0) = \int_0^t \boldsymbol{a}(\boldsymbol{X}(s))\,\mathrm{d}s + \int_0^t \boldsymbol{b}(\boldsymbol{X}(s))\,\mathrm{d}\boldsymbol{B}(s) \tag{4}$$

of (2) exists and is unique [4]. The integrals $\int_0^t \boldsymbol{a}(\boldsymbol{X}(s))\,\mathrm{d}s$ and $\int_0^t \boldsymbol{a}(\boldsymbol{X}(s))\,\mathrm{d}\boldsymbol{B}(s)$ of (4) are defined in the Riemann sense and the Itô sense, respectively. The Riemann definition cannot be used for $\int_0^t \boldsymbol{X}(\boldsymbol{X}(s))\,\mathrm{d}\boldsymbol{B}(s)$ because the sample paths of the Brownian motion are of unbounded variation [4, 5].

Consider a function $f : \mathbb{R}^{d+1} \to \mathbb{R}$ with continuous second-order partial derivatives. The integral and differential forms of the Itô formula are

$$\begin{aligned} f(\boldsymbol{X}(t)) - f(\boldsymbol{X}(0)) = &\sum_{i=1}^{d+1}\int_0^t \frac{\partial f(\boldsymbol{X}(s))}{\partial x_i}\left[a_i(\boldsymbol{X}(s))\,\mathrm{d}s + \sum_{j=1}^{d'} b_{i,j}(\boldsymbol{X}(s))\,\mathrm{d}B_j(s)\right] \\ &+\frac{1}{2}\sum_{k,l=1}^{d+1}\int_0^t \frac{\partial^2 f(\boldsymbol{X}(s))}{\partial x_k \partial x_l}[\boldsymbol{b}(\boldsymbol{X}(s))\boldsymbol{b}(\boldsymbol{X}(s))^{\mathrm{T}}]_{k,l}\,\mathrm{d}s \end{aligned} \tag{5}$$

and

$$\begin{aligned} \mathrm{d}f(\boldsymbol{X}(t)) = &\sum_{i=1}^{d+1}\frac{\partial f(\boldsymbol{X}(t))}{\partial x_i}\left[a_i(\boldsymbol{X}(t))\,\mathrm{d}t + \sum_{j=1}^{d'} b_{i,j}(\boldsymbol{X}(t))\,\mathrm{d}B_j(t)\right] \\ &+\frac{1}{2}\sum_{k,l=1}^{d+1}\frac{\partial^2 f(\boldsymbol{X}(t))}{\partial x_k \partial x_l}[\boldsymbol{b}(\boldsymbol{X}(t))\boldsymbol{b}(\boldsymbol{X}(t))^{\mathrm{T}}]_{k,l}\,\mathrm{d}t \end{aligned} \tag{6}$$

respectively [4, 5], where $\boldsymbol{b}^{\mathrm{T}}$ denotes the transpose of $\boldsymbol{b}$. The last terms of equations (5) and (6) with coefficient $1/2$ are not present in the classical calculus.

3. Local solution of the Schrödinger equation

Consider a diffusion process $\{\boldsymbol{X}(t) \in \mathbb{R}^{d+1}, t \geqslant 0\}$ defined by the stochastic differential equations

$$\begin{aligned} &\mathrm{d}X_i(t) = \mathrm{d}B_i(t) \qquad i = 1, \ldots, d \\ &\mathrm{d}X_{d+1}(t) = q(X_1(t), \ldots, X_d(t))X_{d+1}(t)\,\mathrm{d}t \end{aligned} \tag{7}$$

in which q is the function considered in (1) and $\boldsymbol{B} = (B_1, \ldots, B_d)$ denotes a Brownian motion process consisting of d one-dimensional independent Brownian motion processes. The definition of $\boldsymbol{X}$ given by (7) shows that (i) the first d elements of $\boldsymbol{X}$ coincide with the Brownian motion process $\boldsymbol{B} \in \mathbb{R}^d$ and (ii) the integral form of the last equality, called the Feyman–Kac functional [4], is

$$X_{d+1}(t) = \exp\left[\int_0^t q(X_1(s), \ldots, X_d(s))\,\mathrm{d}s\right] = \exp\left[\int_0^t q(\boldsymbol{B}(s))\,\mathrm{d}s\right] \tag{8}$$

for the initial condition $X_{d+1}(0) = 1$.

