Diagonalization of Hamiltonians for Many-Body Systems by Auxiliary Field Quantum Monte Carlo Technique

Michio Honma,[1] Takahiro Mizusaki,[2] and Takaharu Otsuka[2,3]

[1]*Center for Mathematical Sciences, University of Aizu, Tsuruga, Ikki-machi Aizu-Wakamatsu, Fukushima 965, Japan*

[2]*Department of Physics, University of Tokyo, Hongo, Tokyo 113, Japan*

[3]*The Institute of Physical and Chemical Research (RIKEN), Hirosawa, Wako-shi, Saitama 351-01, Japan*

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We propose a Monte Carlo method for solving the quantum many-body interacting systems. Mean fields dominating the structure of low-lying states are selected by a Monte Carlo method, which generates optimum many-body basis states for diagonalizing the Hamiltonian consisting of one- and two-body terms. Not only the ground state but also low-lying excited states are obtained with their wave functions. Results are examined by comparison to exact values.

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Recently active developments have been made in the stochastic approaches to the study of nuclear structure [1,2]. For instance, the quantum Monte Carlo (QMC) method, which was first proposed for the condensed matter problem, has been applied to the nuclear shell model [1]. In the many-body problem, the dimension of Hilbert space rapidly grows as the particle number increases. Therefore, the direct diagonalization of the Hamiltonian matrix can be carried out only for very restricted systems because the maximum tractable dimension of the matrix is limited. The QMC method enables us to overcome this difficulty. However, because of the so-called "minus-sign" problem, the form of the Hamiltonian is rather restricted for performing a stable calculation. Furthermore, in the QMC shell model [1], the structure of excited states can be seen only through response functions.

For the study of a many-body system, the simplest and most precise method is the diagonalization of the Hamiltonian. For the diagonalization in the shell model or the boson model [3], we usually use the complete bases of a given Hilbert space, although the amplitudes of the wave function distribute over almost all the bases, in general. Consequently, a huge model space is required. On the other hand, the coherent states have been known to give a good approximation, in particular, for low-lying states. Therefore, it is expected that, once appropriate coherent states are selected as many-body basis states, the Hamiltonian can be diagonalized in a reasonable approximation in a subspace spanned by such basis states. The number of basis states can then be made much smaller, so that the practical calculation becomes feasible. In this Letter we propose a method of choosing the many-body basis states in the form of coherent states by using the auxiliary field Monte Carlo technique.

We make use of the interacting boson model (IBM) [3] as an easily accessible, yet still realistic, many-body system. The bosons are denoted as b_i $(i = 1, \ldots, N_{\rm sp})$. In the IBM-1, $N_{\rm sp} = 6$ and $b_1 = s$, $b_2 = d_{-2}$, ..., $b_6 = d_2$. The IBM Hamiltonian consists of single-particle energies and a two-body interaction

$$H = \sum_{i,j=1}^{N_{\rm sp}} \epsilon_{ij} b_i^\dagger b_j + \frac{1}{4} \sum_{i,j,k,l=1}^{N_{\rm sp}} v_{ijkl} b_i^\dagger b_j^\dagger b_k b_l \,. \quad (1)$$

This Hamiltonian can be rewritten in the quadratic form of one-body operators O_α,

$$H = \sum_{\alpha=1}^{N_f} (E_\alpha O_\alpha + \tfrac{1}{2} V_\alpha O_\alpha^2) \,, \quad (2)$$

where the number of the O_α's, called N_f, can be at most $N_{\rm sp}^2$ and usually appears to be much smaller. We consider the imaginary time evolution operator $e^{-\beta H}$, and divide the imaginary time β into N_t steps,

$$e^{-\beta H} = \prod_{n=1}^{N_t} e^{-\Delta\beta H} \,, \quad (3)$$

where $\Delta\beta = \beta/N_t$. According to Ref. [1], by applying the Hubbard-Stratonovich transformation [4] at each time step, this operator can be expressed as an integral of one-body evolution operators with respect to the auxiliary fields $\sigma_{\alpha n}$,

