Monte Carlo Hamiltonian from Stochastic Basis

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Abstract

We further develop the recently proposed Monte Carlo Hamiltonian. We suggest to construct an effective low energy Hamiltonian via a stochastic selection of basis states. We test the method by computing thermodynamical observables like specific heat and average energy in 1-D quantum systems.

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1 Introduction

Path integral quantization in the Lagrangian formulation and canonical quantization in the Hamiltonian formulation are two ways to quantize classical systems. Either one has advantages and disadvantages. The Lagrangian formulation is suitable for numerical simulations on a computer via Monte Carlo. The enormous success of lattice gauge theory over the last two and half decades is certainly due to the fact that the Monte Carlo method with importance sampling is an excellent technique to compute high dimensional (and even "infinite" dimensional) integrals.

Unfortunately, using the Lagrangian formulation it is difficult to estimate wave functions and the spectrum of excited states. 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\cite{1} 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.

In the Hamiltonian formulation, one can obtain the ground state energy, but also wave functions and the spectrum of excited states. Often, and in particular in the case of many-body systems, it is difficult to solve the stationary Schrödinger equation. Recently, we have suggested how to construct an effective Hamiltonian via Monte Carlo\cite{2} to describe the low energy spectrum and wave functions. The method has been tested in 1-D for quantum mechanics, namely for the free system, the harmonic oscillator and other local potentials. In those cases, the exact results were well reproduced.

The purpose if this paper is the following: (a) Firstly, we report further studies to test the viability of the Monte Carlo method at hand of two potentials which generate a bound state spectrum only: $V(x) = |x|/2$, and $V(x) = x^2/2 + x^4/4$. These two models have their own interest in quantum mechanics. In the first case, the potential has the form of a static quark-antiquark confining potential occurring in QCD. The second potential represents an anharmonic oscillator. In field theory this corresponds to a scalar $\phi^4$ theory, which plays a role in the Higgs sector of the electro-weak standard model.

(b) If one wants to construct the Monte Carlo Hamiltonian in the case of high dimensional systems or for many-body systems (field theory) this becomes a formidable problem. In order to solve the many-body problem it has been suggested to construct an effective Hamiltonian in some model space. An example is the folded diagram technique \cite{3}. Here
we suggest a new idea to treat the many-body problem: We try to mimic the success of
the Monte Carlo method with importance sampling in solving Euclidean path integrals in
the Lagrange formulation. There one constructs a ”small” number of representative (equi-
librium) configurations and computes the expectation value of an observable by summing
the observable over those configurations. We draw a parallel between those equilibrium
configurations and stochastically chosen representative basis states. This allows us to con-
struct an effective Hamiltonian from transition matrix elements of stochastically chosen
basis states. As ultimate goal one hopes to be able to solve a full many-body problem
by construction of the effective Hamiltonian in such a ”model space”. One expects the
dimension of the effective Hamiltonian to be in the same order as the typical number of
configurations (100-1000) used in computing path integrals in lattice field theory. Here we
will present results showing that the effective Hamiltonian in conjunction with a stochastic
basis works in quantum mechanics. We apply the Monte Carlo technique twice, once for
the construction of the stochastic basis, and second for the evaluation of the path integral
of the transition matrix elements.

(c) Finally, we present an analysis of statistical errors of the spectrum of the Monte Carlo
Hamiltonian. We compute energy spectra, wave functions and thermodynamical observ-
able like average energy and specific heat.

2 Effective Hamiltonian

The construction of an effective Hamiltonian starting from a regular basis in position space
has been proposed in Ref. [2]. Using Feynman’s path integral formulation [4], we consider
the transition amplitude in imaginary time between time $t = 0$ and $t = T$. Using imagi-
nary time makes the path integral mathematically well defined, and renders it amenable to
numerical simulations by Monte Carlo. Because the effective Hamiltonian is time indepen-
dent, its construction in imaginary time should give the same result as in real time. We
consider the transition amplitude for all combinations of positions $x_i, x_j \in \{x_1, \ldots, x_N\}$,