Let $f : \mathbb{R}^{d+1} \to \mathbb{R}$ be a function defined by

$$f(\boldsymbol{X}(t)) = \psi(X_1(t), \ldots, X_d(t))X_{d+1}(t) = \psi(\boldsymbol{B}(t))X_{d+1}(t) \tag{9}$$

depending on the diffusion process of equation (7) and a function ψ assumed to have continuous second-order partial derivatives. The Itô formula of equation (5) applied to $f(\boldsymbol{X})$ and $\boldsymbol{X}$ defined by (7) and (9) gives

$$\begin{aligned} f(\boldsymbol{X}(t)) - f(\boldsymbol{X}(0)) &= \int_0^t \frac{\partial f(\boldsymbol{X}(s))}{\partial x_{d+1}} q(X_1(s), \ldots, X_d(s))X_{d+1}(s)\,\mathrm{d}s \\ &\quad + \sum_{i=1}^{d} \int_0^t \frac{\partial f(\boldsymbol{X}(s))}{\partial x_i}\,\mathrm{d}B_i(s) + \frac{1}{2}\sum_{i=1}^{d}\int_0^t \frac{\partial^2 f(\boldsymbol{X}(s))}{\partial x_i^2}\,\mathrm{d}s \end{aligned} \tag{10}$$

because $\boldsymbol{X}$ has the drift and diffusion coefficients $a_i(\boldsymbol{x}) = 0$ for $i = 1, \ldots, d$; $a_{d+1}(\boldsymbol{x}) = q(x_1, \ldots, x_d)x_{d+1}$; $b_{i,i}(\boldsymbol{x}) = 1$ for $i = 1, \ldots, d$; and $b_{i,j}(\boldsymbol{x}) = 0$ for all the other values of i and j in $\{1, \ldots, d+1\}$. The Itô formula of equation (10) becomes

$$\begin{aligned} \psi(\boldsymbol{B}(t))X_{d+1}(t) - \psi(\boldsymbol{B}(0)) &= \int_0^t \psi(\boldsymbol{B}(s))q(\boldsymbol{B}(s))X_{d+1}(s)\,\mathrm{d}s \\ &\quad + \sum_{i=1}^{d}\int_0^t \frac{\partial\psi(\boldsymbol{B}(s))}{\partial x_i} X_{d+1}(s)\,\mathrm{d}B_i(s) + \frac{1}{2}\int_0^t \Delta\psi(\boldsymbol{B}(s))\,X_{d+1}(s)\,\mathrm{d}s \end{aligned} \tag{11}$$

by the definitions of $\boldsymbol{X}$ and f (equations (7) and (9)) and the initial condition $X_{d+1}(0) = 1$ (equation (8)). The average of equation (11) is

$$E[\psi(\boldsymbol{B}(t))X_{d+1}(t)] - E[\psi(\boldsymbol{B}(0))] = E\left[\int_0^t X_{d+1}(s)\left(\frac{1}{2}\Delta\psi + q\psi\right)(\boldsymbol{B}(s))\,\mathrm{d}s\right] \tag{12}$$

because the Brownian motion has independent increments with mean zero so that the expectation $E[\sum_{i=1}^{d}\int_0^t(\partial\psi(\boldsymbol{B}(s))/(\partial x_i)X_{d+1}(s)\,\mathrm{d}B_i(s)]$ is zero.