$$e^{-\beta H} \approx \int_{-\infty}^{\infty} \prod_{\alpha,n} d\sigma_{\alpha n} \left(\frac{\Delta\beta |V_\alpha|}{2\pi} \right)^{1/2} G(\sigma) \prod_n e^{-\Delta\beta h(\vec{\sigma}_n)} \,, \quad (4)$$

where $\vec{\sigma}_n$ means a set of auxiliary fields of the nth time step, $\vec{\sigma}_n = (\sigma_{1n}, \sigma_{2n}, \ldots, \sigma_{N_f n})$, and σ denotes the assembly of the auxiliary fields over all the time steps, $\sigma = \{\vec{\sigma}_1, \vec{\sigma}_2, \ldots, \vec{\sigma}_{N_t}\}$. The Gaussian weight factor $G(\sigma)$ is defined by

$$G(\sigma) = e^{-\sum_{\alpha,n} (\Delta\beta/2) |V_\alpha| \sigma_{\alpha n}^2} \,, \quad (5)$$

and the one-body Hamiltonian $h(\vec{\sigma}_n)$ is defined by

$$h(\vec{\sigma}_n) = \sum_\alpha (E_\alpha + s_\alpha V_\alpha \sigma_{\alpha n}) O_\alpha \,, \quad (6)$$

where $s_\alpha = 1$ $(= i)$ if $V_\alpha < 0$ (> 0).

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If the $(N_t \times N_f)$-dimensional integral is treated with sufficient accuracy, we can obtain the ground state wave function by operating (4) with sufficiently large β on any initial state $|\Psi\rangle$ that is not orthogonal to the ground state. In numerical calculations the integral is evaluated by discretizing the $\sigma_{\alpha n}$ variables, and the integrand is computed for several specific sets σ. In the Monte Carlo integration, each set of σ is generated stochastically according to some weight functions. Then many sets of auxiliary fields are generated, and the corresponding wave functions should be added with an equal weight. In many cases this integral does not converge with a tractable number of sets σ, since the variance of the integrand is in general too large. This difficulty can be avoided by considering only the expectation values [1]. This treatment, in turn, gives rise to the minus-sign problem.

In general, the structure of low-lying states of nuclei is dominated by some intrinsic mean fields. Each intrinsic mean field generates intrinsic wave functions as its eigenstates or excitation modes. Since the intrinsic mean fields do not have to be scalar, the intrinsic wave functions are not necessarily eigenstates of the angular momentum. The intrinsic mean fields are rather common for the low-lying states of nuclei, but those states are actually split in energy according to certain quantum numbers, including the angular momentum. This splitting is due to subtle superposition of various intrinsic wave functions, some of which may be different (mainly) only in the orientation. This subtle superposition, which is a very quantum-mechanical effect, is crucial for good angular momentum and orthogonality, but may not be achieved so easily in a stochastic way. On the other hand, such superposition may be carried out to a good approximation by diagonalizing the Hamiltonian in a small subspace spanned by appropriate intrinsic states. Based on this expectation, we propose a new method, consisting of the following steps.

(1) We take an initial coherent state

$$|\Psi^{(0)}\rangle = \frac{1}{\sqrt{N_B!}}\left(\sum_{i=1}^{N_{\rm sp}} x_i b_i^\dagger\right)^{N_B}|0\rangle, \tag{7}$$

where $|0\rangle$ is the boson vacuum and the (generally complex) amplitudes x_i can be determined by a variation method. Then the initial energy $E^{(0)} = \langle\Psi^{(0)}|H|\Psi^{(0)}\rangle$ is calculated.

(2) A set of the auxiliary fields σ is given stochastically according to the Gaussian weight function (5). Note that it is practically easy and fast to generate random numbers obeying Gaussian distribution.

