Green Function Monte Carlo Method for Excited States of Quantum System

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A novel scheme to solve the quantum eigenvalue problem through the imaginary-time Green function Monte Carlo method is presented. This method is applicable to the excited states as well as to the ground state of a generic system. We demonstrate the validity of the method with the numerical examples on three simple systems including a discretized sine-Gordon model.

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The stochastic quantization has been successfully applied in recent years to the various problems of physics ranging from quantum chromo-dynamics to the plasmon oscillation [1, 2]. While it can handle very complex system which is usually beyond the approach either by the direct diagonalization or by the perturbation, it has been only applicable to the calculation of the ground state properties of the system. In this paper, we propose a new method based on the imaginary-time Green function Monte Carlo approach, which is extended to the excited states of Hamiltonian systems. We envision the application of the method both in non-relativistic quantum few-body problems [3, 4], and in lattice field theories [5]. The method is illustrated through the examples of a Morse oscillator, of a simple schematic deformed shell model with two interacting particles in two-dimension, and of sine-Gordon coupled oscillators.

Let us suppose that we want to solve an eigenstate problem of a Hamiltonian \( H \), namely

\[
H |\psi_\alpha\rangle = E_\alpha |\psi_\alpha\rangle. \tag{1}
\]

We assume that each eigenstate is normalized to unity. The evolution operator with imaginary time \( \tau \) acts on an arbitrary state \( |\phi_1\rangle \) as

\[
e^{-\tau H} |\phi_1\rangle = \sum_\alpha e^{-\tau E_\alpha} |\psi_\alpha\rangle \langle \psi_\alpha |\phi_1\rangle. \tag{2}
\]

If we discretize the imaginary time \( \tau \) with the unit \( \Delta \tau \), and call the state at the \( n \)-th step of the evolution \( |\phi_1^{(n)}\rangle \equiv \exp(-n\Delta \tau H) |\phi_1\rangle \), the evolution at each step \( \Delta \tau \) is described by

\[
|\phi_1^{(n+1)}\rangle = e^{-\Delta \tau H} |\phi_1^{(n)}\rangle. \tag{3}
\]

After sufficient number of steps, the state with the lowest energy is filtered out:

\[
|\phi_1^{(n)}\rangle \rightarrow e^{-n\Delta \tau E_1} |\psi_1\rangle \langle \psi_1 |\phi_1\rangle \quad (n \rightarrow \infty). \tag{4}
\]

We consider the second sequence of states \( |\phi_2^{(n)}\rangle \) which satisfy the evolution equation

\[
|\phi_2^{(n+1)}\rangle = e^{-\Delta \tau H} |\phi_2^{(n)}\rangle - |\phi_1^{(n+1)}\rangle \frac{\langle \phi_1 | e^{-\Delta \tau H} |\phi_2^{(n)}\rangle}{\langle \phi_1 | \phi_1^{(n+1)}\rangle}. \tag{5}
\]

The states \( |\phi_1^{(n)}\rangle \) and \( |\phi_2^{(n)}\rangle \) at adjacent time steps satisfy the orthogonality \( \langle \phi_1^{(n)} | \phi_2^{(n+1)}\rangle = 0 \). Expanding eq. (5) in the first order of \( \Delta \tau \), we have

\[
|\phi_2^{(n+1)}\rangle \approx e^{-\Delta \tau H} \times \left\{ 1 - |\phi_1^{(n)}\rangle \langle \phi_1^{(n)} | \langle \phi_1^{(n)} | \phi_1^{(n+1)}\rangle \right\} |\phi_2^{(n)}\rangle
\]

\[
\approx (1 - |\psi_1\rangle \langle \psi_1 |) e^{-\Delta \tau H} |\phi_2^{(n)}\rangle
\]

\[
= e^{-\Delta \tau H} (1 - |\psi_1\rangle \langle \psi_1 |) |\phi_2^{(n)}\rangle
\]

whose \( \Delta \tau \)-dependent term in the first line vanishes at the large time step because of eq. (4). It is now clear that the repeated operation of eq. (5) filters out the first excited state, namely:

\[
|\phi_2^{(n)}\rangle \approx \left[ (1 - |\psi_1\rangle \langle \psi_1 |) e^{-\Delta \tau H} \right]^n |\phi_2\rangle \tag{7}
\]

\[
= (1 - |\psi_1\rangle \langle \psi_1 |) e^{-n\Delta \tau H} |\phi_2\rangle
\]

\[
= e^{-n\Delta \tau H} (1 - |\psi_1\rangle \langle \psi_1 |) |\phi_2\rangle
\]

\[
\rightarrow e^{-n\Delta \tau E_2} |\psi_2\rangle \langle \psi_2 |\phi_2\rangle \quad (n \rightarrow \infty).
\]

