Quantum Theory with Many Degrees of Freedom from Monte Carlo Hamiltonian

Xiang-Qian Luo a, C.Q. Huang b, J.Q. Jiang c, H. Jirari c, H. Kröger d, K. J.M. Moriarty e

aDepartment of Physics, Zhongshan University, Guangzhou 510275, China
and National Center for Theoretical Sciences, Hsinchu, Taiwan 30043, China

bDepartment of Physics, Foshan Science and Technology College, Foshan 528000, China

cDepartment of Physics, Guangdong Institute of Education, Guangzhou 510303, China

dDépartement de Physique, Université Laval, Québec, Québec G1K 7P4, Canada

eDepartment of Mathematics, Statistics and Computational Science, Dalhousie University, Halifax, Nova Scotia B3H 3J5, Canada

With our recently proposed effective Hamiltonian via Monte Carlo, we are able to compute low energy physics of quantum systems. The advantage is that we can obtain not only the spectrum of ground and excited states, but also wave functions. The previous work has shown the success of this method in (1+1)-dimensional quantum mechanical systems. In this work we apply it to higher dimensional systems.

1. Introduction

Monte Carlo (MC) method with importance sampling is an excellent technique to calculate high dimensional integrals, and has successfully been applied to Lagrangian lattice gauge theory. Recently, we proposed an algorithm to compute the MC Hamiltonian [1]. The advantage, in comparison with the standard Lagrangian MC approach, is that one can obtain not only the spectrum of ground and excited states, but also the wave functions. The method has been tested in quantum mechanics (QM) in 1+1 dimensions, where the exact results were reproduced with high precision [1-3]. In this paper, we apply this algorithm to QM in 2+1 dimensions. The motivation is as follows. (a) A number of algorithms for solving the Schrödinger equation in lower dimensions (e.g. Runge-Kutta) do not work in 2+1 dimensions. Our method works in 2+1 dimensions, it is likely to work also in higher dimensions. (b) The ultimate goal of the algorithm is to study structure function, the S matrix, QCD at finite density as well as systems with many degrees of freedom. QM in 2+1 dimensions is a simple example.

2. Algorithm

Let’s review briefly the basic ideas [1]. According to Feynman’s path integral approach to QM, the (imaginary time) transition amplitude between an initial state at position $x_i$, and time $t_i$, and final state at $x_f$, $t_f$ is related to the Hamiltonian $H$ by

$$<x_f, t_f | x_i, t_i> = <x_f | e^{-\frac{H(t_f-t_i)}{\hbar}} | x_i>$$

$$= \sum_{\nu=1}^{\infty} <x_f | E_\nu > e^{-E_\nu T/\hbar} <E_\nu | x_i>, \quad (1)$$

where $T = t_f - t_i$. The starting point of our method, as described in detail in [1] is to construct an effective Hamiltonian $H_{eff}$ (finite $N \times N$ matrix) by

$$<x_f | e^{-\frac{H(t_f-t_i)}{\hbar}} | x_i> \approx <x_f | e^{-\frac{H_{eff} T}{\hbar}} | x_i>$$

$$= \sum_{\nu=1}^{N} <x_f | E^eff_{\nu} > e^{-E^eff_{\nu} T/\hbar} <E^eff_{\nu} | x_i>. \quad (2)$$

$H_{eff}$ can be found by MC simulation using the following procedure:
(a) Discretize the continuous time.
(b) Generate configurations \([x]\) obeying the Boltzmann distribution
\[ P(x) = \frac{\exp(-S[x]/\hbar)}{\int [dx] \exp(-S[x]/\hbar)}. \tag{3} \]
(c) Calculate the transition matrix elements
\[ M_{fi} = \langle x_f | e^{-\mathcal{H}_{eff}T/\hbar} | x_i \rangle \tag{4} \]
between \(N\) discrete \(x_i\) points and \(N\) \(x_f\) points. Note that the matrix \(M\) is symmetric.
(d) Diagonalize \(M\) by a unitary transformation
\[ M = U^\dagger DU, \tag{5} \]
where \(D = \text{diag}(e^{-E_1^{eff}T/\hbar}, \ldots, e^{-E_N^{eff}T/\hbar}).\) Steps (a) and (b) are the same as the standard MC method. Step (c) is the essential ingredient of our method, from which we can construct \(\mathcal{H}_{eff},\) and obtain the eigenvalues \(E_n^{eff}\) and wavefunction \(|E_n^{eff}\rangle\) through step (d). Once the spectrum and wave functions are available, all physical information can be retrieved. Since the theory described by \(H\) is now approximated by a theory described by a finite matrix \(H_{eff},\) the physics of \(H\) and \(H_{eff}\) might be quite different at high energy. Therefore we expect that we can only reproduce the low energy physics of the system. This is good enough for our purpose.