(3) We calculate a wave function $|\Phi(\sigma)\rangle$ for the present set σ:

$$|\Phi(\sigma)\rangle \propto \prod_{n=1}^{N_t} e^{-\Delta\beta h(\vec{\sigma}_n)}|\Psi^{(0)}\rangle. \tag{8}$$

In principle, if an infinite number of auxiliary fields is generated and the corresponding wave functions of this type are added for infinitesimal $\Delta\beta$, the exact time-evolved wave function is obtained. Note that since the initial state is a coherent state and $h(\vec{\sigma}_n)$ is a one-body operator, the state $|\Phi(\sigma)\rangle$ is also a coherent state. Namely, the operation of $\exp(T)$ on $|\Psi\rangle$ is equivalent to the transformation of the amplitudes x_i by a matrix T_{ij}, where $T = \sum_{i,j=1}^{N_{\rm sp}} T_{ij} b_i^\dagger b_j$.

(4) The state $|\Phi(\sigma)\rangle$ is orthonormalized, by means of the Schmidt method, with respect to all other basis states obtained previously, and a new basis $|\Phi'\rangle$ is determined.

(5) By including the new basis state obtained in step (4), we diagonalize the Hamiltonian H, and obtain an improved ground state energy E and its wave function $|\Psi\rangle$.

(6) Steps from (2) to (6) are repeated until the ground state energy E converges. We can also confirm the convergence by calculating the expectation value of the angular momentum operator.

In order to accelerate the convergence, the following process can be added to step (4) according to Ref. [5]. The energy decrease ΔE which originates in the new basis $|\Phi'\rangle$ can be estimated by $\Delta E \sim \frac{1}{2}\{E - E_1 + \sqrt{(E - E_1)^2 + 4|E_2|^2}\}$, where E denotes the ground state energy obtained in the previous step, $E_1 = \langle\Phi'|H|\Phi'\rangle$, and $E_2 = \langle\Psi|H|\Phi'\rangle$. If ΔE is too small, for example, less than 10% in comparison to the energy decrease in the previous steps, the state $|\Phi'\rangle$ is discarded, and we return to step (2).

We refer to the present method as the quantum Monte Carlo diagonalization (QMCD) method. We emphasize that energies and wave functions are determined by the diagonalization, and that we can obtain excited states as well as the ground state. As mentioned before, since the mean fields are similar for low-lying states, several lowest excited states are expected to be obtained with similar accuracies using the same dimension of the basis states.

As a demonstration of the QMCD method, we solve the *sdg*-IBM with the following Hamiltonian:

$$H = -\kappa Q \cdot Q + \kappa' L \cdot L, \tag{9}$$

where the quadrupole operator Q is defined by

$$Q = s^\dagger\tilde{d} + d^\dagger s + \chi_1[d^\dagger\tilde{d}]^{(2)} + \chi_2[d^\dagger\tilde{g} + g^\dagger\tilde{d}]^{(2)} + \chi_3[g^\dagger\tilde{g}]^{(2)}, \tag{10}$$

and L stands for the angular momentum operator.

First we consider the SU(3) limit of the *sdg*-IBM, which corresponds to the axially symmetric rotor and is specified by $\chi_1 = -11\sqrt{10}/28$, $\chi_2 = 9/7$, $\chi_3 = -3\sqrt{55}/14$. Figure 1 shows the energies of the ground and first excited states as a function of the QMCD basis dimension for two cases of $N_B = 10$ and 20. The adopted values of other parameters are shown in the figure caption. The energies come down rapidly as more bases are included. Note that the energies of initial coherent states are -28.909 and -114.892 for these two cases. The dimension of the *m*-scheme basis in the exact diagonalization of the Hamiltonian matrix appears to be 92 123 and 39 180 981 for $N_B =$

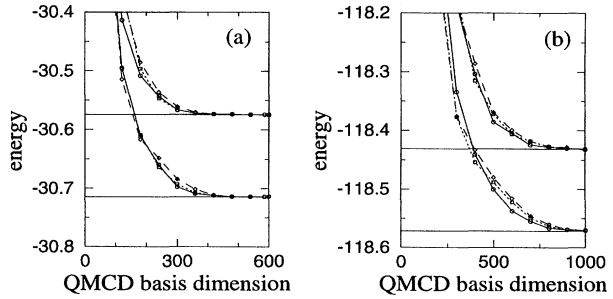

FIG. 1. Energies of the lowest two states for (a) $N_B = 10$ and (b) $N_B = 20$ as a function of QMCD basis dimension, in the SU(3) limit of the *sdg*-IBM. The parameters used are $\Delta\beta = 16$, $N_t = 20$, $\kappa = 0.1$, and $\kappa' = 0.01$. The solid, dashed, and dotted lines stand for different sets of the σ's. The exact values are shown by horizontal lines.

