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Calculation of Positive Spectrum for the Higher Excited States Using Grimm and Storer Diffusion Method

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Abstract

In this work the Grimm and Storer method is employed to calculate all the higher excited states wave functions and their corresponding energy eigenvalues , for the first time by modifying the iterative numerical procedure. Using symmetry arguments of an even Hamiltonian, the even and odd excited states can be calculated separately.

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

المستخلص

في هذه الورقة تم توظيف طريقة جريم وستورير لحساب الدوال الموجية لحالات الاثارة العالية والقيم الذاتية المصاحبة لها لأول مرة وذلك بتعديل الاجراء التكراري العددي. وباستخدام التماثل للهاملتون الزوجي يمكن حساب كل من الحالات الزوجية والحالات الفردية منفصلتين.

Introduction

The Grimm and Storer method is a numerical method that is usually used to solve the Schrödinger equation in the imaginary time domain to obtain the ground state of bound quantum system. The Schrödinger differential equation is transformed into an integral equation that can be solved iteratively. Because of the diffusion nature in the imaginary time only lowest physical state (ground state) is obtained by this procedure [1].

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Using symmetry arguments for even parity potential in one dimension leads to the extraction of the first excited state instead of the ground state [2]. Numerical removal of any lower states by Gram-Schmidt orthogonalization procedure can also lead to the next excited state as well [3]. In this work a new simple numerical iteration procedure is used to obtain any desired quantum state (if it exists) directly without using other numerical expensive techniques. The harmonic potential in one dimension is used to illustrate this technique.

General Theory

The time dependent Schrödinger equation $\hat{H}\ \Psi = i\hbar\frac{\partial\Psi}{\partial t}$ can be rewritten as a diffusion type equation by performing a transformation from real time domain to imaginary time τ domain as follows

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

where $\hat{H}$ is the Hamiltonian of the system, and the parameter $\beta = {}^{\tau}/_{\hbar}$.
The solution of equation (1) can be written as

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

where $\Psi_0(x) = \Psi(x,\beta = 0)$, and β is a real parameter related to the temperature T by $\beta = {}^{1}/_{kT}$ where k is Boltzman constant, so the iterative process can be viewed physically as cooling the system to the ground state.
The Green's function in an integral form is given by

$$G(x,x_0,\beta) = < x\left|e^{-\beta\hat{H}}\right|x_0 >. \tag{3}$$

Equation (2) can be transformed into more convenient iterative form

$$\Psi(x,n\beta) = \int_{-\infty}^{\infty} G(x,x_0,\beta)\Psi\,(x_0,(n-1)\beta)dx_0, \tag{4}$$

where n is an integer representing the number of iterations and β can assume any value.
For even potential we can classify the eigenfunctions to even and odd functions, and by replacing the integral form in equation (4) from $-\infty$ to ∞ by 0 to ∞ we get

$$\Psi(x,n\beta) = \int_{0}^{\infty} [G(x,x_0,\beta) \pm G(x,x_0,\beta)]\,\Psi(x_0,(n-1)\beta)dx_0, \tag{5}$$

where the + sign used for even functions and the – sign used for odd functions.

The solution for any β can be found if the Green's function can be solved exactly but this is difficult and an approximation for the Green's function for small β is used instead by expanding Hamiltonian in equation (1) as $\widehat{H} = \widehat{H}_0 + \widehat{H'}(x)$ to get [1,4]

$$G(x, x_0, \beta) \approx e^{-\frac{\beta}{2}\widehat{H\prime}(x)}\, G_0(x, x_0, \beta)\, e^{-\frac{\beta}{2}\widehat{H\prime}(x_0)} + O(\beta^3)$$

where $G_0(x, x_0, \beta)$ is the Green's function solution of the equation

$$G_0(x, x_0, \beta) = < x\left|e^{-\beta\widehat{H_0}}\right|x_0 >$$

and in one dimension [2[

$$G_0(x, x_0, \beta) = \frac{1}{\sqrt{4\pi\beta}} e^{-\frac{(x - x_0)^2}{4\beta}} .$$

