Calculations for a delta function of Hamiltonian by the Suzuki-Trotter decomposition

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We suggest a new method to calculate an expectation value of a delta function, $\langle\Psi \mid \delta(\hat{H}-E) \mid \Psi\rangle$. The delta function can be replaced by a Gaussian function, $\sqrt{\frac{\beta}{\pi}}\exp[-\beta(\hat{H}-E)^2]$, with large β. Then we apply the Suzuki-Trotter decompositions to this Gauss function of the Hamiltonian. $\exp[-\beta(\hat{H}-E)^2] = \lim_{N\to\infty}\{\exp[-\frac{\beta}{N}\hat{A}_1]\cdots\exp[-\frac{\beta}{N}\hat{A}_M]\}^N$, $(\hat{H}-E)^2 = \hat{A}_1+\cdots+\hat{A}_M$. Approximate calculations with finite N are made, whose the error is estimated to be $O(\frac{1}{N^2})$. Calculations of $\langle\Psi \mid \sqrt{\frac{\beta}{\pi}}\exp[-\beta(\hat{H}-E)^2] \mid \Psi\rangle$ are performed for quantum mechanical problems. We present detailed descriptions on our methods and the numerical results for harmonic oscillator problems in one- and three-dimensions.

Introduction

In the quantum physics some dynamical quantities in the matter [1] can be expressed by

$$\begin{aligned} a(E) &= \mathrm{Im}\{\langle\Psi \mid \hat{A}^\dagger \frac{1}{\hat{H}-E-i\epsilon}\hat{A} \mid \Psi\rangle\} \\ &= \pi\langle\Psi \mid \hat{A}^\dagger\delta(\hat{H}-E)\hat{A} \mid \Psi\rangle\}. \end{aligned} \tag{1}$$

Examples of them are the density of states and the forward scattering amplitude. In this study we replace the delta-function by the Gaussian function,

$$a(E) = \lim_{\beta\to\infty}\ \pi\langle\Psi \mid \hat{A}^\dagger\sqrt{\frac{\beta}{\pi}}e^{-\beta(\hat{H}-E)^2}\hat{A} \mid \Psi\rangle. \tag{2}$$

Although the Gaussian function with finite β is not exactly equal to the delta-function, it is justified to use the former instead of the latter in the calculation because β^{-1} can be interpreted as the resolution in the actual observations.

Let us consider to calculate the following wave function,

$$\mid \phi'\rangle = e^{-\beta(\hat{H}-E)^2} \mid \phi\rangle. \tag{3}$$

We apply the Suzuki-Trotter decomposition to calculate $\exp(-\beta(\hat{H}-E)^2)$. It is well known in the work based on the quantum Monte Carlo methods [2] that this method is quite stable. Calculating $\exp(-i\hat{H}t)$ by this method has been also extensively studied.[3]

Methods

Our study here will be limited to the quantum mechanics, *i.e.* to the one particle problems.

First we describe the method in the one-dimensional case for simplicity. The Hamiltonian is given by

$$\hat{H} = -\frac{d^2}{dx^2} + V(x). \tag{4}$$

Here we adopt units of $\hbar = 1$ and $m = 1/2$. Then it follows

$$\hat{H}^2 = \frac{d^4}{dx^4} - \frac{d^2}{dx^2}V(x) - V(x)\frac{d^2}{dx^2} + V(x)^2. \tag{5}$$

Next we employ the discrete space representation,

$$\begin{aligned} &x_i = (i-1)\Delta + x_{\min}, \qquad i = 1,\cdots,L, \\ &\Delta = (x_{\max} - x_{\min})/L. \end{aligned}$$

The wave function $\phi(x) = \langle x \mid \phi\rangle$ is replaced by $\phi(x_i)$, which is denoted as ϕ_i hereafter. Then the differentials become

$$\frac{d^2\phi(x)}{dx^2} \to \frac{1}{\Delta^2}(\phi_{i+1}+\phi_{i-1}-2\phi_i), \tag{6}$$

$$\frac{d^4\phi(x)}{dx^4} \to \frac{1}{\Delta^4}(\phi_{i+2}+\phi_{i-2}-4\phi_{i+1}-4\phi_{i-1}+6\phi_i), \tag{7}$$

$$\begin{aligned} &V(x)\frac{d^2\phi(x)}{dx^2} + \frac{d^2V(x)\phi(x)}{dx^2} \to \\ &\quad \frac{1}{\Delta^2}\{(V(x_{i+1})+V(x_i))\phi_{i+1} \\ &\quad +(V(x_i)+V(x_{i-1}))\phi_{i-1} - 4V(x_i)\phi_i\}. \end{aligned} \tag{8}$$