It is important to notice that the orthogonralization at each time step, eq. (5) is essential in actual calculation, because the single Schmidt subtraction either at the starting or at the end of the repeated iteration is impractical with finite accuracy numerics. One can generalize eqs. (3) and (5) to obtain the evolution equation for the \( \alpha \)-th energy eigenstate \( \alpha = 1, 2, 3, \ldots \) as

\[
|\phi_\alpha^{(n+1)}\rangle = e^{-\Delta \tau H} |\phi_\alpha^{(n)}\rangle - \sum_{\beta=1}^{\alpha-1} |\phi_\beta^{(n+1)}\rangle \frac{\langle \phi_\beta | e^{-\Delta \tau H} |\phi_\alpha^{(n)}\rangle}{\langle \phi_\beta | \phi_\beta^{(n+1)}\rangle}. \tag{8}
\]

Then, with the step-wise asymptotic orthogonal conditions \( \langle \phi_\beta | \phi_\alpha^{(n+1)}\rangle \rightarrow 0 \quad (n \rightarrow \infty) \) for different states \( \alpha \) and \( \beta \), one can recursively filter out the \( \alpha \)-th energy eigenstate as
\[ |\phi_\alpha^{(n)}\rangle \rightarrow e^{-n\Delta \tau E_\alpha} |\psi_\alpha\rangle \langle \psi_\alpha | \phi_\alpha \quad (n \rightarrow \infty). \] (9)

We work in configuration space, and adopt the usual notation \( \phi_\alpha^{(n)}(\vec{q}) \equiv \langle \vec{q} | \phi_\alpha^{(n)} \rangle \) where \( \vec{q} \) signifies the coordinate vector of the problem. The straightforward evaluation of integrals in the evolution equation is impractical except for the case of very low dimension. Instead, we consider, for given \( n \) and \( \alpha \), a set of vectors \( \{\vec{q}_{\alpha i}^{(n)}(i = 1...M)\} \) distributed according to the probability distribution

\[ P(\vec{q}) = \left| \phi_\alpha^{(n)}(\vec{q}) \right| \cdot \left\{ \int d\vec{q}' \left| \phi_\alpha^{(n)}(\vec{q}') \right| \right\}^{-1} \] (10)

and try to represent the wave function by the method of importance sampling. The sign information of \( \phi_\alpha^{(n)}(\vec{q}) \), which is missing in eq. (10), can be recovered by defining a real number

\[ s_{\alpha i}^{(n)} \equiv \text{sgn} \left( \phi_\alpha^{(n)}(\vec{q}) \right) \times \left\{ \int d\vec{q}' \left| \phi_\alpha^{(n)}(\vec{q}') \right| \cdot \left\{ \sum_i \left| \phi_\alpha^{(n)}(\vec{q}_{\alpha i}^{(n)}) \right| \right\}^{-1} \right\}^{-1} \] (11)

for each point \( \vec{q}_{\alpha i}^{(n)} \). One can evaluate any integral involving the wave function \( \phi_\alpha^{(n)}(\vec{q}) \) using the set \( \{\vec{q}_{\alpha i}^{(n)}, s_{\alpha i}^{(n)}\} \) \( (i = 1...M) \). The most relevant example is the coordinate representation of the evolution equation eq. (8), which now reads

\[ \phi_\alpha^{(n+1)}(\vec{q}) = \int d\vec{q}' K_{\Delta \tau}(\vec{q}', \vec{q}) \phi_\alpha^{(n)}(\vec{q}') - \sum_{\beta=1}^{\alpha-1} \int d\vec{q}' K_{\Delta \tau}(\vec{q}', \vec{q}''') \phi_\beta^{(n)}(\vec{q}') \cdot \frac{\lambda_{\beta \alpha}}{\lambda_{\beta \beta}} \approx \sum_i K_{\Delta \tau}(\vec{q}, \vec{q}_{\alpha i}^{(n)}) s_{\alpha i}^{(n)} \] (12)

