# Nuclear Shell Model by the Quantum Monte Carlo Diagonalization Method

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The feasibility of shell-model calculations is radically extended by the quantum Monte Carlo diagonalization method with various essential improvements. The major improvements are made in the sampling for the generation of shell-model basis vectors, and in the restoration of symmetries such as angular momentum and isospin. Consequently the level structure of low-lying states can be studied with realistic interactions. After testing this method on $^{24}$Mg, we present first results for energy levels and $E2$ properties of $^{64}$Ge, indicating its large and $\gamma$-soft deformation. [S0031-9007(96)01252-5]

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The nuclear shell model has been successful in the description of various aspects of nuclear structure, partly because it is based on a minimum number of natural assumptions. Although the direct diagonalization of the Hamiltonian matrix in the full valence-nucleon Hilbert space is desired, the dimension of such a space is too large in many cases, preventing us from performing the full calculations. The direct diagonalization has been carried out up to $^{48}$Cr [1]. Recently, in order to relax this restriction drastically, stochastic approaches, for instance, the shell-model Monte Carlo (SMMC) method [2], have been investigated. In fact, ground-state [3] and thermal properties [4] have been well described by the SMMC method.

We have presented the quantum Monte Carlo diagonalization (QMCD) method [5] by utilizing the auxiliary field Monte Carlo technique as in the SMMC method, but in a quite different way. In general, low-lying states of nuclei are described to a good extent in terms of static and/or dynamic mean fields and their fluctuations. The basic idea of the QMCD method is to diagonalize the shell-model Hamiltonian, by using this property, in a subspace spanned by a small number of selected basis states obtained by stochastically generated one-body fields. Thus, the ground state and several excited states can be obtained. The QMCD method has been applied to the interacting boson model [5,6]. In this Letter the QMCD method is revised considerably in various aspects so as to be capable of performing large-scale shell-model calculations with realistic nuclear forces. As examples, $^{24}$Mg and $^{64}$Ge are taken. In particular, $^{64}$Ge is an $N = Z$ proton-rich unstable nucleus manifesting a $\gamma$-soft structure, with a wide range of theoretical interpretations (see Ref. [7]). Thus, the shell-model calculation can play a crucial role for clarifying the level structure, but so far such attempts have been impossible due to the large dimension ($\sim 1 \times 10^9$).

We first sketch the QMCD process very briefly, referring to relevant equations of Ref. [5]. More details on certain basic points can be found in Ref. [5]. The shell-model Hamiltonian consisting of single-particle energies and a two-body interaction can be written in the quadratic form of $N_f$ one-body operators $O_\alpha$:

$$H = \sum_{\alpha=1}^{N_f} \left( E_\alpha O_\alpha + \frac{1}{2} V_\alpha O_\alpha^2 \right). \tag{1}$$

We consider the imaginary time evolution operator $e^{-\beta H}$ with $N_t$ slices: $e^{-\beta H} = \prod_{n=1}^{N_t} e^{-\Delta\beta H}$, where $\Delta\beta = \beta/N_t$. By applying the Hubbard-Stratonovich transformation at each time slice [8,9], $e^{-\beta H}$ can be expressed as the integral of an operator, $\prod_{n=1}^{N_t} e^{-\Delta\beta h(\vec{\sigma}_n)}$, over $N_f \times N_t$ auxiliary fields $\sigma_{\alpha n}$ [see Eq. (4) of Ref. [5]] with the Gaussian weight factor $G(\sigma) = \exp(-\sum_{\alpha,n} \Delta\beta/2|V_\alpha|\sigma_{\alpha n}^2)$. The one-body Hamiltonian $h(\vec{\sigma}_n)$ is defined by

$$h(\vec{\sigma}_n) = \sum_\alpha (E_\alpha + s_\alpha V_\alpha \sigma_{\alpha n}) O_\alpha \,, \tag{2}$$

where $s_\alpha = \pm 1$ ($= \pm i$) if $V_\alpha < 0$ ($>0$). In the QMCD method, by generating a new set of values for $\sigma = \{\sigma_{\alpha n}\}$ stochastically according to $G(\sigma)$, a new many-body state is created as

$$|\Phi(\sigma)\rangle \propto \prod_{n=1}^{N_t} e^{-\Delta\beta h(\vec{\sigma}_n)} |\Psi^{(0)}\rangle \,, \tag{3}$$

where $|\Psi^{(0)}\rangle$ is an appropriate initial state. The Hamiltonian is diagonalized in the Hilbert subspace spanned by this state and the basis states previously obtained. If this new state improves the result of the diagonalization sufficiently well, this state is added to the basis states. The number of such basis states is referred to as the QMCD basis dimension, and is increased until reasonable convergence is achieved.

