Monte Carlo Hamiltonian: Inverse Potential

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Abstract

The Monte Carlo Hamiltonian method developed recently allows to investigate ground state and low-lying excited states of a quantum system, using Monte Carlo algorithm with importance sampling. However, conventional MC algorithm has some difficulties when applying to inverse potentials. We propose to use effective potential and extrapolation method to solve the problem. We present examples from the hydrogen system.

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1 Introduction

There are two standard approaches in quantum theory: Hamiltonian and Lagrangian formulations. A comparison is given in Tab.\textsuperscript{1} The Lagrangian formulation is very suitable for applying the Monte Carlo (MC) method to systems with many degrees of freedom, and in the last two decades, it has been widely applied to lattice gauge theory\textsuperscript{1,2,3}. In the standard Lagrangian MC method, however, it is extremely difficult to compute the spectrum and wave function beyond the ground state.

Wave functions in conjunction with the energy spectrum contain more physical information than the energy spectrum alone. Although lattice QCD simulations in the Lagrangian formulation give good estimates of the hadron masses, one is yet far from a comprehensive understanding of hadrons. Let us take as example a new type of hardrons made of gluons, the so-called glueballs. Lattice QCD calculations\textsuperscript{4,5} predict the mass of the lightest glueball with quantum number $J^{PC} = 0^{++}$, to be $1650 \pm 100 \text{MeV}$. Experimentally, there are at least two candidates: $f_0(1500)$ and $f_J(1710)$. The investigation of the glueball production and decays can certainly provide additional important information for experimental determination of a glueball. Therefore, it is important to be able to compute the glueball wave function.

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Table 1: Comparison of the conventional methods in the standard formulations.

| Formulation | Hamiltonian | Lagrangian |
|-------------|-------------|-------------|
| Approach    | Schrödinger Eq. | Path Integral |
|             | $H|E_n⟩ = E_n|E_n⟩$ | $⟨O⟩ = \frac{\int [dx] O[x] \exp(-S[x]/\hbar)}{\int [dx] \exp(-S[x]/\hbar)}$ |
| Algorithm   | Series expansion, variational, Runge-Kutta ... | MC with importance sampling |
| Advantage   | Both the ground state, and the excited states can be computed. | It generates the most important configs. for the measurements. |
| Disadvantage| Analytical methods are too tedious for many body systems; Runge-Kutta works only in 1-D. | It is difficult to study the excited states. |

A natural question is whether in Lagrangian MC simulations one can construct an effective Hamiltonian? We have recently proposed a new approach [6] (named Monte Carlo Hamiltonian method) to investigate this problem. We start out from the action of the theory. We compute the transition matrix for all transitions using MC with importance sampling, where the states are taken from a basis in Hilbert space. As a result, we find an effective Hamiltonian, i.e. its spectrum and eigen states. A lot of models [6, 7, 8, 9, 10, 11, 12, 13] in quantum mechanics (QM) have been used to test the method. This method has also been applied to scalar field theories [14, 15, 16, 17].

Although MC with importance sampling has been very successful for QM with many local potentials, it is very difficult for QM with inverse potentials, due to the singularity. In this paper, we propose effective potential and extrapolation method to solve the problem. The hydrogen system is used as an example.

The rest of the paper is organized as follows. In Sect. 2 and Sect. 3 the basic ideas of MC Hamiltonian are reviewed. In Sect. 4 we describe a method to analyze the errors of the spectrum and wave functions. In Sect. 5 a method to investigate the inverse potential is presented. The numerical results for the hydrogen system are given in Sect. 6 and summarized in Sect. 7.

## 2 Effective Hamiltonian

Let us discuss the construction of the effective Hamiltonian in several steps [6]. First, consider in quantum mechanics in 1-dim the motion of a single particle of mass $m$ under the influence of a local potential $V(x)$. Its classical action is given by

$$ S = \int dt \left( \frac{m}{2} \dot{x}^2 - V(x) \right). \tag{1} $$
Given the classical action, one can determine Q.M. transition amplitudes. Like in Lagrangian lattice field theory, we use imaginary time in what follows. We consider the transition amplitude for some finite time \( T \) \((t_{in} = 0, \ t_{fi} = T)\) and for all combinations of positions \( x_i, x_j \). Here \( x_i, x_j \) run over a finite discrete set of points \( \{x_1, \ldots, x_N\} \) located on the real axis. Suppose these points are equidistantly distributed (spacing \( \Delta x \)) over some interval \([-L, +L]\). The transition amplitudes are given by the (Euclidean) path integral,