3. Results

We consider the following examples in \(D = 2:\)

3.1. Uncoupled harmonic oscillator

The Euclidean action is given by
\[ S = \int_0^T dt \left[ \frac{m}{2}(\dot{x}^2 + \dot{y}^2) + \frac{m\omega^2}{2}(x^2 + y^2) \right]. \tag{6} \]
The spectrum is degenerate and exactly known:
\[ E_{n_1, n_2} = \omega_1 \hbar (n_1 + 1/2) + \omega_2 \hbar (n_2 + 1/2), \tag{7} \]
\(n_1, n_2 = 0, 1, 2, \ldots,\)

3.2. Coupled harmonic oscillator

The Euclidean action is given by
\[ S = \int_0^T dt \left[ \frac{m}{2}(\dot{x}^2 + \dot{y}^2) + \frac{m\omega^2}{2}(x^2 + y^2) + \lambda xy \right], \tag{8} \]
for \(0 < \lambda < m\omega^2.\)
The spectrum is also exactly known:
\[ E_{n_1, n_2} = \omega_1 \hbar (n_1 + 1/2) + \omega_2 \hbar (n_2 + 1/2), \tag{9} \]
\(n_1, n_2 = 0, 1, 2, \ldots,\)
where \(\omega_1 = \sqrt{\omega^2 + \frac{\lambda}{m}}\) and \(\omega_2 = \sqrt{\omega^2 - \frac{\lambda}{m}}.\)

3.3. Summary

Tabs. 1 and 2 compare the spectrum from \(H_{eff}\) with the exact results. Figs. 1-4 show the first two wave functions. They are in very good agreement with the exact ones, at least in the low energy domain. In Ref. [4], more results for wave functions of higher excited states, and thermodynamical quantities such as the average energy and specific heat, were reported. However, the CPU time is much longer than in 1-dimensional systems. We need to find a better (stochastic) way to select the basis in Hilbert space in step (c) of Sect. 2, before extending the method to quantum field theory. We are curious to see if our method can resolve the long standing problem of QCD at finite density. It is worth mentioning the recent analytical [3] and numerical [2] efforts in Hamiltonian formulation.

X.Q.L. is supported by the National Science Fund for Distinguished Young Scholars, supplemented by National Natural Science Foundation, fund for international cooperation and exchange, Ministry of Education, and Hong Kong Foundation of Zhongshan University Advanced Research Center. We also thank the Lat’99 organizers and NCTS, Taiwan for partial support. H.K. would like to acknowledge support by NSERC Canada.

REFERENCES

1. H. Jirari, H. Kröger, X.Q. Luo, K. Moriarty, Phys. Lett. A258 (1999) 6.
2. H. Kröger, these proceedings.
3. C.Q. Huang et al., in preparation.
4. J.Q. Jiang et al., in preparation.
5. X.Q. Luo et al., in preparation.
6. M. Creutz, hep-lat/9905021.
Table 1
Spectrum of *uncoupled* harmonic oscillator.

| $n_1, n_2$ | $E_{MC}^{(n_1, n_2)}$ | $E_{Exact}^{(n_1, n_2)}$ |
|------------|-----------------------|------------------------|
| 0, 0       | 0.9975 ± 0.0258       | 1.0000                 |
| 0, 1       | 1.9902 ± 0.0420       | 2.0000                 |
| 1, 0       | 2.0022 ± 0.0468       | 2.0000                 |
| 0, 2       | 2.9499 ± 0.0393       | 3.0000                 |
| 2, 0       | 2.9815 ± 0.0550       | 3.0000                 |
| 1, 1       | 3.0014 ± 0.0546       | 3.0000                 |
| $n_1 + n_2 = 3$ | 3.9718 ± 0.0496 | 4.0000                 |
| $n_1 + n_2 = 3$ | 3.9853 ± 0.0626 | 4.0000                 |
| $n_1 + n_2 = 3$ | 4.0547 ± 0.0611 | 4.0000                 |
| $n_1 + n_2 = 3$ | 4.0713 ± 0.0851 | 4.0000                 |

Figure 1. $\psi_{n_1 n_2}(x, y)$ vs. $x$ at $y = -1$ for *uncoupled* harmonic oscillator with $n_1 = n_2 = 0$.

Figure 2. $\psi_{n_1 n_2}(x, y)$ vs. $x$ at $y = -1$ for *uncoupled* harmonic oscillator with $n_1 = 0, n_2 = 1$.

Table 2
Spectrum of *coupled* harmonic oscillator.

| $n_1, n_2$ | $E_{MC}^{(n_1, n_2)}$ | $E_{Exact}^{(n_1, n_2)}$ |
|------------|-----------------------|------------------------|
| 0, 0       | 0.9640 ± 0.0245       | 0.9659                 |
| 0, 1       | 1.6693 ± 0.0335       | 1.6730                 |
| 1, 0       | 2.1843 ± 0.0535       | 2.1907                 |
| 0, 2       | 2.3650 ± 0.0363       | 2.3801                 |
| 1, 1       | 2.8818 ± 0.0553       | 2.8978                 |
| 0, 3       | 3.0883 ± 0.0447       | 3.0872                 |
| 0, 3       | 3.0883 ± 0.0447       | 3.0872                 |
| 2, 0       | 3.4049 ± 0.0532       | 3.4154                 |
| 1, 2       | 3.6275 ± 0.0526       | 3.6049                 |
| 0, 4       | 3.7414 ± 0.0327       | 3.7944                 |

Figure 3. $\psi_{n_1 n_2}(x, y)$ vs. $x$ at $y = -1$ for *coupled* harmonic oscillator with $n_1 = n_2 = 0$.

Figure 4. $\psi_{n_1 n_2}(x, y)$ vs. $x$ at $y = -1$ for *coupled* harmonic oscillator with $n_1 = 0, n_2 = 1$. 