To show the argument of the reduction to the ground state one expands $\Psi_0(x)$ in a complete set of eigenfunctions of the Hamiltonian $\widehat{H}$ ie

$$\Psi_0(x) = \sum_{i=0}^{\infty} a_i u_i(x), \qquad (6)$$

where u_i are the stationary eigenstates of the Hamiltonian ie $\widehat{H} u_i = E_i u_i$.
By pluging equation (6) into equation (2) and using equation (3) we get [2]

$$\Psi(x, \beta) = \sum_{i=0}^{\infty} a_i e^{-\beta E_i}\, u_i(x). \qquad (7)$$

The solution for large β leads to the smallest eigenstate with the smallest eigenvalue E_0 or equivalently small β with large *n* as is shown in Fig.1.

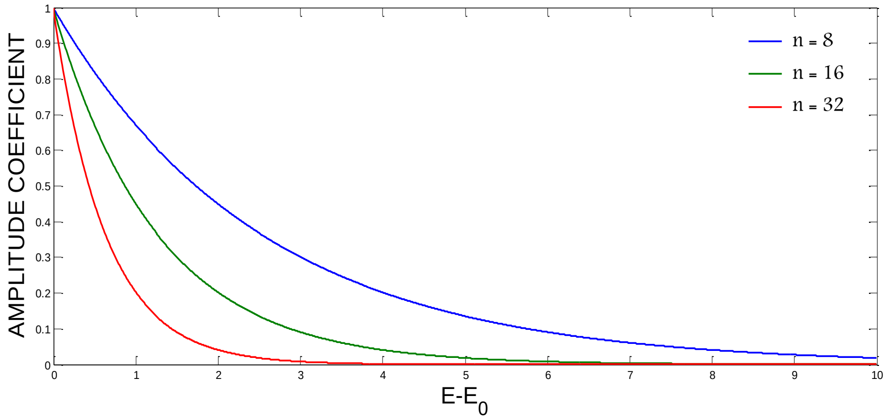

Figure 1. The amplitude coefficient of other states relative to that of the ground state plotted VS E-E_0 at β = 0.05 and different number of iterations

$$\lim_{n\to\infty} \sum_{i=0}^{\infty} a_i e^{-n\beta E_i} u_i \ \approx \ a_0 e^{-n\beta E_0} u_0 \,. \tag{8}$$

So the normalized amplitude of any other state can be written as

$$b = e^{-n\beta(E-E_0)}. \tag{9}$$

This coefficient damps faster than that of the ground state, with half width δE of (spread) depending on the number of the iteration *n* and β by $\delta E = \frac{1}{n\beta}$.

In Fig.1 the blue line for n=8 with $\delta E = 2.5$, the green line for n=16 with $\delta E = 1.25$, and the red line for *n*=32 with δE =0.625.

The new iterative procedure employed in this paper to get the higher excited states involves the following, after n-cooling iterations one extra iteration step using numerical differentiation of the last cooling step with respect to β

$$\chi = -\frac{\partial \Psi}{\partial \beta} = \lim_{\beta' \to 0} \frac{\Psi(x, n\beta) - \Psi(x, n\beta + \beta')}{\beta'}$$

as a heating iterative step is used between the cooling steps and this amounts to an introduction of an extra dependence on E_i for the eigenstate coefficients such that

$$\chi = -\frac{\partial \Psi}{\partial \beta} = \sum_{i=0}^{\infty} E_i a_i e^{-\beta E_i} \ u_i(x)\,, \tag{10}$$

and it acts like heating the system.

Repeating the process every *n*-cooling steps for *M* times the amplitude coefficient for each eigenstate becomes

$$b' = E^M e^{-Mn\beta E}\,, \tag{11}$$

which has the maximum value at

$$\bar{E} = \frac{1}{n\beta}\,. \tag{12}$$

The normalized amplitude has a spread of δE which depends on the number of heating steps by $\delta E = \frac{\bar{E}}{\sqrt{M}}$ as shown in Fig.2, so the more heating steps used the closer and larger growth of the amplitude of the state with energy $\bar{E}$ to the value of $\frac{1}{n\beta}$ as shown in Fig.3.

In Fig.3 the blue line for *n*=2 with $\bar{E} = 2.5$, the green line for *n*=4 with $\bar{E} = 1.25$, and the red line for *n*=8 with $\bar{E}$ =0.625.