\[ - \sum_{\beta=1}^{\alpha-1} \frac{\lambda_{\beta \alpha}}{\lambda_{\beta \beta}} K_{\Delta \tau}(\vec{q}, \vec{q}_{\beta i}^{(n)}) s_{\alpha i}^{(n)} \] (13)

where \( K_{\Delta \tau}(\vec{q}, \vec{q}') \equiv \langle \vec{q}' | \exp(-\Delta \tau H) | \vec{q}' \rangle \) is the step propagator in \( q \)-representation. The overlap matrix \( \Lambda_{\beta \gamma} \) is given by

\[ \Lambda_{\beta \gamma} \equiv \langle \phi_\beta | e^{-\Delta \tau H} | \phi_\gamma \rangle^{(n)} \] (14)

\[ \approx \sum_{i,j} K_{\Delta \tau}(\vec{q}_{\beta i}^{(n)}, \vec{q}_{\gamma j}^{(n)}) s_{\beta i}^{(n)} s_{\gamma j}^{(n)} \] (15)

and

\[ E_\alpha^{(n)} \equiv \int d\vec{q} \phi_\alpha^{(n)}(\vec{q}) H \phi_\alpha^{(n+1)}(\vec{q}) \int d\vec{q} \phi_\alpha^{(n+1)}(\vec{q}) \]

\[ \approx \frac{1}{N_s} \sum_{n=n_0}^{n_0+N_s} E_\alpha^{(n)} \]

\[ \text{TABLE I. The energy eigenvalue of the first five states of the Morse system. The raw [a] is the results with } \Delta \tau = 0.5, \text{ } M = 200 \text{ and } N = 400, \text{ while [b] is with } \Delta \tau = 0.2, \text{ } M = 1000 \text{ and } N = 80. \]

| \alpha | 1 | 2 | 3 | 4 | 5 |
|-------|---|---|---|---|---|
| [a]   | -7.00 | -5.29 | -3.90 | -2.86 | -1.84 |
| [b]   | -7.01 | -5.27 | -3.79 | -2.56 | -1.53 |
| (Exact) | (-7.031) | (-5.281) | (-3.781) | (-2.531) | (-1.531) |
\[ H = \frac{1}{2} \frac{\partial^2}{\partial q^2} + 8e^{-q^2/2} - 16e^{-q}. \]  

In Table 1, the first five eigenvalues evaluated with two sets of sampling parameters \((M = 200, N_s = 400, \Delta \tau = 0.5)\) and \((M = 1000, N_s = 80, \Delta \tau = 0.2)\) are tabulated. Statistical errors are estimated to be 0.2% at most for both cases. One can see, in the table, that the results do converge toward the analytical value \(E_n = -(17 - 2\alpha)^2/32\) with larger \(M\) and smaller \(\Delta \tau\).

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{fig1.png}
\caption{The profile of the first five wave function calculated with Monte Carlo technique.}
\end{figure}

In Fig. 1, we plot the wave functions, which are obtained as suitably normalized probability distributions of sampling points taken separately for \(S_\alpha^{(n)} = 1\) and \(S_\alpha^{(n)} = -1\). Their satisfactory quality is visually evident.

We look at another numerical example of two identical particles in a common two-dimensional asymmetric harmonic potential, mutually interacting through a Gaussian force. This can be regarded as a simplified, but non-trivial prototype of the deformed shell model. The model Hamiltonian is

\begin{equation}
H = \sum_{k=1}^{2} \left\{ -\frac{\partial^2}{\partial x_k^2} - \frac{\partial^2}{\partial y_k^2} + \frac{x_k^2 + 25y_k^2}{16} + v_0 \exp \left\{ \frac{(x_1-x_2)^2 + (y_1-y_2)^2}{a^2} \right\} \right\} + \sum_{i=1}^{N_s} \{ \phi_{ud}(q_{(1)}, q_{(2)}) - \phi_{du}(q_{(1)}, q_{(2)}) \} u_1 d_2 + \{ \phi_{ud}(q_{(1)}, q_{(2)}) - \phi_{du}(q_{(1)}, q_{(2)}) \} d_1 u_2 \end{equation}

