Monte Carlo Hamiltonian - From Statistical Physics to 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 some areas of application to quantum theories computational progress has been slow. Here we present a recently developed approach: the Monte Carlo Hamiltonian method, designed to overcome the difficulties of the conventional approach.

1 Introduction

The Monte Carlo (MC) method with importance sampling is an excellent technique to study systems with many degrees of freedom. It has been widely applied to statistical physics and quantum theories. There are two formulations of quantum theory: the Hamiltonian formulation and the Lagrangian formulation. A comparison of the conventional approaches is given in Tab. 1. A natural question is whether one can perform efficiently MC simulations combined with the Hamiltonian formulation. If so, the disadvantages of the Hamiltonian formulation might be overcome. Our motivation is to construct an effective Hamiltonian via MC simulation starting from the original action.

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Table 1
Comparison of Hamiltonian and Lagrangian formulations.

| Formulation | Hamiltonian | Lagrangian |
|-------------|-------------|------------|
| Approach    | Solving Schrödinger Eq. $H|E_n> = E_n|E_n>$ | Computing Path Integral $<O> = \frac{\int d[x]|O[x]\exp(-S[x]/\hbar)}{\int dx \exp(-S[x]/\hbar)}$ |
| Algorithm   | variational, series expansion, coupled cluster expansion ... | Monte Carlo simulation as in *Stat. Phys.* |
| Advantage   | can obtain not only energies of ground & excited states, but also wavefunctions | use computer to generate the most important configs. obeying Boltzmann’s law |
| Disadvantage| methods above are too tedious for realistic applications | difficult to obtain: wavefunction, excited states, $S$ matrix, finite density QCD |

2 Algorithm

Let us review briefly the basic ideas [1]. According to Feynman’s path integral approach to quantum mechanics, 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

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

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

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

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

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

$H_{eff}$ can be found by MC simulation using the following procedure:

(a) Discretize the continuous time.

(b) Generate configurations $[x]$ obeying the Boltzmann distribution
\[ P(x) = \frac{\exp(-S[x]/\hbar)}{\int [dx] \exp(-S[x]/\hbar)}. \]  
\hspace{1cm} (3)

(c) Calculate the transition matrix elements

\[ M_{fi} = \langle x_f | e^{-H_{eff}T/\hbar} | x_i \rangle \]  
\hspace{1cm} (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

\[ M = U^\dagger D U, \]  
\hspace{1cm} (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 \( H_{eff} \), and obtain the eigenvalues \( E_{\nu}^{eff} \) and wave-function \( |E_{\nu}^{eff}\rangle \) 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 Testing the Method

We have tested a number of quantum mechanical models in both 1+1 dimensions [1–3] and 2+1 dimensions [4,5]. Here we will show some new results for a model in 1+1 dimensions with the following potential

\[ V(x) = x^2/2 + x^4/4. \]  
\hspace{1cm} (6)

The Euclidean action is given by \( S = \int_0^T dt [m \dot{x}^2/2 + V(x)] \). This model is not exactly solvable. We have compared the results from our method with those from a standard algorithm (Runge-Kutta algorithm plus node theorem). The first three eigenvalues are given in Tab. 2. The parameters are \( m = 1, T = 1, \hbar = 1, \Delta x = 1, N = 21 \). The results for the first two wave functions are shown in Figs. 1 and 2. Besides the eigenvalues \( E_{\nu}^{eff} \) and wave functions \( |E_{\nu}^{eff}\rangle \), we have computed thermodynamical quantities such as the partition function \( Z \), average energy \( \overline{E} \) and specific heat \( C \). Since we have approximated \( H \) by \( H_{eff} \), we can express those thermodynamical observables via the eigenvalues of the effective Hamiltonian.
Table 2

Spectrum of the model with $V(x) = x^2/2 + x^4/4$. $E_n^{n.t.}$ corresponds to Runge-Kutta plus node theorem and $\Delta E_n^{M.C.}$ is the statistical error.

| n | $E_n^{n.t.}$ | $E_n^{M.C.}$ | $\Delta E_n^{M.C.}$ |
|---|-------------|-------------|------------------|
| 0 | 0.6209      | 0.6197      | 0.0192           |
| 1 | 2.0260      | 2.0427      | 0.0566           |
| 2 | 3.6985      | 3.6060      | 0.0455           |

Fig. 1. Ground state wave function of the model with $V(x) = x^2/2 + x^4/4$.

$$Z(\beta) = \sum_{\nu=1}^{N} e^{-\beta E_{\nu}^{eff}}$$

$$\overline{E}(\beta) = \sum_{\nu=1}^{N} \frac{E_{\nu}^{eff} e^{-\beta E_{\nu}^{eff}}}{Z(\beta)}$$,

$$C(\beta) = k_B \beta^2 \left( \sum_{\nu=1}^{N} \frac{(E_{\nu}^{eff})^2 e^{-\beta E_{\nu}^{eff}}}{Z(\beta)} - \overline{E}^2(\beta) \right),$$

where $\beta = T/\hbar$. The results for the average energy and specific heat are shown in Figs. 3 and 4, where the solid lines corresponds to the standard algorithm. Within statistical errors, our results are consistent with those from the standard algorithm.
4 Summary and Outlook

We have presented the basic ideas and some new results from our recently proposed Monte Carlo effective Hamiltonian method. We found that the method works well also for the \( V \sim x^4 \) potential, allowing to compute excited states and thermodynamical observables. In the previous simulations, the initial and final positions \( x_i \) and \( x_f \) were chosen to be uniformly distributed. As can be seen, for a given dimension of the Hilbert space \( N \), the results break down if \( \beta \) is too small. Increasing \( N \) requires larger CPU time. For quantum mechanics
in 3+1 dimensions or quantum field theories, a stochastic basis will be necessary to select the most important contributions to the transition matrix $M_{fi}$. Such a work is in progress [3].

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