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 Tab. 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 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.

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

$$M_{fi} = \langle x_f,t_f | x_i,t_i \rangle = \langle x_f | e^{-H(t_f-t_i)\hbar} | x_i \rangle \quad (1)$$

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:

$$M_{fi} = \int [dx] \exp\left( -S(x) / \hbar \right) \langle x_f | e^{H(t_f-t_i)\hbar} | x_i \rangle. \quad (2)$$

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

$$M_{fi} = \langle x_f | e^{-H_{eff}T\hbar} | x_i \rangle$$

Table 1. Comparison of the conventional methods.

| Formulation | Hamiltonian | Lagrangian |
|-------------|-------------|------------|
| Approach    | Schrödinger Eq. | Path Integral |
| $H|E_n >= E_n|E_n >$ | $< O >= \int dx |O| \exp(-S(x) / \hbar) / \int dx \exp(-S(x) / \hbar)$ |
| 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. |

$x_f$ and $t_f$ is related to the Hamiltonian $H$ by

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

$$= \sum_{n=1}^{\infty} \langle x_f | E_n > e^{-\frac{E_n T \hbar}{\hbar}} < E_n | x_i \rangle, \quad (1)$$

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:

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

$$M = U^\dagger DU,$$

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

Since the theory described by $H$, which basis in Hilbert space is infinite, is now approximated by a theory described by a finite matrix $H_{\text{eff}}$, which basis is finite, the physics of $H$ and $H_{\text{eff}}$ 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 (Tab. 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     | $V(x) = 0$                                      |
|                 | $V(x) = \frac{1}{2}m\sigma^2x^2$               |
|                 | $V(x) = -V_0 \text{sech}^2(x)$                 |
|                 | $V(x) = \frac{1}{2}x^2 + \frac{1}{4}x^4$      |
|                 | $V(x) = \frac{2}{3}|x|$                        |
|                 | $V(x) = \{\infty$, $x < 0$                     |
|                 | $F_x$, $x \geq 0$                              |
| Q.M. in 2-D     | $V(x,y) = \frac{1}{2}m\sigma^2x^2 + \frac{1}{2}m\sigma^2y^2$ |
|                 | $V(x,y) = \frac{1}{2}m\sigma^2x^2 + \frac{1}{2}m\sigma^2y^2 + \lambda xy$ |
| Q.M. in 3-D     | $V(x,y,z) = \frac{1}{2}m\sigma^2x^2 + \frac{1}{2}m\sigma^2y^2 + \frac{1}{2}m\sigma^2z^2$ |

**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 $|e_n\rangle$, $n = 1, \ldots, N$. In position space, it can be expressed as

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

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

The simplest choice is a basis with $\Delta x_n = \text{const.}$, 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 important sampling, in Refs. (8, 9), we proposed to select a basis from the Boltzmann weight proportional to the transition amplitude between $x_{t_0} = 0$ at $t_i'$, and $x_{f'} = x_n$ at some $t_f'$. In a free particle or harmonic oscillator case, the distribution is just a Gaussian

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

where $\sigma = \sqrt{h\omega/m}$ for the free case and $\sigma = \sqrt{\text{sinh}(\omega f')/(m\omega)}$ for the harmonic oscillator. 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 $\langle x_{t_i'}, t_f'| x_n, t_i \rangle$ by

$$M_{n'f} = \langle e_{n'}, T | e_n, 0 \rangle = \int x_{n'+1} x_{n'-1} \int x_{n'+1} x_{n'} \frac{dx'}{\sqrt{\Delta x_{f'}}} \frac{dx}{\sqrt{\Delta x_{i'}}} \frac{\langle x', t_f' | x', t_i \rangle}{\langle x', t_f' | x', t_i \rangle} \approx \frac{\sqrt{\Delta x_{f'} \Delta x_n}}{\sqrt{\Delta x_{i'} \Delta x_n}} \langle x_{t_i'}, t_f' | x_n, t_i \rangle,$$

where $\langle x_{t_i'}, t_f' | x_n, t_i \rangle$ can be calculated using MC simulations as follows:

(a) Discretize the continuous time.

(b) Generate free configurations $|x\rangle$ between $t_0$ and $t_f$. Let $P_0[x]$ denote the Boltzmann distribution

$$P_0[x] = \frac{\exp(-S_0[x]/\hbar)}{\int dx \exp(-S_0[x]/\hbar)} e^{S[x_{t_f}]},$$

where $S_0 = \int dt m\dot{x}^2/2$.

(c) Measure

$$\langle x_{t_i'}, t_f' | x_n, t_i \rangle = \langle x_{t_i'}, t_f' \rangle \int dx \exp(-\int dt V(x)/\hbar) P_0[x]$$

The path integral in Eq. (7) is then

$$\langle x_{t_i'}, t_f' | x_n, t_i \rangle = \langle x_{t_i'}, t_f' \rangle \int dx \exp(-\int dt V(x)/\hbar) P_0[x] \times \exp(-m/2\hbar t) (x_{t_f} - x_n)^2.$$
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

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

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:

$$ E_n = \sum_{n_k} \left( n_k + \frac{1}{2} \bar{h} \omega_k \right), $$

$$ \omega_k = \sqrt{\Omega^2 (2 \sin k/2)^2 + \Omega_0^2}, $$

where $n_1, ..., n_{N_{osc}} = 0, 1, ..., k = 2\pi l/N_{osc}$ 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 $\sigma$, we use the distribution for the uncoupled oscillators at $t'_f = t_f$ for simplicity. (Of course, one should study systematically the dependence of the results on $\sigma$).

Tab. 3 compares the spectrum from the MC Hamiltonian with the analytical results for the first 20 states with $\Omega = 1, \Omega_0 = 2, m = 1, \bar{h} = 1, T = 2$. They agree very well with the exact ones.

| $n$ | $E_{n}^{eff}$ | $E_{n}^{Exact}$ |
|-----|-------------|------------|
| 1   | 10.904663192168 | 10.94060480668 |
| 2   | 12.956830557337 | 12.94060480668 |
| 3   | 12.985023578737 | 13.057803869484 |
| 4   | 13.44311582647 | 13.057803869484 |
| 5   | 13.299967341242 | 13.232160193330 |
| 6   | 13.345480638394 | 13.321601933380 |
| 7   | 13.552194613687 | 13.589811791733 |
| 8   | 13.58794986361 | 13.589811791733 |
| 9   | 13.680136748933 | 13.75108478745 |
| 10  | 13.744919087477 | 13.75108478745 |
| 11  | 14.984737011385 | 14.94060480668 |
| 12  | 15.01239383145 | 15.057803869484 |
| 13  | 15.07295761044 | 15.057803869484 |
| 14  | 15.108904652020 | 15.171547258300 |
| 15  | 15.12556713561 | 15.171547258300 |
| 16  | 15.187413290039 | 15.171547258300 |
| 17  | 15.308536490102 | 15.321601933380 |
| 18  | 15.396255686587 | 15.321601933380 |
| 19  | 15.420708031412 | 15.435345382196 |
| 20  | 15.432823810789 | 15.435345382196 |

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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