where \(u\) and \(d\) represent the \(S_z = 1/2\) and \(S_z = -1/2\) states of individual particles respectively. From eq. (19), we can construct the totally antisymmetric state

\begin{equation}
\{ \phi_{ud}(q_{(1)}, q_{(2)}) - \phi_{du}(q_{(1)}, q_{(2)}) \} u_1 d_2 + \{ \phi_{ud}(q_{(1)}, q_{(2)}) - \phi_{du}(q_{(1)}, q_{(2)}) \} d_1 u_2
\end{equation}

which contains all the physical states. Let us assume that the wave functions \(\phi_{ud}\) and \(\phi_{du}\) are sampled respectively by the sets \(\{q_{ud}(l)_i, q_{ud}(2)_i, s_{udi} \} (i = 1\ldots M)\) and \(\{q_{du}(l)_i, q_{du}(2)_i, s_{dui} \} (i = 1\ldots M)\). Clearly, one can sample each term of eq. (20) by enlarging the sets to include 2\(M\) elements with appropriate signs: Namely, for the first term, \(\{q_{ud}(l)_i, q_{ud}(2)_i, s_{udi} \} \oplus \{q_{du}(2)_i, q_{du}(l)_i, -s_{dui} \} (i = 1\ldots M)\), and for the second, \(\{q_{du}(l)_i, q_{du}(2)_i, s_{dui} \} \oplus \{q_{ud}(2)_i, q_{ud}(l)_i, -s_{udi} \} (i = 1\ldots M)\). The operation of enlarging the sampling points for antisymmetrization should be carried out at each step of the evolution in eq. (13). Otherwise, the system would pickup the small contamination of other symmetries, and quickly evolve into the lowest energy state of any symmetry, namely the totally symmetric state. This scheme for the treatment of the exchange symmetry is generalizable, in principle, to the system with arbitrary number of particles.

The results of the calculation for the Hamiltonian eq. (13) is summarized in Table 2. The values for the interaction parameters are taken to be \(v_0 = 1\) and \(a = 0.5\). The sampling number 2\(M\) is set to 1600. The time step is chosen to be \(\Delta \tau = 0.5\). The sampling point from \(N_s = 40\) iterations (after the initial iterations of several hundred) are included. The first line is the energy eigenvalue of first five states. The second line lists the value of 4\(S(S + 1)\) which should serve as a barometer for the quality of wave functions with respect to the separate spatial and spin symmetries: It should be 0 for spatially symmetric \(S = 0\) states, and 8 for spatially antisymmetric \(S = 1\) states. It appears that the third state still contains contamination of other symmetries, and quickly evolve into the lowest energy state of any symmetry, namely the totally symmetric state. The overall feature of the eigenstates are reasonably well captured even at this level. The one-body density profiles calculated from the sampled points are depicted in Fig. 2. Because of the repulsive two body force, the spatially symmetric states are pushed up in the energy compared to the antisymmetric companion states.

\begin{table}[h]
\centering
\begin{tabular}{|c|c|c|c|c|c|}
\hline
\(\alpha\) & 1 & 2 & 3 & 4 & 5 \\
\hline
\(E\) & 2.44 & 3.34 & 3.43 & 3.56 & 3.69 \\
\hline
\(4S^+\) & 0.11 & 7.56 & 0.73 & 7.27 & 0.28 \\
\hline
\end{tabular}
\caption{The energy eigenvalue and the total spin of the first five states of the Gaussian coupled two particles in two-dimensional oscillators. The truncation parameters are \(\Delta \tau = 0.5\) and 2\(M = 1600\).}
\end{table}
Finally, we look at a linear array of oscillators whose Hamiltonian is given by

\[ H = \sum_{k=1}^{N} \left\{ \frac{1}{2} \Pi_k^2 + \frac{1}{2a^2} (\phi_{k+1} - \phi_k)^2 + U(\phi_k) \right\} a \]  

(21)

where \( \phi_k \) and \( \Pi_k = \dot{\phi}_k \) are the amplitude and the conjugate momentum of the \( k \)-th oscillator, and \( a \) is the common distance between the neighboring oscillators. The coupling between adjacent oscillator is given by a trignometric form

\[ U(\phi) = \frac{m}{\beta^2} (1 - \cos \beta \phi). \]  

(22)