It is convenient to adopt basis states in the form of Slater determinants: $\prod_{\alpha=1}^{N} a_\alpha^\dagger |-\rangle$, where $N$ denotes the number of valence nucleons, $|-\rangle$ is an inert spherical core, and $a_\alpha^\dagger$ represents the nucleon creation operator in a canonical single-particle state $\alpha$, which is a linear combination of the spherical bases. Note that, if $|\Psi^{(0)}\rangle$

  

is a Slater determinant, $|\Phi(\sigma)\rangle$ in Eq. (3) remains in the form of a Slater determinant.

While the QMCD method outlined so far is applicable to fermion systems, its capability is limited to simple cases, for instance, a single-$j$ model. Difficulties arise, for example, due to finite single-particle energies. Thus, a substantial further improvement of the method is required for realistic shell-model calculations. Such improvements are that (i) the sampling scheme is modified, and (ii) additional processes are included to restore symmetries.

We start with the sampling. In the original version of the QMCD method, a rather naive sampling is performed [see Eq. (4) of Ref. [5]]. This sampling creates many unnecessary basis vectors in general, and, indeed, the actual sampling has to be modified for large-scale realistic shell-model calculations so that important basis vectors are generated still stochastically but more efficiently by considering the many-body dynamics.

The modification regarding the sampling consists of two parts. In the first part, the basis state generation is refined so as to make use of the local Hartree-Fock (HF) energy minima. In the QMCD calculation, one has to generate good basis states (i.e., Slater determinants in deformed bases) which have (i) low values of diagonal matrix elements and/or (ii) large off-diagonal matrix elements of the Hamiltonian. The point (i) can be fulfilled by using, as $|\Psi^{(0)}\rangle$ in Eq. (3), a deformed HF solution within the present shell-model space. The QMCD process is comprised practically of several segments starting with different initial states, which are HF states at different local minima. States around a minimum satisfy point (ii) in most cases. We then rearrange the one-body evolution process so that the basis states are sampled most frequently near the HF local minima, accelerating the generation of state vectors having larger overlap with eigenstates of interest.

The Hamiltonian is rewritten, by introducing the constants $c_\alpha$, as

$$H = \sum_\alpha \left[ E_\alpha O_\alpha + \frac{1}{2} V_\alpha (O_\alpha - c_\alpha)^2 + V_\alpha c_\alpha O_\alpha \right], \tag{4}$$

where a constant term is omitted. After the HS transformation, the one-body Hamiltonian becomes

$$h(\vec{\sigma}_n) = \sum_\alpha [(E_\alpha + V_\alpha c_\alpha) O_\alpha + s_\alpha V_\alpha \sigma_{\alpha n} O_\alpha], \tag{5}$$

where the $c$-number $-\sum_\alpha s_\alpha V_\alpha \sigma_{\alpha n} c_\alpha$ is omitted since it does not change the wave functions apart from the normalization. In this expression, the modified one-body term $\sum_\alpha (E_\alpha + V_\alpha c_\alpha) O_\alpha$ includes effects coming from the two-body interaction. The $c_\alpha$'s are taken in such a way that this term becomes the HF single-particle Hamiltonian, $h_{\rm HF}$. With this $h_{\rm HF}$, the QMCD basis state takes the form

$$|\Phi(\sigma)\rangle \propto \prod_{n=1}^{N_t} e^{-\Delta\beta\left(h_{\rm HF} + \sum_\alpha s_\alpha V_\alpha \sigma_{\alpha n} O_\alpha\right)} |\Psi^{(0)}\rangle. \tag{6}$$

Thus, we simply replace the single-particle energy $\sum_\alpha E_\alpha O_\alpha$ by $h_{\rm HF}$. If $|\Psi^{(0)}\rangle$ is the HF state being considered, the sampling around $\sigma = 0$ generates various states around this HF state, including Tamm–Dancoff-type states to first order in $\sigma$, and so on. This treatment is possible for all HF local minima.