$$M_{ij}(T) = \langle x_i | e^{-HT/\hbar} | x_j \rangle = \int [dx] \exp[-S_E[x]/\hbar] |_{x_i,T}^{x_i,0},$$

where $S_E$ denotes the Euclidean action. From the transition amplitudes $M_{ij}(T)$, one can
construct the matrix

$$M(T) = [M_{ij}(T)]_{N \times N}. \tag{2}$$

$M(T)$ is a positive, Hermitian matrix. $M$ can be factorized into a unitary matrix $U$ and a
real diagonal matrix $D(T)$, such that

$$M(T) = U^\dagger D(T)U. \tag{3}$$
Note that in order to be rigorous this requires to define the transition amplitude between normalized Hilbert states (see sect.3). Then from Eq.(1), Eq.(3) one can identify

\[ U_{ik}^\dagger = \langle x_i | E_{eff}^k >, \quad D_k(T) = e^{-E_{eff}^k T/\hbar}. \]  

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

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

We compute the matrix element \( M_{ij}(T) \) directly from the action via Monte Carlo with importance sampling. For details see ref.[2].

### 3 Stochastic basis

Let us start out by considering a set of nodes in position space \( \{x_1, \ldots, x_{N+1}\} \). We construct a basis of Hilbert states defined as characteristic states located at \( x_i \). Those basis states are denoted by \( |e_i \rangle >, i = 1, \ldots, N \). They are defined in position space by \( e_i(x) = 1/\sqrt{\Delta x_i} \) in the interval \( I_i = [x_i, x_{i+1}] \), and zero else. \( \Delta x_i = x_{i+1} - x_i \). Those states are normalized to unity. In the numerical calculations we have used equidistant spacing, i.e. \( \Delta x_i = \text{const} \).

Let us call this the regular basis. The matrix element can be written for a given \( N \) as

\[ M_{ij}(T) = \langle e_i, T | e_j, 0 > = \frac{1}{\sqrt{\Delta x_i} \sqrt{\Delta x_j}} \int dx' dx'' \int [dx] \exp[-S[x]/\hbar] \bigg|_{x_j,0}^{x_i, T} \]

\[ = \sqrt{\Delta x_i \Delta x_j} \int [dx] \exp[-S[x]/\hbar] \bigg|_{x_j,0}^{x_i, T} + O(\Delta x^2), \quad i, j \in 1, 2, \ldots, N. \]  

Here \( S \) denotes the Euclidean action for a given path \( x(t) \) going from \( x_j, t = 0 \) to \( x_i, t = T \),

\[ S[x(t)] = \int_0^T dt \left( \frac{1}{2} m \dot{x}^2 + V(x) \right). \]  

Suppose we intend to apply this to a system with many degrees of freedom (many-body system). It is evident that the above basis construction becomes prohibitively large. For example, in a spin model of a 1-dimensional chain of 30 atoms with spin 1/2, one has a Hilbert space basis of dimension \( 2^{30} = 1073741824 \). For such situations we desire to construct a small basis which gives an effective Hamiltonian which reproduces well low-energy observables. Why should such a basis exist? The heuristic argument is the Euclidean
path integral, which, when evaluated via Monte Carlo with importance sampling, gives a good answer for the transition amplitude. In particular, this is possible by taking into account a "small" number of configurations (e.g. in the order of 100 - 1000). In a crude way the configurations correspond to basis functions. Thus we expect that suitably chosen basis functions exist, the number of which is in the order of 100 - 1000, which yields a satisfactory effective low energy Hamiltonian. Note, however, that this will be the case only when the basis functions are chosen in the "right" way.