Therefore $(\hat{H}-E)^2$ becomes a matrix $H_2 = [h_{2i,j}]$. In order to calculate $e^{-\beta H_2}$ using the Suzuki-Trotter decomposition, we divide the Hamiltonian squared H_2 into four matrices, $H_2^{(k)}$ $(k = 1,2,3,4)$, which are formed by aligning the 4×4 matrices along the diagonal line.

$$H_2 = H_2^{(1)} + H_2^{(2)} + H_2^{(3)} + H_2^{(4)}. \tag{9}$$

It is easy to calculate the exponential of the 4×4 matrix. Then we carry out approximate calculations of $e^{-\beta H_2}$ by

$$\begin{aligned} &\{\exp(-\frac{\beta}{2N_t}H_2^{(1)})\exp(-\frac{\beta}{2N_t}H_2^{(2)})\exp(-\frac{\beta}{2N_t}H_2^{(3)}) \\ &\exp(-\frac{\beta}{N_t}H_2^{(4)})\exp(-\frac{\beta}{2N_t}H_2^{(3)})\exp(-\frac{\beta}{2N_t}H_2^{(2)}) \\ &\exp(-\frac{\beta}{2N_t}H_2^{(1)})\}^{N_t} \end{aligned} \tag{10}$$

with the finite Trotter number N_t. The error by this approximation is $O(\frac{1}{N_t^2})$, as is well known.

Let us show numerical results for the harmonic oscillator

$$V(x) = \lambda x^2. \tag{11}$$

In order to estimate errors owing to the decompositions only, we compare our numerical results with those obtained by the diagonalization of H_2.

We assume $x_{\min} = -25$, $x_{\max} = 25$ and $L = 500$. The initial state ϕ_i^I is parametrized by

$$\phi_i^I = \phi_i^{(1)} C_1 + ... + \phi_i^{(L)} C_L, \tag{12}$$
$$C_1^2 + ... + C_L^2 = 1.$$

Here $\phi^{(l)}$ is the eigenstate of the Hamiltonian with the eigenvalue E_l. Also we assume the ordering $E_l < E_{l+1}$.

Errors on

$$I(E) \equiv \langle \phi | e^{-\beta(\hat{H}-E)^2} | \phi \rangle, \tag{13}$$

are shown in Fig. 1 for the two initial wave functions. One of them, which we will call the wave function (a), is given by

$$C_n = \frac{1}{\sqrt{20}} \quad \text{for} \quad n \leq 20,$$

$$C_n = 0 \quad \text{for} \quad n \geq 21.$$

For another one, the wave function (b), we employ

$$C_n = C(\frac{1}{\sqrt{20}} + \frac{1}{100}) \quad \text{for} \quad n \leq 20,$$

$$C_n = C/100 \quad \text{for} \quad 21 \leq n \leq 100,$$

$$C_n = 0 \quad \text{for} \quad n \geq 101,$$

where C is the normalization factor. The latter state is useful to study the effects due to the highly excited states. Here the error is defined as ratios of (the approximate value $-$ the exact value) to the exact value of $I(E)$.

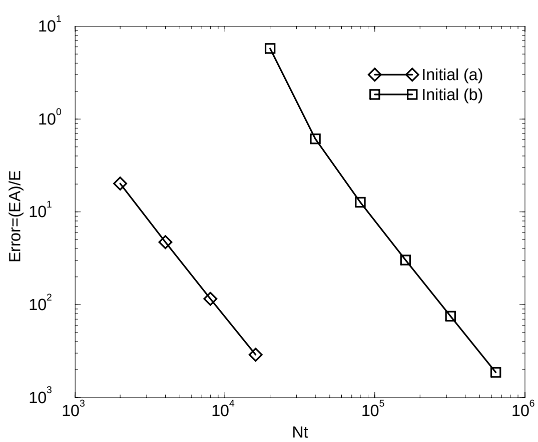

Fig. 1. The error of $I(E)$ versus the Trotter number N_t for two initial wave functions. β and E are 200 and 0.094716 for the wave function (a), while they are 2000 and 0.094716 for the wave function (b).

