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Application of Grimm-Storer Diffusion Approximation Method to Schrödinger Equation With Short Range Potential in One Dimension

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Abstract

In this research we consider a system of one particle moving under the influence of short range potential. The applicability of solving Schrödinger equation by the method of diffusion due to Grimm-Storer approximation for a short range potential is investigated. Schrödinger equation can be solved to get the ground state and first excited state wave function and their Eigenvalues using other methods, like the finite difference method and in some cases the analytic solution if available. Both methods were used to compare solutions to that derived by the diffusion approximation method. In this study an exponential and a square well potential are taken as examples.

المستخلص

في هذا البحث تم افتراض نظام من جسم واحد يتحرك تحت تأثير جهد قصير المدى وتحري مدى قابلية حل معادلة شرودنجر بطريقة الانتشار التقريبية المقدمة من جرم وستورر للجهد قصير المدى. يمكن حل معادلة شرودنجر لإيجاد معادلة الموجة للحالة الارضية وحالة الاثارة الاولى وكذلك القيم الذاتية التابعة لها باستخدام طرق اخرى مثل طريقة الفروق المحدودة وفي بعض الحالات طريقة الحل التحليلي التام, كلتا الطريقتين استخدمت لمقارنة الحلول المتحصل عليها باستخدام طريقة الانتشار التقريبية. في هذا البحث تم اخذ الجهد الاسي وبئر الجهد كأمثلة تطبيقية.

Key words: Diffusion method; Schrödinger equation; Integral solution; Green's function

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Introduction

The diffusion approximation method is based on numerical solution of the diffusion like equation:

$$\hat{H}\,\Psi = -\frac{\partial\Psi}{\partial\beta} \tag{1}$$

Where $\hat{H}$ is the Hamiltonian for the system of one particle satisfying certain boundary condition, and β is a real parameter . It is a numerical method that was established by Grimm and Storer [1], and it involves the use of Green's functions and converts Schrödinger equation into an integral equation. The integral equation is then solved iteratively for small β and by expanding the initial guess function $\Psi_0(x)$ in a complete set of Eigenfunctions of the Hamiltonian. This iterative procedure converges the solution which approaches the ground state or the first excited state in the special case of even potential where the wave functions can be classified into even and odd functions. The whole process is based on this expansion of the complete set of the wave functions associated with the Hamiltonian. For short range potentials only few bound states can exist so the notion of expanding of the initial guess wave function is not appropriate because of the lack of the complete set of Eigenfunctions. This raises the question, is this method applicable to short range potential or not. It was demonstrated, here, that it is possible to get the ground state and the first excited state wave function for the short range potential which does not have a complete set of Eigenfunctions.

General Theory

The solution to the operator equation (1) can be found in terms of the Green's function as:

$$\Psi(x,\beta) = \int_{-\infty}^{\infty} G(x,x_0,\beta)\Psi_0(x_0)dx_0 \tag{2}$$

Where $G(x,x_0,\beta) = < x\left|e^{-\beta\hat{H}}\right|x_0 >$ is the Green's function of equation (1) for any β , with the initial condition $G(x,x_0,0) = \delta(x-x_0)$ [2]. And

$\Psi_0(x) = \Psi(x,\beta=0)$ ≡ an initial guess.

The operator $\widehat{H}$ can be written into the form $\widehat{H} = \widehat{H}_0 + \widehat{V}(x)$, so equation (2) can be transformed into an iterative form [3]:

$$\Psi(x,n\beta) = e^{-\frac{\beta}{2}V(x)} \int_0^{\infty} [G_0(x,x_0,\beta) \pm G_0(-x,x_0,\beta)]\, e^{-\frac{\beta}{2}V(x_0)}\, \Psi(x_0,(n-1)\beta)dx_0 \tag{3}$$

Where $G_0(x,x_0,\beta) = \langle x | e^{-\beta\widehat{H_0}} | x_0 \rangle = \frac{1}{\sqrt{4\pi\beta}} e^{-\frac{(x-x_0)^2}{4\beta}}$ is the Green's function of the equation $\widehat{H_0}G_0 = -\frac{\partial G_0}{\partial\beta}$ and $\widehat{\mathrm{H}_0} = -\frac{d^2}{dx^2}$.
For even potentials $V(x)$ the + sign is used for the even wave function $\Psi_{\mathrm{e}}(x)$ which corresponds to the ground state wave function, and the – sign is used for the odd wave function $\Psi_{\mathrm{o}}(x)$ which corresponds to the first excited state wave function. Convergence is expected for large iterative steps n.

Applications

A - Short Range Exponential Potential.

