Algorithm for Computing Excited States in Quantum Theory

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Abstract. Monte Carlo techniques have been widely employed in statistical physics as well as in quantum theory in the Lagrangian formulation. However, in the conventional approach, it is extremely difficult to compute the excited states. Here we present a different algorithm: the Monte Carlo Hamiltonian method, designed to overcome the difficulties of the conventional approach. As a new example, application to the Klein-Gordon field theory is shown.

INTRODUCTION

There are two standard formulations in quantum theory: Hamiltonian and Lagrangian. A comparison of the conventional approaches is given in Table 1.

Monte Carlo (MC) method with importance sampling is an excellent non-perturbative technique to calculate path integrals in quantum theory. In the last two decades, it has successfully been applied to Lagrangian lattice gauge theory [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. On the other hand, the standard Hamiltonian formulation is capable of doing it.

Recently, we proposed an algorithm to construct an effective Hamiltonian from Lagrangian MC simulations in Ref. [4]. We called it the MC Hamiltonian method. The advantage, in comparison with the standard Lagrangian MC approach, is that one can obtain the spectrum and wave functions beyond the ground state. It also allows to do thermodynamics. In this paper, we briefly review what we have done, and present some new results.

Table 1. Comparison of the conventional methods.

Formulation	Hamiltonian	Lagrangian
Approach	Schrödinger Eq. $H\|E_n>=E_n\|E_n>$	Path Integral $<O>=\frac{\int d[x]O[x]\exp(-S[x]/\hbar)}{\int[dx]\exp(-S[x]/\hbar)}$
Algorithm	Series expansion, variational approx., Runge-Kutta ...	MC simulation with importance sampling
Advantage	Both ground state, & excited states can be computed.	It generates the important configurations
Problem	Difficult for many body systems.	Difficult for excited states.

ALGORITHM

Effective Hamiltonian

Let us review briefly the basic ideas of our approach. The (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 is related to the Hamiltonian H by

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

$$=\sum_{n=1}^{\infty}<x_f|E_n>e^{-E_nT/\hbar}<E_n|x_i>, \tag{1}$$

where $T=t_f-t_i$. According to Feynman's path integral formulation of quantum mechanics (Q.M.), the transition amplitude is also related to the path integral:

$$M_{fi}=\int[dx]\exp(-S[x]/\hbar)|_{x_i,t_i}^{x_f,t_f}. \tag{2}$$

The starting point of our method, as described in detail in Ref. [4] is to construct an effective Hamiltonian H_{eff} (finite $N\times N$ matrix) by

$$M_{fi}=<x_f|e^{-H_{eff}T/\hbar}|x_i>$$

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$$= \sum_{n=1}^{N} < x_f|E_n^{eff} > e^{-E_n^{eff} T/\hbar} < E_n^{eff}|x_i > . \quad (3)$$

The eigenvalues E_n^{eff} and wave function $|E_n^{eff} >$ can be obtained, by diagonalizing M using a unitary transformation

$$M = U^\dagger D U, \quad (4)$$

where $D = diag(e^{-E_1^{eff} T/\hbar}, ..., e^{-E_N^{eff} T/\hbar})$. Once the spectrum and wave functions are available, all physical information can also be obtained.

Since the theory described by H, whose basis in Hilbert space is infinite, is now approximated by a theory described by a finite matrix H_{eff}, whose basis is finite, 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. In Refs. [4, 5, 6, 7], we investigated many 1-D, 2-D and 3-D Q.M. models (Table 2) using this MC Hamiltonian algorithm. We computed the spectrum, wave functions and some thermodynamical observables. The results are in very good agreement with those from analytical and/or Runge-Kutta methods.

Table 2. Q.M. systems, investigated by the MC Hamiltonian method using the regular basis.

System	Potential
Q.M. in 1-D	$V(x) = 0$
	$V(x) = \frac{1}{2} m\omega^2 x^2$
	$V(x) = -V_0 \mathrm{sech}^2(\mathrm{x})$
	$V(x) = \frac{1}{2} x^2 + \frac{1}{4} x^4$
	$V(x) = \frac{1}{2}\|x\|$
	$V(x) = \{ \begin{array}{ll} \infty, & x < 0 \\ Fx, & x \geq 0 \end{array}$
Q.M. in 2-D	$V(x,y) = \frac{1}{2} m\omega^2 x^2 + \frac{1}{2} m\omega^2 y^2$
	$V(x,y) = \frac{1}{2} m\omega^2 x^2 + \frac{1}{2} m\omega^2 y^2 + \lambda xy$
Q.M. in 3-D	$V(x,y,z) = \frac{1}{2} m\omega^2 x^2 + \frac{1}{2} m\omega^2 y^2 + \frac{1}{2} m\omega^2 z^2$

Basis in Hilbert Space

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

$$e_n(x) = \{ \begin{array}{ll} 1/\sqrt{\Delta x_n}, & x \in [x_n, x_{n+1}] \\ 0, & x \notin [x_n, x_{n+1}] \end{array} \quad (5)$$

where $\Delta x_n = x_{n+1} - x_n$.

The simplest choice is a basis with $\Delta x_n = const.$, which is called the " regular basis". In Refs. [4, 5, 6, 7], the regular basis is used. For many body system or quantum field theory, the regular basis will encounter problem. For example, in a system with a 1-D chain of oscillators (see later), if the number of oscillators is 30, the minimum non-trivial regular basis is $N = 2^{30} = 1073741824$, which is prohibitively large for numerical calculations.