How can we construct such a "small" basis? Let us consider first the most simple case, i.e., a free particle in \( D = 1 \) dimension. Let us take as "large" basis the regular basis, described above. Suppose \( N \) is large (\( N >> 1 \)). The idea is to make a selection guided by the Euclidean quantum mechanical transition amplitude. Recall: For the free system it reads

\[
G_{\text{Eucl}}(x, T; y, 0) = \sqrt{\frac{m}{2\pi \hbar T}} \exp[-\frac{m}{2\hbar T} (x - y)^2].
\]

(8)

Note that this function is positive for all \( x, y, T \). It can be used as a probability density. We put \( y = 0 \) and define a probability density \( P(x) \) by

\[
P(x) = \frac{1}{Z} G_{\text{Eucl}}(x, T; 0, 0),
\]

\[
Z = \int dx G_{\text{Eucl}}(x, T; 0, 0).
\]

(9)

Then we define a selection process as follows: Using a random process with probability density \( P(x) \) one draws a "small" set of samples \( \{x_\nu\}_{\nu=1,\ldots,N_{\text{eff}}+1} \), where \( N_{\text{eff}} << N \).

In the case of the free particle, \( P(x) \) is a Gaussian,

\[
P(x) = \frac{1}{\sqrt{2\pi\sigma}} \exp[-\frac{x^2}{2\sigma^2}], \quad \sigma = \sqrt{\frac{\hbar T}{m}}.
\]

(10)

In other words, we select \( \{x_\nu\} \) by drawing from a Gaussian distribution. We draw \( N_{\text{eff}} + 1 \) samples, giving \( N_{\text{eff}} \) states, where \( N_{\text{eff}} \) is considerably smaller than \( N \), the original size of the basis. The width \( \sigma \) is a parameter, which will be discussed in sect. 5.

Let us give some thought to the question: Is such probability density physically reasonable? Firstly, consider the case when \( T \) is large. The Boltzmann-Gibbs distribution

\[
P_{BG}(E) = \frac{1}{Z} \exp[-E T / \hbar]
\]

(11)

projects onto the ground state when \( T \rightarrow \infty \). For the free system the ground state energy is \( E = 0 \). I.e., the distribution \( P_{BG}(E) \) has a strong peak at \( E = 0 \) (when \( T \rightarrow \infty \)). On the other hand, when \( T \rightarrow \infty \), then \( \sigma \) given by Eq.(10) is large. Thus the density \( P(x) \),
from which we draw the \( x_\nu \) is a broad Gaussian. In the limit \( \sigma \to \infty \), it becomes a uniform distribution. Now we go over from \( P(x) \) to \( \tilde{P}(k) \), related via Fourier transformation. If \( P(x) \) is uniform, then \( \tilde{P}(k) \propto \delta(k) \). Thus it gives the energy \( E_k = \frac{k^2}{2m} |_{k=0} = 0 \), which is the correct ground state energy eigenvalue. Thus, in the extreme low-energy regime, the distribution \( P(x) \) gives a result consistent with the Boltzmann-Gibbs distribution. This is a good indication that \( P(x) \) will generate an effective Hamiltonian useful for the computation of thermodynamical observables.

Although less relevant for our purpose, it is instructive to look what happens in the opposite situation, i.e., when \( T \) is small. In the limit \( T \to 0 \), the Boltzmann-Gibbs distribution is approximately a constant. All energies occur with equal probability. Thus \( \sigma \) is also small. The distribution \( P(x) \) behaves like \( P(x) \propto \delta(x) \). The Fourier transform yields \( \tilde{P}(k) = \text{const} \), i.e. a uniform distribution. Then \( E_k = \frac{k^2}{2m} \) is distributed like \( 1/\sqrt{E} \). This is not the same as the Boltzmann-Gibbs distribution. But for small \( T \), which means large energy \( E \), it is qualitatively comparable to that of Boltzmann-Gibbs.

Next we ask: What do we do in the case when a local potential is present? The definition of the probability density \( P(x) \) given by Eq.(9) generalizes to include also local potentials. In order to construct a stochastic basis one can proceed via the following steps: (i) Compute the Euclidean Green’s function \( G_E(x,t;0,0) \), e.g., by solving the diffusion equation and compute \( P(x) \). (ii) Find an algorithm giving a random variable \( x \) distributed according to the probability density \( P(x) \) and draw samples from this distribution, giving nodes, say \( x_\nu \). Finally, one obtains the stochastic basis by constructing the corresponding characteristic states from the nodes \( x_\nu \).