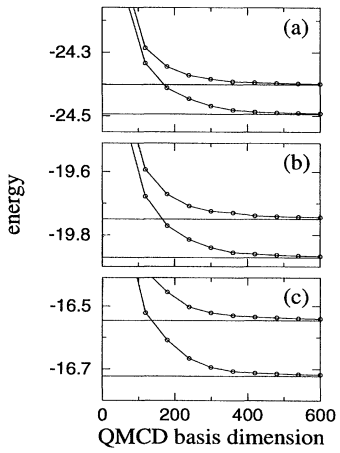

FIG. 2. Energies of the lowest two states as a function of QMCD basis dimension for (a) $q = 0.8$, (b) $q = 0.6$, and (c) $q = 0.4$. The parameters used are $N_B = 10$, $N_t = 20$, $\kappa = 0.1$, $\kappa' = 0$, and $\Delta\beta = 80$ for (a), 40 for (b), 20 for (c). The exact energies are shown by horizontal lines.

10 and 20, respectively, in the case of the total magnetic quantum number $M = 0$. The exact numerical diagonalization is already very difficult in the former case, and is indeed practically impossible in the latter case. In Fig. 1, the exact energies are calculated analytically. We can see that in the QMCD the convergence is attained at about 400 and 900 basis states for these two cases, respectively. Although the number of QMCD basis states increases as N_B increases, this increase is much slower than that of the dimension of the entire Hilbert space. The ground state expectation values of the $L \cdot L$ operator are 0.003 and 0.037 for these two cases, respectively, while they are 6.002 and 6.017 for the first 2^+ state. These results confirm that the convergence of the angular momentum is fulfilled. Since these values are 74.474 and 154.641 for initial coherent states, we can see that the restoration of the angular momentum is significant. This feature is also found in the expectation value of the quadrupole operator $Q_{\mu=0}$. In one of the calculations with $N_B = 10$, this value starts from -9.501 (intrinsic state value), and ends at 0.004 for the resultant ground state. We repeated the calculation using different sets of σ. The results are shown by the various lines in Fig. 1. We find that all lines converge to the same value.

We next change the structure by multiplying the SU(3) values of the χ_i $(i = 1, 2, 3)$ by a common parameter q. As an example we take $N_B = 10$. In Fig. 2 the energies of the ground and first excited 2^+ state are shown for several q values as a function of the QMCD basis dimension. As q becomes smaller than unity, the system loses the character of the axially symmetric rotor and becomes more γ unstable. The exact eigenvalues are also shown in Fig. 2. The convergence point is shifted as the parameter q decreases. However, the deviation of the energy from the exact values is less than 0.006 for all cases.

Next we consider excited states and $E2$ transition matrix elements. Note that, in the QMCD, stochastic procedures are utilized not for calculating matrix elements but for generating basis state vectors. Since random numbers are generated with the Gaussian distribution, the minus-sign problem which appears in many quantum Monte Carlo methods including the QMC shell model for bosons disappears in the QMCD for any interaction. Therefore we can modify the Hamiltonian and change the order of energy levels. For example, by adding an artificial term $\gamma(L_z - M)^2$ with positive γ and some integer M, all states with $L_z \neq M$ can be pushed up. Therefore we can distill lowest eigenstates of a given L_z. These states can be used for the calculation of transition matrix elements.

