Improving the Effective Hamiltonian*

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Abstract: The effective Hamiltonian method is useful for describing the physics in the low energy regime. The basic idea is to construct the effective Hamiltonian from the quantum transition matrix elements. The transition matrix is calculated more precisely than before in order to improve the precision of the relative physics value. A simple 1-spatial dimension quantum mechanical system is considered as an example.

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One of the most popular non-perturbative methods in quantum theory is to do numerical simulation on an Euclidean lattice. In the standard Lagrangian formulation, it is very difficult to study excited states. To solve this problem, a new approach (so called effective Hamiltonian)[1] was proposed recently. In Refs [2—8], we investigated many quantum mechanical models using this effective Hamiltonian algorithm. We computed some thermodynamical observables such as the average energy, and specific heat. For the free particle system, we calculated the spectrum and wave-functions in the low energy regime. The results are in very good agreement with those obtained using analytical and/or Runge-Kutta methods.

The calculation of the quantum transition matrix elements is an essential ingredient of the algorithm. In those previous papers, we made an approximation for the matrix elements. In the current paper, we try to calculate the matrix elements using a more precise method. A simple quantum mechanical system is used as an example. The results indicate improvement.

1 Algorithm

The basic idea of the effective Hamiltonian method for one body quantum mechanics has been described in details in Ref. [1]. What is new in our method[1] is to construct an effective Hamiltonian $H_{\rm eff}$ (finite $N\times N$ matrix) through calculation of (imaginary time) transition amplitude between an initial state at position x_i, and time t_i, and final state at x_f and t_f.

$$M_{fi}=\int[{\rm d}x]\exp\left(-\frac{S[x]}{\hbar}\right)_{x_i,t_i}^{x_f,t_f}=\sum_{n=1}^{N}\langle x_f\mid E_n^{\rm eff}\rangle\exp\left(-\frac{E_n^{\rm eff}}{\hbar}\right)\langle E_n^{\rm eff}\mid x_i\rangle \qquad (1)$$

where $S=\int_{t_i}^{t_f}{\rm d}t\left[\frac{m\dot{x}^2}{2}+V(x)\right]$ is the action for a given path, and $T=t_f-t_i$ is the time difference. In (1), $E_n^{\rm eff}$ and $\mid E_n^{\rm eff}\rangle$ are the corresponding nth eigenvalue and eigenvector.

$$H_{\rm eff}=\sum_{n=1}^{N}\mid E_n^{\rm eff}\rangle E_n^{\rm eff}\langle E_n^{\rm eff}\mid \qquad (2)$$

$H_{\rm eff}$ is the effective Hamiltonian. Since the theory described by H, which has an infinite basis in Hilbert space, is now approximated by a theory described by $H_{\rm eff}$ which has a finite basis, the physics of H and $H_{\rm eff}$ might be quite different at high energy. Therefore, we expect that we can only reproduce the low energy physics of the system.

To get the correct scale for the spectrum, the position state $\mid x_n\rangle$ at initial time t_i or final time t_f (Bargman states or box states) should be properly normalized. We denote a normalized basis of Hilbert states as $\mid e_n\rangle$, $n=1,\cdots,N$. In position space, it can be expressed as

$$e_n(x)=\begin{cases}1/\sqrt{\Delta x_n} & x\in[x_n,x_{n+1}]\\ 0, & x\notin=[x_n,x_{n+1}]\end{cases} \qquad (3)$$

where $\Delta x_n=x_{n+1}-x_n$. There is some arbitrariness in choosing a basis for the initial and final states. The simplest choice is a basis with $\Delta x_n=$const., which is called

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the "regular basis".

As explained above, the calculation of the transition matrix elements is an essential ingredient of our method. The matrix element in the normalized basis is related to $\langle x_{n'}, t_f \mid x_n, t_i \rangle$ by

$$M_{n'n} = \langle e_{n'}, t_f \mid e_n, t_i \rangle = \int_{x'_n}^{x_{n'+1}} \mathrm{d}x' \int_{x_n}^{x_{n+1}} \mathrm{d}x'' \frac{\langle x', t_f \mid x'', t_i \rangle}{\sqrt{\Delta x_{n'} \Delta x_n}} \tag{4}$$

Only in a few cases, the transition amplitude $\langle x', t_f \mid x'', t_i \rangle$ can be computed analytically. In most cases, Monte Carlo algorithm has to be employed. Details can be found in our previous papers.

In the previous papers [1—8], we approximated the integral in (4) by the integrand multiplied by the upper and lower limits, i.e.,

$$M_{n'n} \approx \sqrt{\Delta x_{n'} \Delta x_n} \langle x_{n'}, t_f \mid x_n, t_i \rangle \tag{5}$$

It is as an approximation method. In this paper, the 2-dimensional integral in (4) will be calculated by numerical integration.