This potential is a good example to test the applicability of the diffusion method to short range smooth potential given by:

$$V(x) = -V_0 e^{-\frac{|x|}{a}} \qquad -\infty < x < \infty \tag{4}$$

In Fig. 1 (a,b) we show the ground state and the first excited state wave function respectively calculated using finite difference method, diffusion method, and the analytic solution with $\text{ט}_0 = \frac{2ma^2}{\hbar^2} V_0 = 100$ which are in good agreement. The initial guess wave function was a small square well.

The red line is for the wave function calculated using finite difference method, while the black line is for the wave function calculated using this diffusion approximate method, and the blue line is for the wave function calculated using the analytic method.

In tables 1(a,b) we show the numerically calculated Eigenvalues for the ground state and the first excited state respectively with different ט_0 . The first column shows the results of the finite difference method calculated numerically when

$\Psi(x)$ calculated at mesh point $x_n = \Delta n, n \geq 0$ [4,5], where $\Psi(x_n) = \Psi_n$ and Δ is the distance between adjacent points $x_{n+1} - x_n = \Delta$.

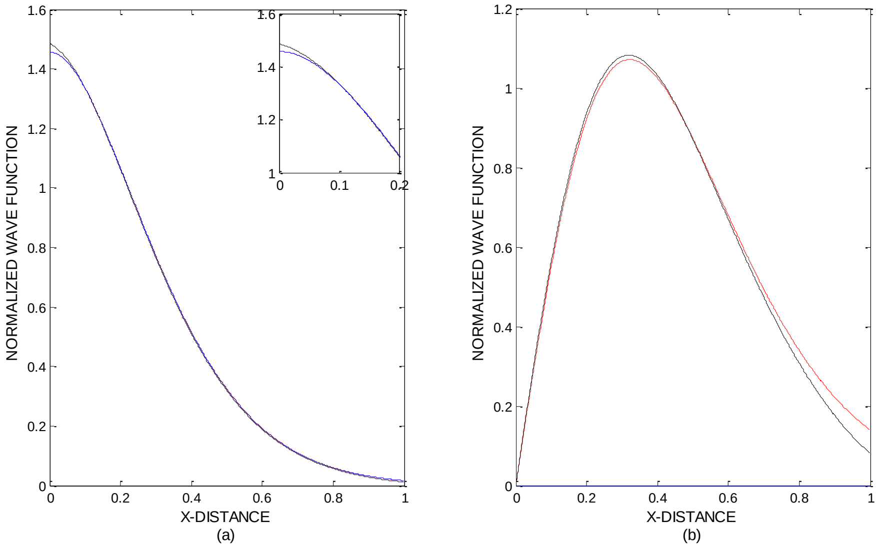

Figure 1. a) The normalized ground state wave function and b) first excited wave function of short range exponential potential.

$$\Psi_{n+1} = \left[2 + \Delta^2\left(\upsilon_0 e^{-\Delta n} - \varepsilon\right)\right]\Psi_n - \Psi_{n-1} \qquad (5)$$

For $\upsilon_0 = \frac{2ma^2}{\hbar^2} V_0$ and $\varepsilon = \frac{2ma^2}{\hbar^2} |E|$.

For ground state wave function we choose the initial values of the wave function as:

$$\Psi(x_0) = \Psi_0 = 1.0 \quad \text{and} \quad \Psi(\Delta) = \Psi_1 = 1.0 + \left(\frac{\varepsilon - \upsilon_0}{2}\right)\Delta^2 \qquad (6)$$

And for the first excited state wave function we choose initial values of the wave function as:

$$\Psi(x_0) = \Psi_0 = 0.0 \quad \text{and} \quad \Psi(\Delta) = \Psi_1 = c \qquad (7)$$

Where c is a small constant.

The second column shows the results using diffusion approximate method with $\beta = 0.001$ and $\Delta = 0.001$ where Δ is the mesh size of the coordinate x ie $x_n = n\Delta$. For the diffusion approximate method the initial guess wave function is compact in small range near a square well, so the iterative procedure can be more efficient in reducing the wave function to the ground state or to the first excited state. The distance is measured in units of a, and the units of energy is $\frac{\hbar^2}{2ma^2}$. In these units the Hamiltonian is $\widehat{\mathrm{H}_0} = -\frac{\mathrm{d}^2}{\mathrm{dx}^2}$ and $V(x) = -\upsilon_0 e^{-x}$ where $\upsilon_0 = \frac{2ma^2}{\hbar^2} V_0$.