Let

$$T(\boldsymbol{x}) = \inf\{t \geqslant 0 : \boldsymbol{B}(t) \notin D\} \tag{13}$$

denote the first time when a Brownian motion $\boldsymbol{B}$ starting at $\boldsymbol{x} \in D$, that is, $\boldsymbol{B}(0) = \boldsymbol{x}$, leaves a bounded domain $D \subset \mathbb{R}^d$. It can be shown that the Itô formula of equation (5) holds for t replaced with the random time $T(\boldsymbol{x})$ defined by equation (13) [4, 5]. If D is the domain of definition of equation (1) and ψ denotes the solution of this equation, then equation (12) with t replaced by $T(\boldsymbol{x})$ gives

$$E[\psi(\boldsymbol{B}(T(\boldsymbol{x})))X_{d+1}(T(\boldsymbol{x}))] - E[\psi(\boldsymbol{B}(0))] = 0 \tag{14}$$

because $\boldsymbol{B}(s) \in D$ for $s < T(\boldsymbol{x})$ and ψ is the solution of (1) so that $[(1/2)\Delta\psi + q\psi](\boldsymbol{B}(s)) = 0$. Moreover, the expectation $E[\psi(\boldsymbol{B}(0))]$ coincides with $\psi(\boldsymbol{x})$ as the initial value of the Brownian motion $\boldsymbol{B}(0) = \boldsymbol{x}$ is not random and the value

of $\psi(\boldsymbol{B}(T(\boldsymbol{x})))$ is $g(\boldsymbol{B}(T(\boldsymbol{x})))$ by the boundary conditions of (1) and the property $\boldsymbol{B}(T(\boldsymbol{x})) \in \partial D$ (equation (13)). Hence, (14) becomes

$$\psi(\boldsymbol{x}) = E^{\boldsymbol{x}}\left[g(\boldsymbol{B}(T(\boldsymbol{x}))) \exp\left(\int_0^{T(\boldsymbol{x})} q(\boldsymbol{B}(s))\,\mathrm{d}s\right)\right] \tag{15}$$

where $E^{\boldsymbol{x}}$ denotes a conditional expectation corresponding to the initial value of the Brownian motion $\boldsymbol{B}(0) = \boldsymbol{x}$. This equation shows that the value of the solution of (1) at an arbitrary point $\boldsymbol{x}$ of the domain D is equal to an expectation depending on the first time $T(\boldsymbol{x})$ when a Brownian motion $\boldsymbol{B}$ starting at $\boldsymbol{x} \in D$ leaves D and the sample paths of $\boldsymbol{B}$ during the time interval $[0, T(\boldsymbol{x})]$. The formula of equation (15) gives the local solution of (1).

Generally, it is not possible to calculate the expectation of equation (15) in closed form. However, this expectation can be estimated from samples of $\boldsymbol{B}$ generated by Monte Carlo simulation. The generation of samples of the Brownian motion $\boldsymbol{B}$ involves four steps. First, a sequence of discrete times $\{t_k\}$ needs to be defined, for example, $t_0 = 0$ and $t_k = k\,h$, $k = 0, 1, \ldots$, where $h > 0$ is a small time step. Second, a sequence of independent samples $\{\boldsymbol{\xi}_s(\omega)\}$, $s = 1, 2, \ldots$, needs to be generated from a d-dimensional Gaussian vector with mean zero and covariance matrix $h\,\boldsymbol{i}$. Simple methods are available to generate this sequence [7]. The sample path ω of the Brownian motion is equal to

$$\boldsymbol{B}(t_k, \omega) = \boldsymbol{x} + \sum_{s=1}^{k} \boldsymbol{\xi}_s(\omega) \tag{16}$$

at time t_k. Third, the sample values of the exit time $T(\boldsymbol{x}, \omega)$ and the boundary exit point $\boldsymbol{B}(T(\boldsymbol{x}, \omega), \omega)$ need to be recorded. Fourth, the value of ψ at $\boldsymbol{x} \in D$ can be estimated by

$$\hat{\psi}(\boldsymbol{x}) = \frac{1}{n_s}\sum_{\omega=1}^{n_s}\left[g(\boldsymbol{B}(T(\boldsymbol{x}, \omega), \omega)) \exp\left(h\sum_{k=1}^{n(\omega)} q(\boldsymbol{B}(k\,h, \omega))\right)\right] \tag{17}$$

in which n_s denotes the number of samples of $\boldsymbol{B}$ and $n(\omega)$ is the number of time steps to exist from D for sample ω.