In cases of nonspherical nuclei, many Hartree-Fock local minima appear in the search for the initial state. By stochastically taking those local minima as the initial states, it is possible to take into account a wider variety of configurations.

The second major improvement on the sampling is the ordering of one-body fields according to their importance. The QMCD method is a method for generating favorable basis states for diagonalization, and there is no need to carry out the stochastic integration over all auxiliary fields. In constructing the basis states, we start with the most relevant part of the Hamiltonian, which yields fewer auxiliary fields than the whole Hamiltonian. The calculation can then be performed more efficiently. After certain basis states are obtained, we take an enlarged portion of the Hamiltonian, so that other terms of the Hamiltonian can be properly included in constructing the basis states. Eventually the completeness of the QMCD basis is guaranteed for the ground state by taking all fields.

In most cases, the auxiliary fields with large values of $|V_\alpha|$ in Eq. (1) turn out to have quadrupole, hexadecapole, or monopole natures. Therefore it is reasonable to arrange all fields in descending order of $|V_\alpha|$, and take them starting from the largest one. In addition, for a fixed initial state $|\Psi^{(0)}\rangle$, the total strength of each $O_\alpha$ changes due to the Pauli principle and to collective effects. Therefore we consider an excitation sum rule,

$$S_\alpha = \langle\Psi^{(0)}|O_\alpha^\dagger O_\alpha|\Psi^{(0)}\rangle - |\langle\Psi^{(0)}|O_\alpha|\Psi^{(0)}\rangle|^2, \tag{7}$$

and use it as a practical measure of importance of the $O_\alpha$'s. The selection of $O_\alpha$'s according to $|V_\alpha|$ and $S_\alpha$ plays an essential role in the actual calculations.

Incorporating all of the above improvements, the sampling is made much more efficient. Note that this way of sampling clearly differs from that of the SMMC.

We now come to the restoration of symmetries. We implement explicitly kinematic symmetries such as angular momentum and isospin into the QMCD method, since the restoration of such symmetries proceeds only very slowly for wave functions generated stochastically. In the previous paper [6] we have presented the $M$-projection method to restore the magnetic quantum number.

Since a nucleus has rotational symmetry, the restoration of the total angular momentum, denoted as $J$, is quite crucial. In the QMCD method, we diagonalize the Hamiltonian in the laboratory frame by using QMCD bases. If the QMCD bases contain all components (i.e., Slater determinants) required for the coupling to a good angular momentum, the diagonalization restores the rotational symmetry. We accelerate this restoration process by considering rotated states $\exp(-i\theta_y J_y)\exp(-i\theta_z J_z)|\Phi(\sigma)\rangle$

as candidates of new basis states. We have found that the restoration of the angular momentum is remarkably improved by taking only several values of the angle $\theta$'s. We refer to this method as $J$-drive. In addition to this, the $M$ projection [6] is carried out for all bases thus created.

We next discuss isospin. The isospin projection is possible in the same way as the $J$ projection. In this Letter, however, since we consider only $N = Z$ nuclei, we keep good isospin in an alternative way. In the decomposition process, Eq. (1), all one-body operators can be chosen so as to carry a definite isospin $T = 0$ or 1 for the isoscalar Hamiltonian. Since the isoscalar fields are dominant over the isovector ones, particularly, for $T = 0$ states, we start the QMCD basis generation process with the isoscalar fields. Thus, since the initial HF state has $T = 0$, the isospin is conserved at least until the isovector fields are activated. It appears that, in $N = Z$ nuclei, one obtains sufficiently good results by keeping only the isoscalar fields. For $T \neq 0$ states, the isospin projection is definitely needed, and results obtained with this procedure will be presented elsewhere.