This is a discretized version of the one-dimensional sine-Gordon field. The eigen spectra with the periodic boundary condition

\[ \phi_{N+1} = \phi_1 \]  

(23)

give the bosonic excitation modes. There are also soliton modes which are identified as the fermionic excitations. They are given by the twisted boundary condition

\[ \phi_{N+1} = \phi_1 + n_f \frac{2\pi}{\beta} \]  

(24)

where an integer \( n_f \) is the number of kinks, or fermions. Direct extraction of excitation spectra from the Hamiltonian, eq. (21) difficult, because of the existence of translational zero mode of the system. We define an operator \( T \) which shifts the whole system by \( a \) as

\[ T_a \Psi(\phi_1, \phi_2, ..., \phi_{N-1}, \phi_N) = \Psi(\phi_2, \phi_3, ..., \phi_N, \phi_1 + \frac{2\pi n_f}{\beta}) \]  

(25)

where \( \Psi \) is an arbitrary wave function. Clearly, \( T \) commutes with the Hamiltonian \( H \). Therefore, from an arbitrary eigenstates \( \Psi_{n_f, \alpha} \) of \( H \), one can project out the translationally invariant component as

\[ \tilde{\Psi}_{n_f, \alpha} = \left\{ 1 + T_a + T_a^2 + ... + T_a^{N-1} \right\} \Psi_{n_f, \alpha}. \]  

(26)

The projected eigenstates, which are the solutions of the eigenvalue problem

\[ H\tilde{\Psi}_{n_f, \alpha}(\phi_1 \ldots \phi_N) = E_{n_f, \alpha}\tilde{\Psi}_{n_f, \alpha}(\phi_1 \ldots \phi_N), \]  

(27)

are calculated with the iterated Monte Carlo sampling as before. The only complication is that we need to include all \( N \)-cyclic permutations in the set of sampling points at each step of the iteration to ensure the projection, eq. (26): Namely, if \( \Psi_{n_f, \alpha} \) is sampled by a set of \( M \) vectors \( \{\phi_{1i}, \phi_{2i}, ..., \phi_{Ni}, s_i\} \) \((i = 1 \ldots M)\), \( \tilde{\Psi}_{n_f, \alpha} \) can be sampled by \( NM \) vectors \( \{\phi_{1i}, \phi_{2i}, ..., \phi_{Ni}, s_i\} \oplus \{\phi_{2i}, \phi_{3i}, ..., \phi_{(i+1)i}, s_i\} \oplus \cdots \oplus \{\phi_{Ni}, \phi_{1i+1} + n_f \frac{2\pi}{\beta}, s_i\} \) \((i = 1 \ldots M)\). From the eigenvalues \( E_{n_f, \alpha} \), we can extract the mass of bosons as

\[ m_{b1} = E_{0,1} - E_{0,1}, \quad m_{b2} = E_{0,3} - E_{0,1}, \quad \text{etc.} \]  

(28)

where \( m_{b1} \) is the mass of the elementary boson, \( m_{b2} \), the second boson, etc. The mass of the fermion is given by

\[ M_f = E_{1,0} - E_{0,0}. \]  

(29)

![FIG. 2. The one body density profiles of the first five eigenstates of the Hamiltonian eq. (18).](image)

![FIG. 3. (a) The soliton mass \( M_f \) as the function of the coupling \( \beta \) and (b) the bosonic masses \( m_{b1} \) and \( m_{b2} \) as the function of soliton mass \( M_f \) in one dimensional sine-Gordon model.](image)
for $N = 4, 6, 8$ are shown in the figures. In Fig. 3(a), results for different $N$ are practically indistinguishable. For the continuum limit $N \to \infty$, the mass spectra of the sine-Gordon model has been calculated within semi-classical approximation using the trace formula [11]. This analytical result is shown in the figures as the line. The agreement with the numerical results seems to support the assertion by the authors of ref. [11] that their results are exact in full quantum sense.

In above examples, the computational time required for the convergent calculation still tends to exceed the time required for the conventional direct diagonalization approach. However, the expected increase in time and storage for larger degrees of freedom is more modest in the Monte Carlo calculation than in conventional approaches. Also, the Monte Carlo methods have inherent affinity to the computational parallelism. We therefore believe that the results obtained here are sufficiently encouraging for the prospect of tackling more realistic problems both in many-body quantum theories and field theories.

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