The proposed method based on equations (15)–(17) can be generalized to find the local solution of the stochastic version of (1) in which function q is replaced by a real-valued random field Q defined on D. The solution of this generalization of the Schrödinger equation is a random field Ψ. The algorithm for finding statistics of $\Psi(\boldsymbol{x})$ at an arbitrary point $\boldsymbol{x} \in D$ involves three steps. First, samples $\{q(\boldsymbol{x}, \nu)\}$ of $Q(\boldsymbol{x})$, $\boldsymbol{x} \in D$, need to be generated. Second, equation (17) can be applied for each realization $q(\boldsymbol{x}, \nu)$ of $Q(\boldsymbol{x})$ to obtain sample values $\hat{\psi}(\boldsymbol{x}, \nu)$ of the solution $\Psi(\boldsymbol{x})$. Third, statistics of $\Psi(\boldsymbol{x})$ can be inferred from its samples $\{\hat{\psi}(\boldsymbol{x}, \nu)\}$.

4. Generalization

Suppose that ψ is the solution of the generalized version

$$\frac{1}{2}\sum_{i,j=1}^{d} \gamma_{ij}(\boldsymbol{x})\frac{\partial^2\psi(\boldsymbol{x})}{\partial x_i \partial x_j} + \sum_{i=1}^{d} \mu_i(\boldsymbol{x})\frac{\partial\psi(\boldsymbol{x})}{\partial x_i} + q(\boldsymbol{x})\psi(\boldsymbol{x}) = 0 \qquad \boldsymbol{x} \in D \tag{18}$$

of (1), where $D \subset \mathbb{R}^d$ is an open and bounded set and $\psi(\boldsymbol{x}) = g(\boldsymbol{x})$, $\boldsymbol{x} \in \partial D$, on the boundary of D.

Denote by $\boldsymbol{Y}$ and Z the first d elements and the element $d+1$ of the diffusion process $\boldsymbol{X}$ (equation (2)) defined by

$$\begin{aligned} \mathrm{d}\boldsymbol{Y}(t) &= \boldsymbol{\mu}(\boldsymbol{Y}(t))\,\mathrm{d}t + \boldsymbol{\sigma}(\boldsymbol{Y}(t))\,\mathrm{d}\boldsymbol{B}(t) \\ \mathrm{d}Z(t) &= q(\boldsymbol{Y}(t))\,Z(t)\,\mathrm{d}t \end{aligned} \tag{19}$$

where the drift and diffusion coefficients $\boldsymbol{\mu}$ and $\boldsymbol{\sigma}$ of $\boldsymbol{Y}$ are $(d,1)$ and (d,d') matrices related to the coefficients of equation (18) by $\boldsymbol{\mu}(\boldsymbol{y}) = \{\mu_i(\boldsymbol{y})\}$ and $(\boldsymbol{\sigma}(\boldsymbol{y})\,\boldsymbol{\sigma}(\boldsymbol{y})^{\mathrm{T}})_{ij} = \gamma(\boldsymbol{y})_{ij}$ and $\boldsymbol{B} \in \mathbb{R}^{d'}$ consists of d' independent standard Brownian motions. The Itô formula of equation (5) gives

$$\begin{aligned} &\psi(\boldsymbol{Y}(t))\,Z(t) - \psi(\boldsymbol{Y}(0))\,Z(0) \\ &\quad = \int_0^t \left[\sum_{i=1}^{d} \frac{\partial \psi(\boldsymbol{Y}(s))}{\partial y_i} Z(s)\,\mathrm{d}Y_i(s) + q(\boldsymbol{Y}(s))\,Z(s)\psi(\boldsymbol{Y}(s))\,\mathrm{d}s \right] \\ &\qquad + \frac{1}{2} \sum_{i,j=1}^{d} \int_0^t \frac{\partial^2 \psi(\boldsymbol{Y}(s))}{\partial y_i \partial y_j} Z(s)\,\gamma(\boldsymbol{Y}(s))_{ij}\,\mathrm{d}s \end{aligned} \tag{20}$$