The energy Eigenvalue $\mathcal{E}$ for ground state is calculated by means of numerical evaluation of the expectation value of the Hamiltonian for the normalized wave function using Simpson rule:

$$\mathcal{E} = \int_{-\infty}^{\infty} \Psi^*(x)\, \widehat{H} \Psi(x) dx \tag{8}$$

While the energy Eigenvalue for the first excited state is calculated by means of numerical evaluation of the norm of the last convergent wave function by the formula [3]:

$$\mathcal{E} = -\frac{1}{2\beta} ln \int_{-\infty}^{\infty} \Psi^*(x, n\beta) \Psi(x, n\beta) dx \tag{9}$$

The last column shows the exact calculated energy Eigenvalue using an analytic method by converting Schrödinger equation of short range potential to Bessel function of order $2\sqrt{\mathcal{E}}$ by the transformation $z = e^{-x/2a}$ where $\mathcal{E}$ is the energy Eigenvalue written as [6,7]:

$$z^2 \frac{d^2\Psi}{dz^2} + z\frac{d\Psi}{dz} + \left(4\upsilon_0 z^2 - 4\mathcal{E}\right)\Psi = 0 \tag{10}$$

Where $\upsilon_0 = \frac{2ma^2}{\hbar^2} V_0$ and $\mathcal{E} = \frac{2ma^2}{\hbar^2} |E|$
For $x \geq 0$ then $0 < z \leq 1$

equation (10) then has the solution $J_{2\sqrt{\varepsilon}}(2\sqrt{\upsilon_0}\, z)$. The even parity solution would satisfy $J'_{2\sqrt{\varepsilon}}\left(2\sqrt{\upsilon_0}\right) = 0$ where J' is defined as $J' = \frac{dJ}{dz}$, and the odd parity solution satisfies $J_{2\sqrt{\varepsilon}}\left(2\sqrt{\upsilon_0}\right) = 0$. Both conditions are calculated numerically to obtain the Eigenenergies.

Table 1a. The ground state energy eigenvalues for the short range exponential potential using different methods.

υ_0	*Finite difference method*	*Diffusion approximation method*	*Exact solution*
100	-79.7614	-79.7612	-79.7567
200	-167.324	-167.324	-167.316

Table 1b. The first excited state energy eigenvalues for the short range exponential potential using different methods.

υ_0	*Finite difference method*	*Diffusion approximation method*	*Exact solution*
100	-65.2907	-56.2887	-56.2882
200	-128.465	-128.466	-128.458

B - Square Well Potential.

This potential is another good example to test the applicability of the diffusion method to short range but the discontinuous potential is given by:

$$V(x) = \begin{cases} -\upsilon_0 & |x| \le a \\ 0 & |x| > a \end{cases}$$

Where Schrödinger equation is put into the form:

$$\frac{d^2\Psi}{dx^2}+(\mathcal{E}-V(x))\Psi=0$$

In Fig. 2(a) we show the ground state wave function for $ʋ_0 = 100\,, a = 0.1$ calculated using diffusion approximate method and exact analytic solution.

In Fig. 2(b) we show the first excited state wave function for $ʋ_0 = 100\,, a = 0.3$ calculated using diffusion approximate method and exact analytic solution.

The wave functions calculated using the diffusion approximte method have a discontinuity at $x = a$ which caused difficulties in calculating the ground state energy Eigenvalue.

The black line is for the wave function calculated using diffusion approximate method, while the blue line is for the wave function calculated using the analytic method.

In table 2(a,b) we show the numerically calculated Eigenvalues for the ground state and the first excited state respectively with different $ʋ_0$ and a.

The first column shows the results using finite difference method calculated numerically as before with:

$$\Psi_{n+1} = \left[2 + \Delta^2\left(\mathcal{E} - ʋ_0\right)\right]\Psi_n - \Psi_{n-1} \tag{11}$$

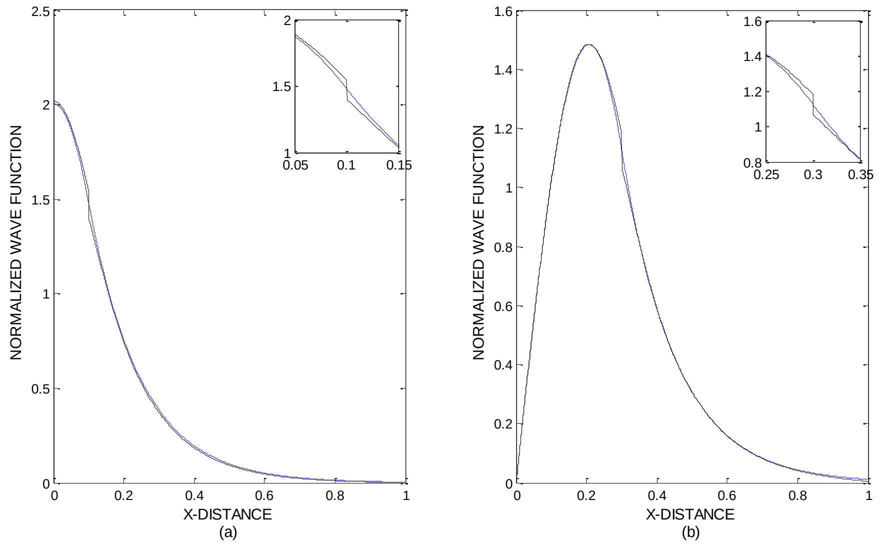

Figure 2. a) The normalized ground state wave function and b) first excited wave function of square well potential.