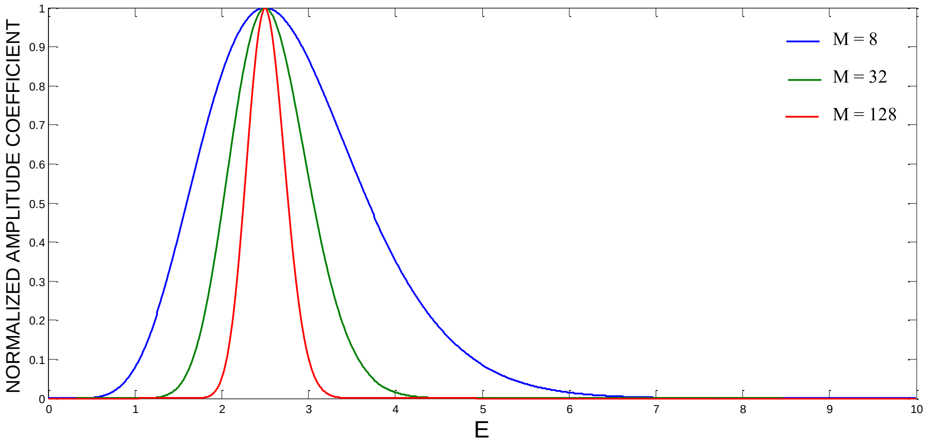

Figure 2. The normalized amplitude coefficient plotted VS E at β = 0.1 and number of iterations n = 4 with different number of M

In Fig.2 the blue line for M=8 with δE =0.88, the green line for M=32 with δE =0.44, and the red line for M=128 with δE =0.22.

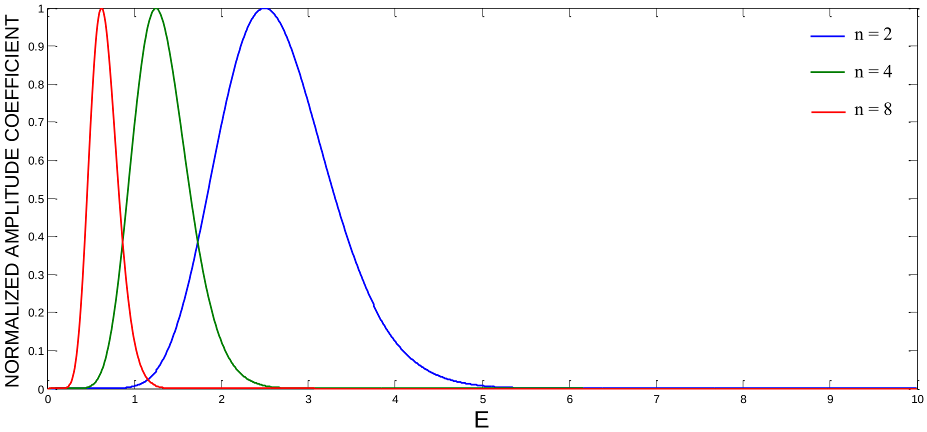

Figure 3. The normalized amplitude coefficient plotted VS E at β = 0.2 and M = 16 with different number of iterations

Fig.3 shows how changing the number of cooling steps n results in different normalized amplitude coefficients centered on different energies and we can expect that the convergence to the lower state needs fewer heating steps while the convergence to the higher states needs more heating steps M because δE is larger for large$\bar{E}$.

elimination of all lower states at each numerical iteration [3], the much simpler iterative technique used in this work decreases greatly the numerical cost and it is much simpler to implement .

Applications

The simple harmonic oscillator is chosen to test this method and to illustrate the effect of cooling and heating steps on the results. If the unit distance is $a = \sqrt{\frac{\hbar}{m\omega}}$ and the unit of energy is $\frac{1}{2}\hbar\omega^2$ the effective potential for simple harmonic oscillator in these units is $\widehat{H'}(x) = V(x) = x^2$. The small values of β can cause a vanishing effect of potential term in Hamiltonian in a small range of x, so for the ground state we used a quite large β and then to get the excited states we chose a suitable values of β and n using equation (12).