As an example of realistic shell-model calculations, we first consider $^{24}$Mg with the USD interaction [10]. Figure 1 shows energies and expectation values of $J \cdot J$, for six low-lying states as a function of the QMCD basis dimension compared with the exact values. In this case we start with five significant fields, and eventually all 144 $T = 0$ one-body operators are activated. In the process of $J$-drive, three values for $\theta_y$ are employed. For 800 QMCD bases, the ground-state energy becomes $-86.91$ MeV, while the exact value is $-87.08$ MeV. The dimension of the $m$-scheme shell-model basis for the ground state is 28 503. Thus the number of bases is reduced by a factor of $1/35$ with a loss of accuracy of only 0.17 MeV in the total energy. The error due to the truncation of the Hilbert space (systematic error) does not exceed 200 keV in the ground-state energy in the present calculations.

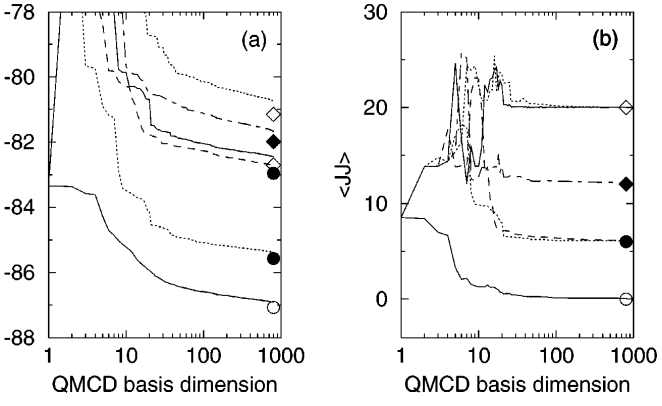


FIG. 1. (a) Energies and (b) expectation values of $J \cdot J$ of the lowest six states of $^{24}$Mg plotted as a function of the QMCD basis dimension, with $N_t = 20$ and $\Delta\beta = 0.07$ (MeV$^{-1}$). The exact values are shown by symbols. Different symbols indicate different angular momenta.

Table I shows the lowest three energy levels, where the QMCD results for 100, 400, and 800 basis dimensions are listed together with the exact results. One finds a remarkable agreement between the QMCD and exact values. Note that the accuracy of these excitation energies is better than that of absolute energies. In fact, the deviations are less than 0.15 MeV with only 400 basis states. In the same table, several $E2$ transition matrix elements and quadrupole moments are compared with the exact values. It can be found that several in-band transition $B(E2)$ values are reproduced well with only 100 basis states, and other matrix elements are also obtained with 400 basis states. Thus the QMCD method turns out to be useful, especially for the study of low-lying collective states.

We now proceed on to full pf shell calculations. We have confirmed the feasibility of the QMCD method by comparing its results with the exact ones [1] for $^{48}$Cr with the KB3 interaction [11], as will be presented elsewhere. In this Letter, we discuss $^{64}$Ge. The $m$-scheme dimension of the $M = 0$ space is 1 087 455 228, which is the second largest one for the $N = Z$ even-even pf shell nuclei. It is larger than the dimension for $^{48}$Cr by a factor of about 550, and the exact diagonalization is hopeless in the near future. This nucleus is one of the proton-rich $N = Z$ unstable nuclei, and experimental data [7] suggest that it is $\gamma$-soft. Thus, it is quite interesting to investigate whether we can reproduce such a structure by using a realistic interaction, the validity of which has been examined at least for the lower part of the pf shell. In this Letter, we adopt the FPD6 interaction [12]. This interaction is derived by fitting experimental data in the mass range 41–49, and is suggested to be suitable for describing nuclei in the upper pf shell [13].