\[
M_{ij}(T) = \int [dx] \exp\left[-S_E[x]/\hbar\right]_{x_i,0}^{x_i,T},
\]

where \( S_E = \int dt \ (m\dot{x}^2/2 + V(x)) \) denotes the Euclidean action. Suppose for the moment that those transition amplitudes were known. From that one can construct an approximate, i.e. effective Hamiltonian. Note that the matrix \( M(T) = [M_{ij}(T)]_{N \times N} \) is a real, positive and Hermitian matrix. It can be factorized into a unitary matrix \( U \) and a real diagonal matrix \( D(T) \),

\[
M(T) = U^\dagger \ D(T) \ U.
\]

Because the matrix \( M(T) \) can be expressed in terms of the full Hamiltonian \( H \) by

\[
M_{ij}(T) = \langle x_i | \exp(-HT/\hbar) | x_j \rangle,
\]

the matrices \( U \) and \( D \) have the following meaning,

\[
U_{ik} = \langle x_i | E_{eff}^k \rangle,
D_k(T) = \exp(-E_{eff}^k T/\hbar),
\]

i.e., the \( k-th \) eigenvector \( |E_{eff}^k\rangle \) of the effective Hamiltonian \( H_{eff} \) can be identified with the \( k-th \) column of matrix \( U^\dagger \) and the energy eigenvalues \( E_{eff}^k \) of \( H_{eff} \) can be identified with the logarithm of the diagonal matrix elements of \( D(T) \). This yields an effective Hamiltonian,

\[
H_{eff} = \sum_{k=1}^{N} |E_{eff}^k\rangle \langle E_{eff}^k| < E_{eff}^k|E_{eff}^k\rangle.
\]

Note that in the above we have been mathematically a bit sloppy. The states \(|x_i\rangle\) are not Hilbert states. We have to replace \(|x_i\rangle\) by some “localized” Hilbert state. This can be done by introducing box states. We associate to each \( x_i \) some box state \( b_i \), defined by

\[
b_i(x) = \begin{cases} 
1/\sqrt{\Delta x_i} & \text{if } x_i < x \leq x_i + 1 \\
0 & \text{else}
\end{cases}
\]

where \( \Delta x_i = x_{i+1} - x_i \). When we use an equidistant distribution of \( x_i \), i.e. \( \Delta x_i = \Delta x \), we refer to the basis of box states as the regular basis.
3 Matrix elements

We compute the matrix element $M_{ij}(T)$ directly from the action via Monte Carlo with importance sampling. This is done by writing each transition matrix element as a ratio of two path integrals.

$S_E = S_0 + S_V$. 

This allows to express the transition amplitude by

$$M_{ij}(T) = M_{ij}^{(0)}(T) \frac{\int_{x_i}^{x_{i+1}} dy \int_{x_j}^{x_{j+1}} dz \int [dx] \exp[-S_V[x]/\hbar] \exp[-S_0[x]/\hbar]|_{y,T}^{y',T}}{\int_{x_i}^{x_{i+1}} dy \int_{x_j}^{x_{j+1}} dz \int [dx] \exp[-S_0[x]/\hbar]|_{y,T}^{y',T}}.$$

Here $\exp(-S_0/\hbar)$ is the weight factor and $\exp(-S_V/\hbar)$ is the observable. $M_{ij}^{(0)}(T)$ stands for the transition amplitude of the noninteracting system, which is (almost) known analytically. For details see ref. [6]. Carrying out these steps allows to construct an effective Hamiltonian, which has turned out to reproduce well low energy physics of a lot of quantum systems [6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17].