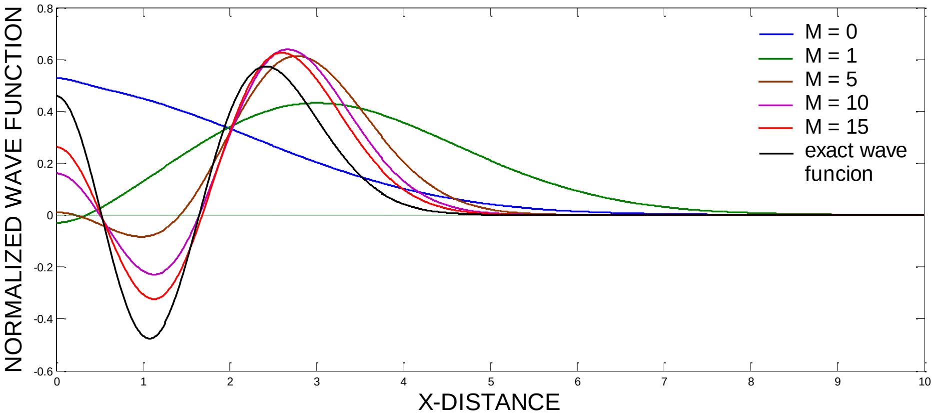

Figure 4a. The development of the normalized 4th excited state wave function of harmonic ocsillator for different M

The development of 4^{th} excited wave functions is shown in Fig.4a at different number of heating steps *M*. The figure illustrates the progression of the wave function toward the exact one. The initial starting guess of the wave function is simply a normalized square box (not shown in Fig.4a) and after *n*=5 of cooling steps, each cooling step is followed by a normalizing step. The resulting shape of the wave function resembles the ground state wave function in this case *M*=0 (the blue curve) where there is growth toward the origin. The next iterative start is the numerical derivative of the blue curve with respect to β resulting in *M*=1 (the green curve), notice the development of first node near the origin, then after few cooling and heating steps a second node develops as shown in Fig.4a at *M*=5, then

M=10, and finally M=15, the amplitudes between the nodes grow in an increasing fashion till finally the shape conformed with the exact wave function (the black curve) that has the closest energy to the value of $\frac{1}{n\beta}$.

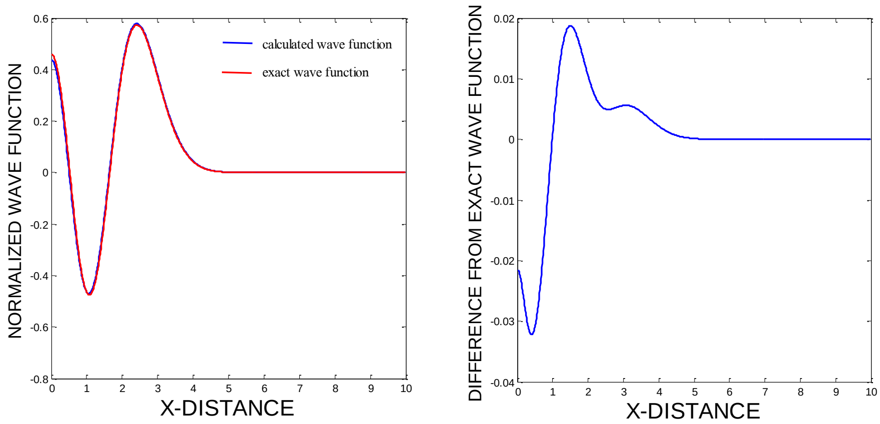

Figure 4b. The normalized 4th excited state wave function of harmonic oscillator for β = 0.02 , n = 5 and M = 50

In Fig. 4b both the numerical calculated wave function after M=50 step and the exact one are shown as well as their differences. The calculated energy of this particular excited state is 9.0001 compared with exact value of 9.0000 [5].