for $\boldsymbol{X}$ defined by equation (19) and $f(\boldsymbol{X}) = \psi(\boldsymbol{Y})Z$. Take $\boldsymbol{x} \in D$ arbitrary and set $\boldsymbol{Y}(0) = \boldsymbol{x}$; $Z(0) = 1$ in equation (20). The corresponding expectation of the resulting equation is

$$\begin{aligned} E^{\boldsymbol{x}}[\psi(\boldsymbol{Y}(T(\boldsymbol{x})))Z(T(\boldsymbol{x}))] - \psi(\boldsymbol{x}) = E^{\boldsymbol{x}} \int_0^{T(\boldsymbol{x})} \Bigg[&\frac{1}{2} \sum_{i,j=1}^{d} \gamma_{ij}(\boldsymbol{Y}(s)) \frac{\partial^2 \psi(\boldsymbol{Y}(s))}{\partial y_i \partial y_j} \\ &+ \sum_{i=1}^{d} \mu_i(\boldsymbol{Y}(s)) \frac{\partial \psi(\boldsymbol{Y}(s))}{\partial y_i} + q(\boldsymbol{Y}(s))\psi(\boldsymbol{Y}(s)) \Bigg] Z(s)\,\mathrm{d}s \end{aligned} \tag{21}$$

in which $T(\boldsymbol{x}) = \inf\{t \geqslant 0 : \boldsymbol{Y}(t) \notin D\}$ denotes the first time the process $\boldsymbol{Y}$ starting at $\boldsymbol{Y}(0) = \boldsymbol{x}$ exists D. If ψ is the solution of equation (18), then (21) simplifies to

$$\psi(\boldsymbol{x}) = E^{\boldsymbol{x}} \left[g(\boldsymbol{Y}(T(\boldsymbol{x}))) \exp\left(\int_0^{T(\boldsymbol{x})} q(\boldsymbol{Y}(s))\,\mathrm{d}s \right) \right] \tag{22}$$

because $\boldsymbol{Y}(s) \in D$ for $s \in [0, T(\boldsymbol{x}))$ so that the right-hand term of (21) is zero, $\boldsymbol{Y}(T(\boldsymbol{x})) \in \partial D$, the unknown function ψ is equal to a specified function g on the boundary of D, and $Z(t) = \exp(\int_0^t q(\boldsymbol{Y}(s))\,\mathrm{d}s)$.

Generally, it is not possible to obtain the expectation of equation (22) in closed form. However, estimates of this expectation can be calculated from samples of $\boldsymbol{Y}$. Estimators as defined by equation (17) can be used to find approximations $\hat{\psi}(\boldsymbol{x})$ of $\psi(\boldsymbol{x})$. Samples of the diffusion process $\boldsymbol{Y}$ can be generated from the finite-difference approximation

$$\boldsymbol{Y}(t+h) = \boldsymbol{Y}(t) + \boldsymbol{\mu}(\boldsymbol{Y}(t))h + \boldsymbol{\sigma}(\boldsymbol{Y}(t))(\boldsymbol{B}(t+h) - \boldsymbol{B}(t)) \qquad \boldsymbol{Y}(0) = \boldsymbol{x} \tag{23}$$

of equation (19), where $h > 0$. More accurate algorithms for generating samples of $\boldsymbol{Y}$ are available [6].

5. Numerical examples

Two one-dimensional examples with known analytical solutions are used to illustrate the proposed local solution and evaluate its accuracy. The Schrödinger operators considered in these examples are identical but satisfy different types of boundary conditions, Dirichlet boundary conditions and Neumann–Dirichlet boundary conditions.