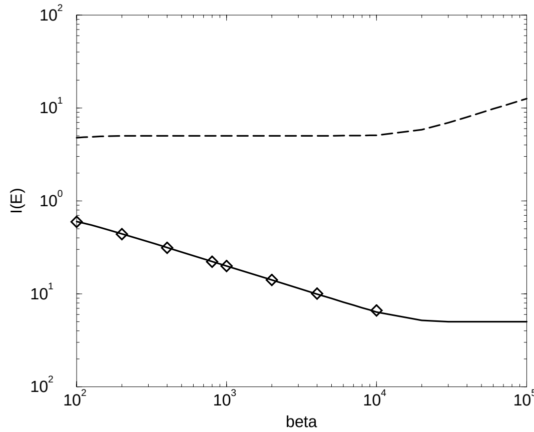

Fig. 2. The numerical data (the diamonds) and the analytic result (the solid line) on $I(E)$. The analytic result on $(\beta/\pi)^{1/2} \cdot I(E)$ are also presented by the dashed line. Here we use the initial wave function (b) with $E = 0.094716$. The Trotter number N_t is fixed to be 20β.

Figure 2 shows the numerical results on $I(E)$ and $\sqrt{\beta/\pi} \cdot I(E)$. (Remember that, in order to approximate the delta function by the Gaussian function, we need the extra factor $\sqrt{\beta/\pi}$.) The diamonds show the numerical data, while the dashed (solid) line is the analytic result with (without) the extra factor. For $50 \leq \beta \leq 50000$, the Gaussian function multiplied by the extra factor is almost flat with the value about 0.5, which is the exact value in the continuum limit $L \to \infty$.

As is expected, the error decreases as $1/N_t^2$. Also one see that the operator $\exp(-\beta(\hat{H} - E)^2)$ can indeed pick up the state with the energy E.

Three-dimensional problems

Next we will discuss on the three-dimensional problems. Here the Hamiltonian is

$$\hat{H} = -\vec{\nabla}^2 + V(\vec{r}). \tag{14}$$

In calculating $e^{-\beta[-\vec{\nabla}^2 + V(\vec{r}) - E]^2}$, we simply extend the method developed in the one-dimensional case and add terms of

$$\frac{d^4}{dx^2 dy^2}, \quad \frac{d^4}{dy^2 dz^2}, \quad \frac{d^4}{dz^2 dx^2}.$$

In the process of including these terms we use

$$\begin{aligned} &\frac{d^4 \phi(x,y,z)}{dx^2 dy^2} \to \\ &\frac{1}{\Delta^4} [\phi_{i+1,j+1,k} + \phi_{i+1,j-1,k} + \phi_{i-1,j+1,k} + \phi_{i-1,j-1,k} \\ &- 2(\phi_{i-1,j,k} + \phi_{i-1,j,k} + \phi_{i-1,j,k} + \phi_{i-1,j,k}) \\ &+ 4\phi_{i,j,k}], \end{aligned} \tag{15}$$

and so on.

Let us now show the numerical results on $I(E)$ for the harmonic oscillator in three dimension. The potential is given

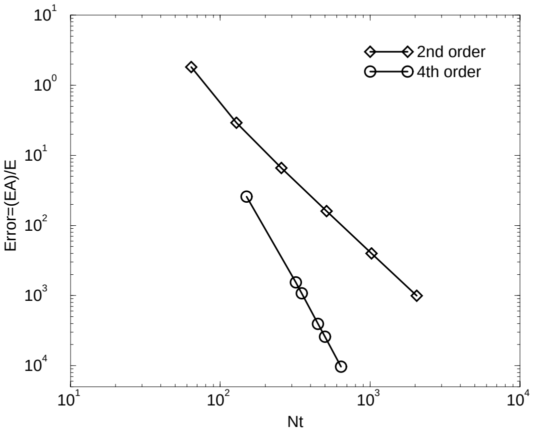

Fig. 3. The error of $I(E)$ versus the Trotter number N_t for the three dimensional harmonic oscillator. Here $L^3 = 32^3$, $x_{\mathbf{max}} = -x_{\mathbf{min}} = 8.0$, $\beta = 4.0$ and $E = 1.1101$. The results from the forth order formula are also plotted.