We choose the initial boundaries for the ground state and first excited state in the form given by equations (6) and (7) respectively.

The second column shows the results using diffusion approximate method with $\beta = 0.0003$, $\Delta= 0.001$ for the ground state, and $\beta = 0.0001$, $\Delta= 0.001$ for the first excited state. The energy Eigenvalues are calculated by evaluating the expectation value of the Hamiltonian for the normalized wave function as [6]:

$$\mathcal{E}_1 = \int_{-\infty}^{\infty} \Psi^*(x)\, \widehat{H}\Psi(x)dx \qquad (12)$$

And this can be transformed by partial integration into

$$\mathcal{E}_2 = \int_{-\infty}^{\infty} ([\Psi'(x)]^2 + V(x)[\Psi(x)]^2)dx \qquad (13)$$

Table 2a. The ground state energy eigenvalues for the square well potential using different methods.

ט$_0$	a	*Finite difference method*	*Diffusion approximate method*			*Exact solution*
			$\mathcal{E}_1$	$\mathcal{E}_2$	$\mathcal{E}_2$'	
100	0.1	-45.3756	-55.7510	-43.8804	-45.3751	-45.3753
200	0.2	-166.852	-193.980	-165.268	-166.851	-166.851

Table 2b. The first excited state energy eigenvalues for the square well potential using different methods.

ט$_0$	a	*Finite difference method*	*Diffusion approximate method*			*Exact solution*
			$\mathcal{E}_1$	$\mathcal{E}_2$	$\mathcal{E}_2$'	
100	0.3	-42.2970	-82.3097	-41.6445	-42.2970	-42.2976
200	0.3	-130.062	-219.871	-129.672	-130.061	-130.062

These two equations didn't result in acceptable results because of the discontinuity of the wave function at $= a$, so we can get acceptable results for ε'_2 by removing the peak in the square differential wave function as shown in Fig 3(b).

The last column shows the exact energy Eigenvalues using the analytic method.

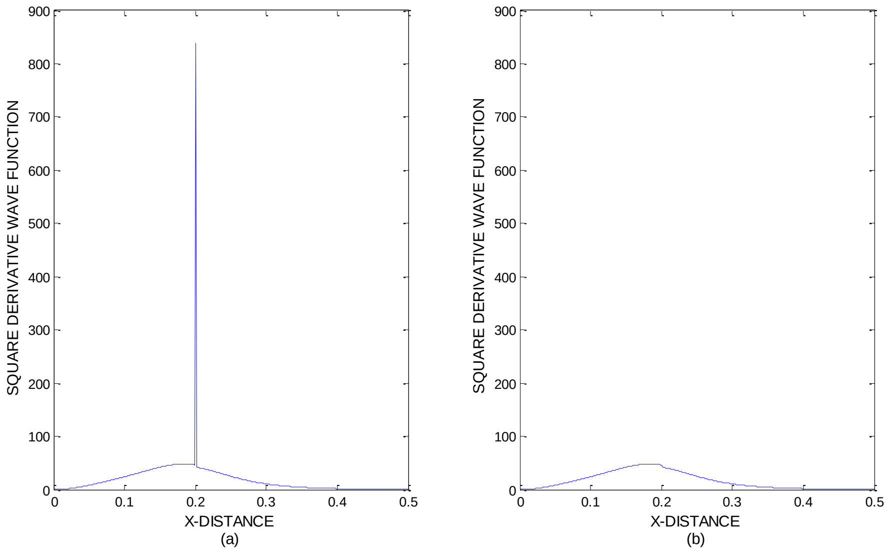

Figure 3. a) The square derivative of wave function and b) singularity removed.

Conclusion

We have used the diffusion approximate method developed by Grimm and Storer to solve the Schrödinger equation to get the ground state and the first excited state for an even short range potential. It was demonstrated, here, that this method is applicable for solving the Schrödinger equation for short range potentials by an appropriate initial guess wave function in a small range near the origin. Discontinuous potentials manifest themselves in the final wave function as the method cannot rid of the discontinuity. Extra care should be taken when evaluating the energy Eigenvalues in this case.

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