The spectrum E_n^{eff} and wave function $\mid E_n^{\mathrm{eff}} \rangle$ of the effective Hamiltonian can be obtained by diagonalizing M using unitary transformation

$$M = U^{\dagger} D U \tag{6}$$

where $D = \mathrm{diag}(\exp(-E_1^{\mathrm{eff}} T/\hbar), \cdots, \exp(-E_N^{\mathrm{eff}} T/\hbar))$. And the wave function is the n-th column of U. Once the spectrum and wave functions are available, all physical information can also be obtained. For example, the thermodynamical quantities can be approximated by

$$\begin{aligned} Z_{\mathrm{eff}}(\beta) &= \sum_{n=1}^{N} \exp(-\beta E_n^{\mathrm{eff}}) \\ U_{\mathrm{eff}}(\beta) &= \sum_{n=1}^{N} \frac{E_n^{\mathrm{eff}} \exp(-2\beta E_n^{\mathrm{eff}})}{Z(\beta)} \\ C_{\mathrm{eff}}(\beta) &= k_{\mathrm{B}} \beta^2 \left(\sum_{n=1}^{N} \frac{(E_n^{\mathrm{eff}})^2 \exp(-\beta E_n^{\mathrm{eff}})}{Z(\beta)} - U_{\mathrm{eff}}^2(\beta) \right) \end{aligned} \tag{7}$$

where $\beta = T/\hbar$ and k_{B} is the Boltzmann constant.

2 Exact results for a simple system

To see how the integration method work, we consider the free particle system. One can get the analytical expression for the transition amplitude

$$\langle x', t_f \mid x'', t_i \rangle = \sqrt{\frac{m}{2\pi\hbar T}} \exp\left(-\frac{m}{2\hbar T} (x' - x'')^2 \right) \tag{8}$$

and the following thermodynamical quantities

$$\begin{aligned} Z(\beta) &= \sqrt{\frac{m}{2\pi\hbar^2\beta}} \int_{-\infty}^{+\infty} \mathrm{d}x \\ U(\beta) &= \frac{1}{2\beta}, \; C(\beta) = \frac{k_{\mathrm{B}}}{2} \end{aligned} \tag{9}$$

For a finite basis, the model is reduced to a system with infinitely deep well potential

$$V_{\mathrm{eff}}(x) = \begin{cases} 0, & x \in [-a/2, a/2] \\ \infty, & x \notin [-a/2, a/2] \end{cases} \tag{10}$$

where $a = N\Delta x$. The n th eigenvalue and wave function are exactly known:

$$\begin{aligned} E_n &= \frac{1}{2n} \left(\frac{n\pi\hbar}{a} \right)^2 \\ \psi_n(x) &= \begin{cases} \sqrt{\frac{2}{a}} \sin\left[\frac{n\pi (x + \frac{a}{2})}{a} \right], & x \in [-\frac{a}{2}, \frac{a}{2}] \\ 0, & x \notin [-\frac{a}{2}, \frac{a}{2}] \end{cases} \end{aligned} \tag{11}$$

The transition amplitude is given by (8) inside the well and vanishes identically outside the well. With the increase of the width of the well $a = N\Delta x$, one should expect that the model will have a tendency towards the free theory. This is indeed observed in our previous calculations.

3 Numerical results from the effective Hamilonian

The input parameters of the model are $m = 1$ and $\hbar = 1$. Because this is a stationary system, we can in principle choose any value of T. Here $T = 0.5$ is considered. Correspondingly, we construct a regular basis of size $N = 100$ and distance $\Delta x_n = \Delta x_{n'} = 1$. This leads to the width of the well $a = 100$. The analytical formula for the transition amplitude (8) is substituted into (4) and then $M_{n'n}$ matrix M is calculated by Simpson's 1/3 quadrature. Using the Jacobi method to diagonalize the $N \times N$ matrix M, we get the eigenvalues and wave functions of the effective Hamiltonian as well as the thermodynamical quantities, as discussed in details in Sect. 2.

The spectrum and wave function from the effective Hamiltonian are consistent with (11). The results for the first three wave functions are plotted in Fig. 1. As one sees, they are in good agreement with the analytical results.

Tables 1 and 2 compare the analytical results of the eigenvalues with those from the effective Hamiltonian with the matrix elements computed by integration and approximated methods. Very small β is equivalent to very high temperature. This regime can not be studied very well, because many higher excited states contribute. (It has been stated that the effective Hamiltonian is good for investigating low energy physics). At some lower temperature or larger β, the results from the effective Hamiltonian approach the exact ones. Mostly, the integration method gives results closer to the analytical data, as shown in Tab. 1 and 2.