In Table I $B(E2)$ values between low-lying states are shown for $q = 0.6$ and 0.2 for $N_B = 10$. The term γL_z^2 is added to the Hamiltonian in order to extract $M = 0$ states. The number of QMCD basis states is taken as 1000. The exact $B(E2)$ values are also shown. We can see that the agreement between the QMCD and the exact values is significant (at most 2% error).

As another demonstration, we consider the O(6) limit in the *sd*-IBM-1. The O(6) limit represents γ-unstable nuclei, and its eigenstates are formed by a superposition of an infinite number of intrinsic states [6]. Although

TABLE I. $E2$ transition matrix elements between low-lying states for the cases of $q = 0.6$ and 0.2. $N_B = 10$, $N_t = 20$, $\kappa = 0.1$, and $\kappa' = 0$ are used, while $\Delta\beta = 40$ (20) for $q = 0.6$ (0.2).

	$q = 0.6$		$q = 0.2$	
Transition	QMCD	Exact	QMCD	Exact
$2_1^+ \rightarrow 0_1^+$	39.2	39.2	27.7	27.8
$2_1^+ \rightarrow 2_1^+$	55.6	55.7	35.1	34.7
$4_1^+ \rightarrow 2_1^+$	54.7	55.4	39.5	39.3
$4_1^+ \rightarrow 4_1^+$	49.5	49.7	26.0	26.2

TABLE II. QMCD calculations for the O(6) Hamiltonian (H) for $N_B = 10$ and 16. The expectation values of $L \cdot L$ and the exact energies are also shown. The parameters are $\kappa = 0.05$, $\kappa' = 0.01$, $N_t = 20$, and $\Delta\beta = 50$.

	$N_B = 10$			$N_B = 16$		
State	H	$L \cdot L$	Exact	H	$L \cdot L$	Exact
0_1^+	−6.999	0.03	−7.000	−15.999	0.02	−16.000
2_1^+	−6.738	6.05	−6.740	−15.739	6.03	−15.740
2_2^+	−6.435	6.11	−6.440	−15.438	6.06	−15.440
4_1^+	−6.292	20.16	−6.300	−15.298	20.05	−15.300

this feature is remedied for small boson numbers due to quantum fluctuations, this feature becomes prominent for $N_B \gtrsim 10$ [7]. We shall see whether the QMCD is still useful for such cases or not, considering the cases of $N_B = 10$ and 16. The Hamiltonian (9) with $Q = s^\dagger \tilde{d} + d^\dagger s$ (i.e., $q = 0$) corresponds to the O(6) limit. In Table II the energies and the expectation values of the $L \cdot L$ operator are shown for the 0_1^+, 2_1^+, and 2_2^+ states. The exact energies are also listed. The QMCD basis dimension is taken to be 500 and 1500 for $N_B = 10$ and 16, respectively. In both cases, we can see a good agreement between the QMCD and the corresponding exact values. Note that the excitation energies of 2_2^+ states are still obtained within 1% errors. It has been shown [7] that the 2_2^+ excitation energy calculated from a single triaxial intrinsic state deviates much more than the present result. Thus, one finds the efficiency of the QMCD also for the states without simple intrinsic structure.

We have compared the QMCD results with those obtained by the variation after the angular momentum projection (VAP) calculation where a single intrinsic coherent state is optimized with respect to the energy calculated by projecting this state onto a good angular momentum. The QMCD always gives significantly better agreement with the exact results than the VAP, in particular, for transition matrix elements.

We are now trying to apply the QMCD to fermion systems. The fermion system can be treated in a quite similar way, because the difference emerges only in the calculation of matrix elements. One option is to take Slater determinants as basis states, as in the Monte Carlo shell model [1]. As another method, we can take condensed states of nucleon pairs in place of Slater determinants.

In summary, we have presented a new method for selecting coherent basis states by using the auxiliary field Monte Carlo technique. We can calculate both the ground and low-lying excited states for any interaction. As the system becomes large, the QMCD basis dimension increases only gradually. The conservation of the angular momentum is built-in. Since the wave function is obtained explicitly, the transition matrix elements, including those between excited states, can be calculated directly.

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