The same goal can be achieved in an elegant and efficient manner via the Euclidean path integral. Writing Eq.(9) as path integral yields

\[
P(x) = \frac{\int [dy] \exp[-S_E[y]/\hbar]}{\int_{-\infty}^{+\infty} dx \int [dy] \exp[-S_E[y]/\hbar]} \bigg|_{0,0}^{x,T} \bigg|_{0,0}^{x,T} \quad (12)
\]

Using a Monte Carlo algorithm with importance sampling (e.g., Metropolis) one generates representative paths, which all start at \( x = 0, t = 0 \) and arrive at some position \( x \) at time \( t = T \). Let us denote those paths (configurations) by \( C_\nu \equiv x_\nu(t) \). We denote the endpoint of path \( C_\nu \) at time \( t = T \) by \( x_\nu \equiv x_\nu(T) \). Those form the stochastically selected nodes, which define the stochastic basis.

4 Estimation of statistical errors

We have computed the transition matrix elements via Monte Carlo. This yields matrix elements \( M_{ij} \) with a statistical error \( \delta M_{ij} \). Using stationary perturbation theory to lowest
order, one can compute the propagation of the statistical errors into the energy eigenvalues and wave functions of the effective Hamiltonian. Here we have estimated the error propagation numerically. We have considered the matrix $M_{ij} \pm \delta M_{ij}$ and diagonalized it and computed correspondingly $H_{\text{eff}}$ via Eqs. (3,4). This gives upper bounds on the error of energy eigenvalues and on the error in the wave functions.

5 Numerical results

First we present results of the Monte Carlo Hamiltonian using the regular basis. We have considered quantum mechanical systems in $D = 1$ dimension, given by the following potentials

$$V(x) = |x|/2,$$

$$V(x) = x^2/2 + x^4/4.$$  (13)  (14)

For the potential $V(x) = |x|/2$ an exact solution of the ground state energy and wave function is analytically known [6]. They are given by

$$E_0 = \frac{|\xi_0|}{2} (\hbar^2/m)^{1/3} = 0.5094 (\hbar^2/m)^{1/3},$$

$$\psi_0(x) = \sqrt{|\xi|} \left[ J_{\frac{2}{3}} \left( \frac{2}{3} |\xi|^{3/2} \right) + J_{-\frac{2}{3}} \left( \frac{2}{3} |\xi|^{3/2} \right) \right],$$

$$\xi = (|x| - 2E_0) \left( m/\hbar^2 \right)^{1/3},$$  (15)

where $\xi_0 = \xi|_{x=0}$, $|\xi_0| = (3z_0/2)^{2/3}$, $z_0$ being the solution of the equation $J_{2/3}(z) - J_{-2/3}(z) = 0$, and $J_{\frac{2}{3}}$ and $J_{-\frac{2}{3}}$ are Airy functions.

We compare two methods: the Monte Carlo Hamiltonian method and as reference solution we take a numerical solution using the Runge-Kutta algorithm and the node theorem with an iterative searching algorithm. This means that we solve the stationary Schrödinger equation expressed as differential equation in position space and search for the discrete eigenvalue $E_n$ corresponding to the number of nodes of the wave function. We have computed the energy spectrum, wave functions as well as thermodynamical observables such as average energy, specific heat and the partition function. The results can be summarized as follows.