4 Error analysis

From errors of the matrix elements $\Delta M$ in Monte Carlo simulations, one can obtain the errors of the eigen value $E_n$ and wave function $\psi_n$ of the effective Hamiltonian. Suppose $H$ is the Hamiltonian of the theory, $H'$ is a perturbation term induced by error in the simulation, then we have the following equation for the transition matrix element

$$\exp \left( -\frac{(H + H')T}{\hbar} \right) \approx \exp \left( -\frac{HT}{\hbar} \right) - \frac{T}{\hbar} \exp \left( -\frac{HT}{\hbar} \right) H',$$

which implies

$$\Delta M = \exp \left( -\frac{(H + H')T}{\hbar} \right) - \exp \left( -\frac{HT}{\hbar} \right)$$

$$\approx -\frac{T}{\hbar} \exp \left( -\frac{HT}{\hbar} \right) H'$$

or

$$H' \approx -\frac{\hbar}{T} M^{-1} \Delta M.$$

According to perturbation theory, the first order correction to the eigen value and wave function is

$$\Delta E_n = H'_{nn} = -\frac{\hbar}{T} \exp(-E_nT/\hbar) \int dx \psi^*_n M \psi_n$$

$$\psi'_n = \sum_{n' \neq n} \frac{H'_{nn'}}{E_n - E_{n'}} \psi_{n'}.$$


where

$$H'_n = \int dx \, \psi_n^* H' \psi_n.$$  \hfill (14)

Eq. (13) gives an estimate of the wave function.

5 Inverse potential: the hydrogen atom

The Schrödinger equation of a hydrogen is

$$-\frac{\hbar^2}{2m} \nabla^2 \Psi(r, \theta, \varphi) + V(r) \Psi(r, \theta, \varphi) = E \Psi(r, \theta, \varphi),$$  \hfill (15)

where

$$V(r) = -\frac{e}{r}.$$  \hfill (16)

Because of the spherical symmetry, the wave function can be factorized as

$$\Psi(r, \theta, \varphi) = \psi(r) Y(\theta, \varphi),$$  \hfill (17)

and the radial wave function satisfies

$$-\frac{\hbar^2}{2m} \left[ r^2 \frac{d}{dr} \left( d\psi(r) \frac{1}{dr} \right) \right] + \left[ V(r) + \frac{l(l+1)\hbar^2}{2mr^2} \right] \psi(r) = E \psi.$$  \hfill (18)

Defining a function $u(r)$ by

$$u(r) = r \psi(r),$$  \hfill (19)

and considering the case of angular-momentum quantum number zero ($l = 0$), one obtains

$$-\frac{\hbar^2}{2m} \frac{d^2 u}{dr^2} + V(r) u = E u$$  \hfill (20)

which reduces to a one dimensional QM problem. This system has the following analytic result for the energy

$$E_n = -\frac{1}{2(n+1)^2},$$  \hfill (21)

where $n = 0, 1, \ldots$ is the principal quantum number and $m = 1$, $e = 1$, $\hbar = 1$ have been chosen. The ground state and first excited state radial wave functions are

$$\psi_0(r) = 2 \exp(-r),$$

$$\psi_1(r) = \frac{1}{\sqrt{2}} (2 - r) \exp(-r/2).$$  \hfill (22)
Our purpose is to investigate the 1-d system NOT by solving Eq. (20), but by MC Hamiltonian method. Unfortunately, due to the divergence of $V(r)$ at $r = 0$, it is not convenient for MC simulations.

To solve the problem, we replace $V(r)$ by an effective potential with cut-off parameter $R$

$$V_R(r) = \frac{\exp(2r/R) - 1}{\exp(2r/R) + 1} V(r).$$

(23)

$V_R(r)$ approaches to $V(r)$ when $R \to 0$ and $V_R(r)$ is analytic for any value of finite $R$, which will be used in numerical simulations.

6 Numerical results

The coordinates for the box state (see Eq. (7)) are chosen to be

$$r_i = i \ast dr, \quad i = 1, 2, ..., N.$$ 

(24)

The simulation parameters are $m = 1$, $e = 1$, $\hbar = 1$, $T = 0.85$, $dr = 0.99$ and $N = 100$. Using the Metropolis algorithm and method described in Sect. 3, we obtain the matrix elements $M_{n'n}$ with potential $V_R(r)$ for some non-zero $R$. Then we compute the eigenvalues and eigenvectors using the method described in Sect. 2 and analyze their errors using the method described in Sect. 4.

Fig. 1 plots the ground state energy of the hydrogen system with effective potential $V_R(r)$ at $R = 0.3, 0.4, 0.5, 0.6, 0.7$ and $0.8$. Between initial and final $r_i$, 600 paths are used in MC simulations. We use the least square method to extrapolate the data to the $R = 0$ limit. The result agrees with the analytic one within large error bar. Fig. 2 plots the first excited state energy. The agreement is greatly improved if more paths (1000) are used in MC simulations. This is shown in Fig. 3 and Fig. 4.