Example 1. Suppose that D is the interval $(0, l)$ of the real line and q is a constant (equation (1)). The corresponding Schrödinger equation

$$\tfrac{1}{2}\psi''(x) + q\psi(x) = 0 \tag{24}$$

has the solution

$$\psi(x) = \alpha\ \cos(\sqrt{2q}x) + \frac{\beta - \alpha\ \cos(\sqrt{2q}l)}{\sin(\sqrt{2q}l)} \sin(\sqrt{2q}x) \tag{25}$$

for the Dirichlet boundary conditions $\psi(0) = \alpha$, $\psi(l) = \beta$, where α, β are real numbers.

The estimate of $\psi(x)$ at an arbitrary point $x \in (0, l)$ is (equation (17))

$$\begin{aligned}\hat{\psi}(x) &= \frac{1}{n_s}\left[\alpha \sum_{\omega'=1}^{n_s'} \exp(q\tau(\omega')) + \beta \sum_{\omega''=1}^{n_s''} \exp(q\tau(\omega''))\right] \\ &= c'(x)\alpha + c''(x)\beta\end{aligned} \tag{26}$$

where n_s' and n_s'' denote the number of samples of the Brownian motion B that exit $D = (0, l)$ through the left and the right ends of this interval, $n_s' + n_s'' = n_s$, and $c'(x)$; $c''(x)$ give the weights of the boundary conditions $\psi(0) = \alpha$; $\psi(l) = \beta$ in the expression of the estimated value of $\psi(x)$. Let $e(x) = 100|\psi(x) - \hat{\psi}(x)|/|\psi(x)|$ be the error of the estimate $\hat{\psi}(x)$ of $\psi(x)$ at an arbitrary point $x \in (0, l)$. The largest error $e_{\max}$ recorded at $x = (k/10)l$, $k = 1, \ldots, 9$, does not exceed 5% for $l = 1$, $\alpha = 1$, $\beta = 2$, $q = 1$, $h = 0.001$, and $n_s = 500$. This error can be reduced by increasing the sample size and/or reducing the time step h used for generating the sample paths of the Brownian motion process. For example, $e_{\max} \leqslant 1.5\%$ for $n_s = 1000$ and $h = 0.0005$.

The estimator $\hat{\psi}$ of equation (26) is less accurate when the domain D and/or the parameter q is large. This unsatisfactory performance is caused by the dependence of $\hat{\psi}(x)$ on $\exp(qT(x))$, a random variable with heavy tail if D and/or q is large. To clarify this statement consider the special case $\alpha = \beta = 1$, $q = 1$, $l = 2a$, and $x = a$ in which $\hat{\psi}(x)$ is equal to the expected value of $\exp(T(a))$. Table 1 gives the estimates of the mean $E[T(a)]$ and the coefficient of variation c.o.v.$[T(a)]$ of $T(a)$ and the coefficient of variation c.o.v.$[\exp(T(a))]$ of $\exp(T(a))$ calculated from 1000 sample paths of the Brownian motion generated with a time step $h = 0.001$, where the coefficient of variation c.o.v.$[U]$ of a random variable U is the ratio of the standard deviation to the mean of U. The relatively large uncertainty in $T(a)$ is amplified by the mapping $T(a) \to \exp(T(a))$, as demonstrated by the coefficients of variation of $\exp(T(a))$ that are much larger than the corresponding coefficients of variation of $T(a)$. The large coefficients of variation of $\exp(T(a))$ are the cause of unstable estimates for the expectation of $\exp(T(a))$. In fact, $E[\exp(T(a))]$ may not even exist. For example, $E[\exp(T(a))]$ is not bounded if $T(a)$ is an exponential random variable with expectation $1/\lambda$ and $0 < \lambda < 1$. In this case, it is not possible to obtain stable estimates of the mean of $\exp(T(a))$ from samples of $T(a)$ [7].