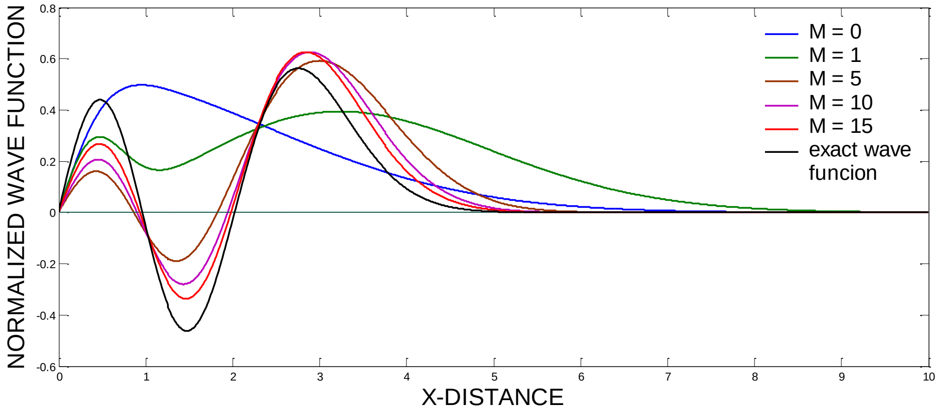

Figure 5a. The development of the normalized 5th excited state wave function of harmonic oscillator for different values of M

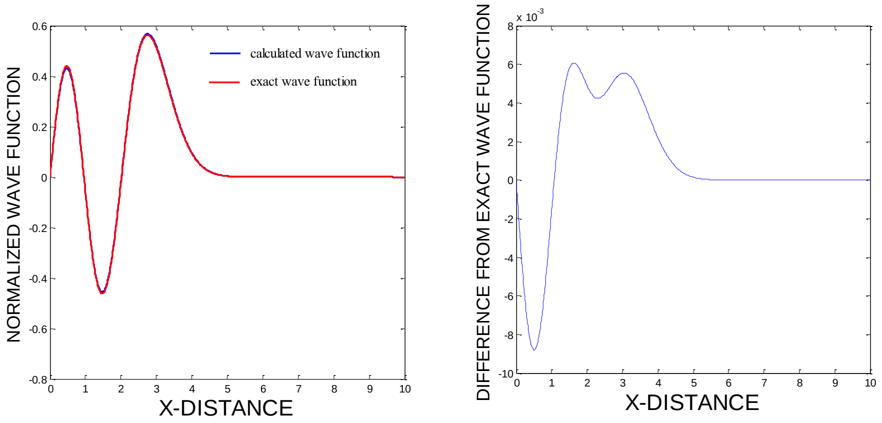

Figure 5b. The normalized 5th excited state wave function of harmonic oscillator for β = 0.01, n = 9 and M = 60

The numerical calculated state wave function after M=60 step and the exact one are shown as well as their difference in Fig.5b.The calculated energy of this particular excited state is 11.0001 which is in a good agreement with exact value of 11.000 [5]. The energy eigenvalues are calculated by evaluating the expectation value of the Hamiltonian for the normalized wave function $E = \int_{-\infty}^{\infty} \Psi^*(x)\,\hat{H}\Psi(x)dx$, where the integrals evaluated using Simpson rule. In table 1 and table 2 we show the energy expectation value of the normalized wave function for the two cases presented here after every 10 heating steps.

Table 1. Calculated Value 0f the 4th State Energy of Harmonic Oscillator with β = 0.02 and n =5

No of heating loop M	*eigenvalue*
10	8.6999
20	9.0418
30	9.0119
40	9.0012
50	9.0001

Table 2. Calculated Value of the 5th State Energy of Harmonic Oscillator with β = 0.01 and n =9

No of heating loop M	*eigenvalue*
10	10.4608
20	10.8452
30	10.9627
40	10.9917
50	10.9985
60	11.0001

Conclusions

In this paper we have presented a detailed account of the diffusion method applied to excited states where we have demonstrated in Fig.1 how the iterative procedure leads to the ground state, then by using a simple numerical procedure based on adding a heating iteration step after *n*-cooling steps and by choosing a proper values of parameter β and number of cooling steps *n* as shown in Fig.3 this developed diffusion method is used for calculating simultaneously the high excited state energy and it's wave function. We have demonstrated the convergence of the iterative wave function to the exact wave function by using more heating steps *M*. This technique offers the advantage over the Gram-Schmidt orthogonalization technique of being less expensive in numerical cost .

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