Fig. 5 plots the ground state wave function of the hydrogen system extrapolated to $R = 0$. Between initial and final $r_i$, 1000 paths are used in MC simulations. Fig. 6 shows the first excited state wave function. They are consistent with the analytic ones.

7 Summary

In the preceding sections, we have extended the effective Hamiltonian method to QM with inverse potentials, and taken the hydrogen system as an example. The results are encouraging. We believe that the application of the algorithm to more complicated systems will be very interesting. It will allow a non-perturbative investigation of physics beyond the ground state.

References

[1] M. Creutz, Quarks, Gluons and Lattices, Cambridge University Press, Cambridge (1983).

[2] H. Rothe, Lattice Gauge Theory: an Introduction, World Scientific, Singapore (1992).
[3] I. Montvay and G. Münster, Quantum Fields on a Lattice, Cambridge University Press, Cambridge (1994).

[4] X.Q. Luo, and Q. Chen, Mod. Phys. Lett. A11 (1996) 2435.

[5] X.Q. Luo, Q. Chen, S. Guo, X. Fang, and J. Liu, Nucl. Phys. B (Proc. Suppl.)53 (1997) 243.

[6] H. Jirari, H. Kröger, X.Q. Luo, and K. Moriarty, Phys. Lett. A258 (1999) 6.

[7] X.Q. Luo, C. Huang, J. Jiang, H. Jirari, H. Kröger, and K. Moriarty, Physica A281 (2000) 201.

[8] X.Q. Luo, J. Jiang, C. Huang, H. Jirari, H. Kröger, and K. Moriarty, Nucl. Phys. B(Proc. Suppl.)83 (2000) 810.

[9] J. Jiang, C. Huang, X.Q. Luo, H. Jirari, H. Kröger, K. Moriarty, Commun. Theor. Phys. 34 (2000) 723.

[10] H. Jirari, H. Kröger, C. Huang, J. Jiang, X.Q. Luo, and K. Moriarty, Nucl. Phys. B(Proc. Suppl.)83 (2000) 953.

[11] C. Huang, J. Jiang, X.Q. Luo, H. Jirari, H. Kröger, and K. Moriarty, High Energy Phys. Nucl. Phys. 24 (2000)478.

[12] X. Q. Luo, H. Xu, J. Yang, Y. Wang, D. Chang, Y. Lin and H. Kroger, Commun. Theor. Phys. 36 (2001) 7.

[13] X. Q. Luo, J. J. Liu, C. Q. Huang, J. Q. Jiang and H. Kroger, Commun. Theor. Phys. 38 (2002) 561

[14] X. Q. Luo, H. Jirari, H. Kroger and K. J. Moriarty, in Non-perturbative methods and lattice QCD, World Scientific, Singapore (2001) 100. [hep-lat/0108026].

[15] C. Q. Huang, X. Q. Luo, H. Kroger and K. J. Moriarty, Phys. Lett. A299 (2002) 483

[16] H. Kroger, X. Q. Luo and K. J. Moriarty, Nucl. Phys. B(Proc. Suppl.)119 (2003) 508.

[17] H. Kroger, X. Q. Luo and K. J. Moriarty, Math. Comput. Simul. 62 (2003) 377.
Figure 1: Ground state energy of the hydrogen system with effective potential $V_R(r)$ at $R = 0.3, 0.4, 0.5, 0.6, 0.7$ and $0.8$. The circle at $R = 0$ is the analytic result and the line is the fitting curve. Between initial and final $r_i$, 600 paths are used in MC simulations.

Figure 2: The same as Fig. 1 but for the first excited state energy.
Figure 3: Ground state energy of the hydrogen system with effective potential $V_R(r)$ at $R = 0.3$, 0.4, 0.5, 0.6, 0.7 and 0.8. The circle at $R = 0$ is the analytic result and the line is the fitting curve. Between initial and final $r_i$, 1000 paths are used in MC simulations.

Figure 4: The same as Fig. 3 but for the first excited state energy.
Figure 5: Ground state wave function of the hydrogen system extrapolated to $R = 0$. The line is the analytical result. Between initial and final $r_1$, 1000 paths are used in MC simulations.

Figure 6: The same as Fig. 5 but for the first excited state wave function.