Table 1. Statistics of $T(a)$ and $\exp(T(a))$.

	Estimates		
a	$E[T(a)]$	c.o.v.$[T(a)]$	c.o.v.$[\exp(T(a))]$
1	1.0097	0.7554	1.7506
2	4.0946	0.7663	31.6228

The performance of the estimator $\hat{\psi}$ of equation (26) can be improved by dividing the domain of integration D into sufficiently small subdomains for which this estimator is accurate. Suppose that $D = (0, l)$ is divided into $m + 1$ equal intervals and let $\alpha_k = \psi(kl/(m + 1))$ be the unknown value of ψ at the division point $x_k = kl/(m + 1)$, $k = 1, \ldots, m$. Relationships $\alpha_k = c'_k\alpha_{k-1} + c''_k\alpha_{k+1}$ between the values of ψ at the division points can be obtained from equation (26) applied in the intervals $((k - 1)l/(m + 1), (k + 1)l/(m + 1))$, $k = 1, \ldots, m$. The unknown values of ψ at the division points can be obtained from these relationships and the boundary conditions giving two additional equations, $\alpha_0 = \alpha$ and $\alpha_{m+1} = \beta$. For example, let $\alpha = 1$, $\beta = 2$, $q = 1$, $l = 2$, and $m = 3$. The relationships between the values of ψ at the division points are $\psi(k/2) = \alpha_k = (\alpha_{k-1} + \alpha_{k+1})/2$, $k = 1, 2, 3$, by the symmetry of the Brownian motion and equation (26). These equations and the boundary conditions give $\alpha_1 = 1.25$, $\alpha_2 = 1.50$, and $\alpha_3 = 1.75$. Suppose that $\psi(0.3)$ needs to be estimated. The estimate of $\psi(0.3)$ can be obtained by the proposed method from equation (26) for the domain $(0, 0.5)$ and the boundary conditions $\psi(0) = 1$, $\psi(0.5) = 1.25$. The error of this estimate is under 1.2% for $n_s = 500$ and $h = 0.0005$.

The partition of the domain of integration in subdomains of sufficiently small size discussed for one-dimensional problems can be extended to solve the Schrödinger equation in higher dimensions. First, the domain D needs to be divided in $m + 1$ sufficiently small subdomains delimited by the boundaries $\{\partial D_k\}$, $k = 1, \ldots, m$. Second, points $\{\boldsymbol{x}_{k,p}\}$ have to be selected on each ∂D_k and spline or other approximations developed for the values of ψ everywhere in ∂D_k depending on the unknown values $\alpha_{k,p} = \psi(\boldsymbol{x}_{k,p})$ of this function at $\{\boldsymbol{x}_{k,p}\}$. Third, the proposed method can be applied to relate the values $\alpha_{k,p}$ with $\alpha_{k-1,p}$ and $\alpha_{k+1,p}$. These relationships and the boundary conditions can be used to estimate $\{\alpha_{k,p}\}$. Fourth, $\psi(\boldsymbol{x})$ can be estimated by applying the proposed method in the subdomain of D including $\boldsymbol{x}$.

Example 2. Consider the Schrödinger operator of equation (24) with the boundary conditions $\psi'(0) = \alpha$ and $\psi(l) = \beta$. The exact solution is

$$\psi(x) = \frac{\beta - (\alpha/\sqrt{2\,q})\sin(\sqrt{2\,q}l)}{\cos(\sqrt{2\,q}l)}\cos(\sqrt{2\,q}x) + \frac{\alpha}{\sqrt{2\,q}}\sin(\sqrt{2\,q}x) \tag{27}$$

for $q > 0$.