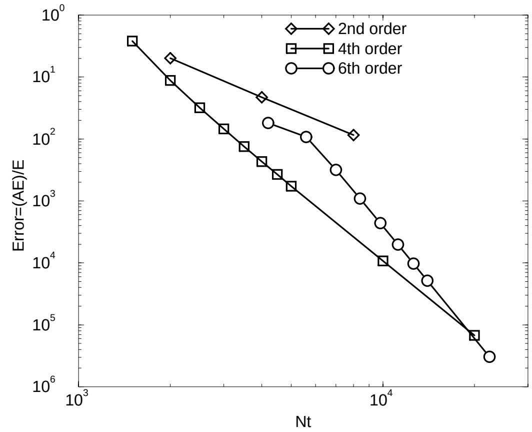

Fig. 4. The error of $I(E)$ versus the Trotter number N_t for the higher order formulae. The data from the second order decomposition are also included for comparison. Parameters are the same as those in Fig. 1.

by

$$V(\vec{r}) = \lambda \mid \vec{r} \mid^2 = \lambda(x^2 + y^2 + z^2). \tag{16}$$

The energy eigenvalues and the eigenstates can be obtained by those in the one-dimensional case. The initial state ϕ is given by

$$\phi^I_{i,j,k} = \sum_{1 \le l,m,n \le L} \phi_i^{(l)} \phi_j^{(m)} \phi_k^{(n)} C_{l,m,n},$$

where $\phi_i^{(l)}$ denotes an eigenstate in the one-dimensional case. Figure 3 plots the results obtained from the initial state with

$$C_{l,m,n} = 1/\sqrt{1000} \quad \text{for } l \le 10, \quad m \le 10, \quad n \le 10,$$

which indicates that the error is $O(1/N_t^2)$ in this case, too.

Higher order decompositions

In the Ref. 4 the higher order decompositions have been suggested. Here we will apply some of these decompositions to our calculations of the delta functions.

For simplicity we explain here only the fourth-order decomposition by two operators $\hat{A}$ and $\hat{B}$. The fourth-order decomposition is based on the second-order decomposition

$$\hat{S}(x) = \exp(\frac{x}{2}\hat{A}) \exp(x\hat{B}) \exp(\frac{x}{2}\hat{A}). \tag{17}$$

The forth-order formula is given by

$$\exp[x(\hat{A} + \hat{B})] = [\hat{S}_4(x/N_t)]^{N_t} + O(x^5/N_t^4), \tag{18}$$

where

$$\hat{S}_4(x) = \hat{S}(p_2 x)^2 \hat{S}((1 - p_2)x) \hat{S}(p_2 x)^2 \tag{19}$$

and $p_2 = (4 - 4^{1/3})^{-1}$.

In Figs. 3 and 4 we plot the results obtained using this formula. It should be noted that the effective number on the products of $\hat{S}(x)$ is used in the axis of abscissas. The results clearly show the error behaves as N_t^{-4}. We also tried to apply the sixth-order decomposition in the one dimensional case, whose results are plotted in Fig. 4. The N_t^{-6} dependence surely can be seen for large values of N_t. Figure 4 indicates, however, the results in the sixth-order decomposition are not so encouraging because the error in this composition exceeds that in the fourth-order decomposition in a wide range of N_t.

Summary

We present detailed descriptions of a new method to calculate an expectation value of a delta function, which can be replaced by a Gaussian function. We apply the Suzuki-Trotter decompositions to the Gauss function of the Hamiltonian and carry out numerical calculations on the quantum mechanical problems. Our results for harmonic oscillator problems in one- and three-dimensions indicate that this method is useful to study the dynamical quantities.

References

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