4 Discussions

In this paper, we have tried to improve the effective

Hamiltonian method by applying the integration method to the computation of the matrix elements $M_{n'n}$. Once $M_{n'n}$ is known, a lot of physical information can be obtained. For the infinitely deep well potential, improvement is observed. We should also note that in general, the transition amplitude $\langle x_{n'}, t_f \mid x_n, t_i \rangle$ in $M_{n'n}$ has to be evaluated by Monte Carlo simulation. In this case, the combination of the integration and Monte Carlo might consume a lot of CPU time. We hope to further investigate this problem in the future.

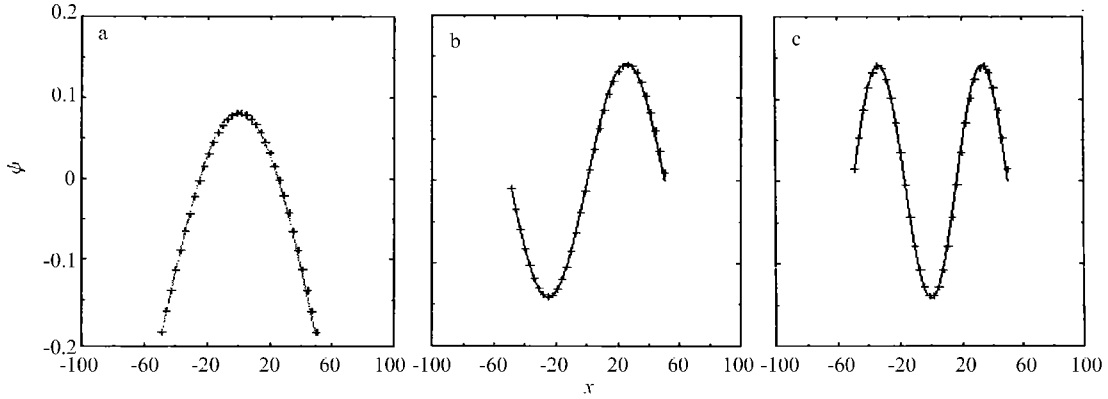

Fig. 1 Wave function of the ground state (a), the first excited state (b) and the second excited state (c)

Tab. 1 Mean energy

β	U^{exact}	U_{eff}^{int}	U_{eff}^{approx}	β	U^{exact}	U_{eff}^{int}	U_{eff}^{approx}
0.1	5.0000	1.7921	1.3310	0.8	0.6250	0.6322	0.6264
0.2	2.5000	1.5226	1.1965	0.9	0.5556	0.5646	0.5677
0.3	1.6667	1.2925	1.0727	1.0	0.5000	0.5091	0.5168
0.4	1.2500	1.1011	0.9605	1.1	0.4545	0.4631	0.4729
0.5	1.0000	0.9445	0.8602	1.5	0.3333	0.3394	0.3474
0.6	0.8333	0.8177	0.7716	2.0	0.2500	0.2548	0.2583
0.7	0.7143	0.7152	0.6939	2.5	0.2000	0.2043	0.2056

Tab 2 Specific heat

β	$\frac{C^{exact}}{k_B}$	$\frac{C_{eff}^{int}}{k_B}$	$\frac{C_{eff}^{ap}}{k_B}$	β	$\frac{C^{exact}}{k_B}$	$\frac{C_{eff}^{int}}{k_B}$	$\frac{C_{eff}^{ap}}{k_B}$
0.1	0.5	0.0288	0.0139	0.8	0.5	0.4777	0.4029
0.2	0.5	0.1000	0.0517	0.9	0.5	0.4944	0.4419
0.3	0.5	0.1893	0.1063	1.0	0.5	0.5038	0.4723
0.4	0.5	0.2771	0.1670	1.1	0.5	0.5086	0.4951
0.5	0.5	0.3520	0.2358	1.5	0.5	0.5094	0.5335
0.6	0.5	0.4097	0.2987	2.0	0.5	0.5057	0.5312
0.7	0.5	0.4507	0.3550	2.5	0.5	0.5048	0.5216

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改进等效哈密顿量

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摘 要: 有效哈密顿方法适用于低能区物理, 以简单的一维量子系统为例, 从量子跃迁矩阵元素出发构造一个等效哈密顿量。通过提高矩阵元的精确度来提高相关物理量的精度, 达到改善计算结果的目的。

关键词: 量子力学; 哈密顿量; 计算物理

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