To incorporate the Neumann boundary condition at $x = 0$ it is necessary to replace the Brownian motion process B used in the previous example with the reflected Brownian motion at zero defined by

$$|B(t)| = \hat{B}(t) + L(t) \tag{28}$$

in which $\hat{B}$ is a Brownian motion and L is a process with increasing continuous sample paths that can have non-zero increments only at the reflection times, that is, at the times when $|B|$ is zero. The process L, called the local time of the Brownian motion at zero, is given by the limit [4, 8]

$$L(t) = \lim_{\varepsilon \downarrow 0} \frac{1}{2\varepsilon}\int_0^t 1_{(-\varepsilon,\varepsilon)}(B(s))\,\mathrm{d}s \tag{29}$$

where $1_{(-\varepsilon,\varepsilon)}(u)$ is one for $u \in (-\varepsilon, \varepsilon)$ and zero otherwise. The Itô formula can be extended to incorporate reflected processes and has the form [8]

$$\psi(|B(t)|)X_2(t) - \psi(x) = \int_0^t \psi'(|B(s)|)X_2(s)\,\mathrm{sign}(B(t))\,\mathrm{d}B(s) + q\int_0^t \psi(|B(s)|)X_2(s)\,\mathrm{d}s + \frac{1}{2}\int_0^t \psi''(|B(s)|)X_2(s)\,\mathrm{d}s + \lim_{\varepsilon\downarrow 0}\frac{1}{2\varepsilon}\int_0^t \psi'(|B(s)|)X_2(s)1_{(-\varepsilon,\varepsilon)}(B(s))\,\mathrm{d}s \tag{30}$$

for $\boldsymbol{X} \in \mathbb{R}^2$ with elements $X_1 = |B|$ and X_2 given by the differential equation $\mathrm{d}X_2(t) = qX_2(t)\,\mathrm{d}t$ [8]. This version of the Itô formula gives

$$\psi(x) = E^x[\psi(|B(T(x))|)\,X_2(T(x))] - \alpha\,E^x\left[\lim_{\varepsilon\downarrow 0}\frac{1}{2\varepsilon}\int_0^{T(x)} 1_{(-\varepsilon,\varepsilon)}(B(s))X_2(s)\,\mathrm{d}s\right] \tag{31}$$

by averaging, where $T(x)$ denotes the first exit time of $|B|$ starting at $|B(0)| = x$ from $D = (0, l)$. The estimates of ψ based on equation (31) and samples of $\boldsymbol{X}$ are in error by less than 2% for $\alpha = 1$, $\beta = 2$, $q = 1$, $l = 1$, $h = 0.0005$, and $n_s = 500$.

6. Conclusions

A local method was developed for solving the Schrödinger equation. The method is local in the sense that the solution of the Schrödinger equation can be obtained at an arbitrary point directly rather than by extracting this value from the field solution. The method is based on properties of diffusion processes, the Itô formula, and Monte Carlo simulation. The essential features of the proposed method are simplicity, accuracy, and generality. The method can be extended to obtain the local solution of the stochastic and generalized versions of the classical Schrödinger equation. Two examples with Dirichlet and Neumann boundary conditions were presented to demonstrate the application and evaluate the performance of the proposed local solution.

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References

[1] Sobczyk K 1985 *Stochastic Waves Propagation* (New York: Elsevier)
[2] Kalos M H and Whitlock P A 1986 *Monte Carlo Methods* (New York: Wiley)
[3] Vrbik J 1985 Monte Carlo technique for finding the lowest eigenvalue of the modified Schrödinger equation *J. Phys. A: Math. Gen.* **18** 1327–35
[4] Chung K L and Williams R J 1990 *Introduction to Stochastic Integration* (Boston: Birkhäuser)
[5] Protter P 1990 *Stochastic Integration and Differential Equations* (New York: Springer)
[6] Kloeden P E and Platen E 1992 *Numerical Solutions of Stochastic Differential Equations* (New York: Springer)
[7] Grigoriu M 1995 *Applied non-Gaussian Processes. Examples, Theory, Simulation, Linear Random Vibration, and MATLAB Solutions* (Englewood Cliffs, NJ: Prentice Hall)
[8] Grigoriu M 1997 Reflected Brownian motion and solution of a class of partial differential equations *Report* 97-1, School of Civil and Environmental Engineering, Cornell University