Guided by the idea of importance sampling, in Refs. [8, 9], we proposed to select a basis from the Boltzmann weight proportional to the transition amplitude between $x_i' = 0$ at $t_i' = 0$ and $x_f' = x_n$ at some t_f'. In one free particle case, the distribution is just a Gaussian

$$P_{basis}[x_n] = \frac{1}{\sqrt{2\pi}\sigma} \exp(-\frac{x_n^2}{2\sigma^2}), \quad (6)$$

where $\sigma = \sqrt{\hbar t_f'/m}$. We call such a basis the "stochastic basis".

Matrix elements

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 $< x_{n'}, t_f | x_n, t_i >$ by

$$\begin{aligned} M_{n'n} &= < e_{n'}, T | e_n, 0 > \\ &= \int_{x_n'}^{x_{n'+1}} dx' \int_{x_n}^{x_{n+1}} dx'' \frac{< x', t_f | x'', t_i >}{\sqrt{\Delta x_{n'} \Delta x_n}} \\ &\approx \sqrt{\Delta x_{n'} \Delta x_n} < x_{n'}, t_f | x_n, t_i >, \end{aligned} \quad (7)$$

where $< x_{n'}, t_f | x_n, t_i >$ can be calculated using MC simulations as follows.
(a) Discretize the continuous time.
(b) Generate free configurations $[x]$ between $t \in (t_i, t_f)$ obeying the Boltzmann distribution

$$P_0[x] = \frac{\exp(-S_0[x]/\hbar)}{\int [dx] \exp(-S_0[x]/\hbar)} \Big|_{x_n, t_i}^{x_{n'}, t_f}, \quad (8)$$

where $S_0 = m\dot{x}^2/2$.
(c) Measure

$$< O_V > = \int [dx] \exp(-V(x)/\hbar) \Big|_{x_n, t_i}^{x_{n'}, t_f} P_0[x] \quad (9)$$

The path integral in Eq. (7) is then

$$\begin{aligned} < x_{n'}, t_f | x_n, t_i > &= < O_V > \times \sqrt{\frac{m}{2\pi\hbar T}} \\ &\times \exp[-\frac{m}{2\hbar T}(x_{n'} - x_n)^2]. \end{aligned} \quad (10)$$

QUANTUM FIELD THEORY

The main purpose of the algorithm is to study many body systems and quantum field theory beyond the ground state. As an example, we consider a chain of N_{osc} coupled oscillators in 1 spatial dimension. Its Hamiltonian is given in Ref. [10] as

$$H = \sum_{j=1}^{N_{osc}} \frac{1}{2}[p_j^2 + \Omega^2(q_j - q_{j+1})^2 + \Omega_0^2 q_j^2], \tag{11}$$

where p_j and q_j are the momentum and displacement of the j-th oscillator respectively. This model is equivalent to the Klein-Gordon field theory on a (1+1)-dimensional lattice.

The spectrum of the system is analytically known:

$$\begin{aligned} E_n &= \sum_{n_k} (n_k + \frac{1}{2})\hbar\omega_k, \\ \omega_k &= \sqrt{\Omega^2(2\sin k/2)^2 + \Omega_0^2}, \end{aligned} \tag{12}$$

where $n_1, ..., n_{N_{osc}} = 0, 1, \ldots$, and $k = 2\pi l / N_{osc}$ with l an integer between $-N_{osc}/2$ and $N_{osc}/2$.

We generate a stochastic basis according to Eq. (6) with N=1000 configurations $[q_1, ..., q_{N_{osc}}]$ for the initial and final states for $N_{osc} = 9$ oscillators. For the adjustable parameter σ, we set $t_f' = t_f$ for simplicity. (Of course, one should study systematically the dependence of the results on σ). Table 3 compares the spectrum from the MC Hamiltonian with the analytical results for the first 20 states with $\Omega = 1$, $\Omega_0 = 2$, $m = 1, \hbar = 1$, and $T = 2$. They agree very well with the exact ones.

SUMMARY

In this paper, we have tested the MC Hamiltonian method with a stochastic basis in a many body Q.M. system with a chain of coupled oscillators: the Klein-Gordon field theory on a (1+1)-dimensional lattice. The results are very encouraging. We believe that the application of the algorithm to more complicated body systems and quantum field theory will be very interesting.

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Table 3. Comparison of the spectrum of the chain of 9 coupled oscillators, between the MC Hamiltonian method with a *stochastic* basis and the analytic ones.

n	E_n^{eff}	E_n^{Exact}
1	10.904663192168	10.944060480668
2	12.956830557334	12.944060480668
3	12.985023578737	13.057803869484
4	13.044311582647	13.057803869484
5	13.299967341242	13.321601993380
6	13.345480638394	13.321601993380
7	13.552195133687	13.589811791733
8	13.585794986361	13.589811791733
9	13.680136748933	13.751084748745
10	13.744919087477	13.751084748745
11	14.984737011385	14.944060480668
12	15.012353803145	15.057803869484
13	15.057295761044	15.057803869484
14	15.108904652020	15.171547258300
15	15.125356713561	15.171547258300
16	15.187413290039	15.171547258300
17	15.308536490102	15.321601993380
18	15.396255686587	15.321601993380
19	15.420708031412	15.435345382196
20	15.432823810789	15.435345382196

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