Fig.[1a] shows the ground state wave function corresponding to the potential $V(x) = |x|/2$. One observes good agreement between the Monte Carlo Hamiltonian result and the exact solution. From the data in the first line of Tab.[1], we find for the ground state energy a deviation of about 1.04% between the result of the Monte Carlo Hamiltonian and the analytic solution. Fig.[1b] shows a similar comparison for the wave function of the first
excited state. Here $E_0^{M.C.}$ denotes the ground spectrum using Monte Carlo Hamiltonian and $E_0^{R.K.}$ denotes the corresponding quantity obtained by the Runge-Kutta algorithm. $E_0^{Exact}$ denotes the analytic solution. Fig.[2a], Fig.[2b] and Tab.[2] show a comparison of the spectrum and wave functions corresponding to the potential $V(x) = x^2/2 + x^4/4$. Here $n$ denotes the quantum number. One can see that there is good agreement in the low energy regime. The partition function is defined by $Z(\beta) = \text{Tr}(e^{-\beta H})$. The average energy is defined by $U(\beta) = \frac{1}{Z} \text{Tr}(He^{-\beta H})$, and the specific heat by $C(\beta) = \frac{\partial U}{\partial T}$. We have used the following notation: $\beta = (k_B T)^{-1}$, $T$ is the temperature and we identify $\beta$ with the imaginary time $T$ by $\beta = T/\hbar$. We have approximated $H$ by $H_{\text{eff}}$. Then corresponding to the effective Hamiltonian we can express the thermodynamical observables via the eigenvalues of the effective Hamiltonian. For example, the partition function is obtained by $Z_{\text{eff}}(\beta) = \sum_{k=1}^{N} e^{-\beta E_{k}^{\text{eff}}}$. Similarly, one computes average energy and specific heat from the effective Hamiltonian (for details see Ref.[2]). The numerical results are shown in Fig.[3] to Fig.[6]. One observes good agreement between the results from the Monte Carlo Hamiltonian and the reference solution.

Secondly, we present results using the stochastic basis. For the case of the harmonic oscillator we have computed the spectrum, average energy and specific heat. Tab.[3] shows the spectrum, comparing the exact result with that of the Monte Carlo Hamiltonian using the stochastic basis. We used a basis of size $N = 100$. We have tuned the parameter $\sigma$, such that the agreement with the exact result is optimal. The thermodynamical observables average energy and specific heat are displayed in Figs.[7,8]. The results for this 1-D system show that the stochastic basis gives results comparable to those of the regular basis, in particular for higher excited states. We want to stress that the advantage of using a stochastic basis is supposed to show up in high-dimensional systems and in many-body systems. This expectation is based on the analogy with integrals, where summation over Monte Carlo nodes wins over fixed node rules for dimensions $D > 6$, as a rule of thumb.

6 Conclusion

We have suggested how to obtain an effective low energy Hamiltonian by constructing via Monte Carlo a stochastic basis. We have shown that this works by computing thermodynamical observables in quantum mechanics.

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sity Advanced Research Center and the Guangdong Provincial Natural Science Foundation of China (proj. 990212).
References


21(1953)1087.

[6] B.C. Qian and J.Y. Zeng, Selected Exercises and Analysis in Quantum Mechanics,
Captions

Tab.1 Spectrum of potential \( V(x) = |x|/2 \).

Tab.2 Spectrum of potential \( V(x) = x^2/2 + x^4/4 \).

Tab.3 Spectrum of harmonic oscillator. \( m = 1, \ h = 1, \ \omega = 0.6 \). Exact and stochastic, respectively, stand for the exact analytical result, and that from the exact matrix elements using a stochastic basis with \( T = 1, \ N = 100 \) and \( \sigma = 6 \).

Fig.1a Ground state wave function \( \psi_0(x) \) of potential \( V(x) = |x|/2 \).

Fig.1b Same as Fig.[1a], first excited state \( \psi_1(x) \).

Fig.2a Ground state wave function \( \psi_0(x) \) of potential \( V(x) = x^2/2 + x^4/4 \).

Fig.2b Same as Fig.[2a], first excited state \( \psi_1(x) \).

Fig.3 Average energy \( U(\beta) \) of potential \( V(x) = |x|/2 \).

Fig.4 Specific heat \( C(\beta) \) of potential \( V(x) = |x|/2 \).

Fig.5 Average energy \( U(\beta) \) of potential \( V(x) = x^2/2 + x^4/4 \).

Fig.6 Specific heat \( C(\beta) \) of potential \( V(x) = x^2/2 + x^4/4 \).

Fig.7 Average energy \( U(\beta) \) of harmonic oscillator.

Fig.8 Specific heat \( C(\beta) \) of harmonic oscillator.