In Fig. 2, calculated low-lying spectra are compared with experimental data. It is remarkable that the calculated levels show a rather good agreement with experiment without any adjustment. The $\gamma$-soft nature is also evident in the calculation. The calculated

TABLE I. Comparison between the QMCD and the exact results for excitation energies (MeV), $B(E2)$ ($e^2$ fm$^4$) and quadrupole moments ($e$ fm$^2$). The effective charges $e_p + e_n = 1.78e$ are used [10].

| Observable | QMCD dimension 100 | 400 | 800 | Exact |
|---|---|---|---|---|
| $E_x(2_1^+)$ | 1.50 | 1.54 | 1.53 | 1.51 |
| $E_x(2_2^+)$ | 4.33 | 4.23 | 4.18 | 4.12 |
| $E_x(4_1^+)$ | 4.54 | 4.50 | 4.46 | 4.37 |
| $B(E2; 2_1^+ \rightarrow 0_1^+)$ | 74.1 | 73.2 | 74.2 | 76.1 |
| $B(E2; 2_2^+ \rightarrow 0_1^+)$ | 7.1 | 7.2 | 7.1 | 6.8 |
| $B(E2; 2_2^+ \rightarrow 2_1^+)$ | 12.1 | 16.8 | 16.2 | 16.6 |
| $B(E2; 4_1^+ \rightarrow 2_1^+)$ | 103.8 | 102.6 | 102.0 | 101.1 |
| $B(E2; 4_1^+ \rightarrow 2_2^+)$ | 1.8 | 0.4 | 0.5 | 0.5 |
| $Q(2_1^+)$ | $-18.7$ | $-18.4$ | $-17.9$ | $-17.1$ |
| $Q(2_2^+)$ | 18.5 | 18.4 | 18.1 | 17.3 |
| $Q(4_1^+)$ | $-21.1$ | $-21.5$ | $-21.2$ | $-20.8$ |

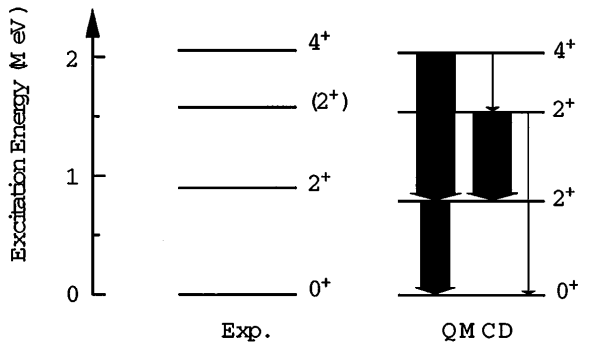


FIG. 2. Experimental and calculated energy levels of $^{64}$Ge. The QMCD parameters are $N_t = 40$ and $\Delta\beta = 0.06$ (MeV$^{-1}$). The arrows designate $E2$ transitions with $B(E2)$'s indicated by their widths.

ratio of excitation energies of $2_2^+$ to $2_1^+$ is 1.9 and that of $4_1^+$ to $2_1^+$ is 2.6. Experimentally, these ratios are 1.75 and 2.27, respectively. The relative magnitudes of $B(E2)$ values are shown in Fig. 2. With $e_p = 1.33e$ and $e_n = 0.64e$, $B(E2; 2_1^+ \rightarrow 0_1^+) = 5 \times 10^2 (e^2\ \mathrm{fm}^4)$ is obtained, which corresponds to $\beta_2 \sim 0.28$. The $B(E2)$ values of the $4_1^+ \rightarrow 2_1^+$ and $2_2^+ \rightarrow 2_1^+$ transitions are about 1.3 times larger than that of $B(E2; 2_1^+ \rightarrow 0_1^+)$, suggesting $\gamma$-softness. We obtain $B(E2; 2_2^+ \rightarrow 0_1^+)/B(E2; 2_2^+ \rightarrow 2_1^+) \sim 2 \times 10^{-3}$, which is quite small similarly to the experimental value, suggesting $\gamma \sim 30°$ in triaxial deformation models [7]. Calculated quadrupole moments appear to be small (typically $|Q| < 10e$ fm$^2$), consistently with $\gamma$-softness.

The convergence of the results in Fig. 2 has been examined by several calculations with different stochastic parameters. The typical deviation among different calculations (statistical error) is about 100 keV for the $2_2^+$ energy level, for instance. The discrepancy between theoretical and experimental results comes partly from the systematic and statistical errors in the present method, and partly from the interaction. The former one is being reduced by improving the method.

Typical occupation numbers of $f_{7/2}$, $p_{3/2}$, $p_{1/2}$, and $f_{5/2}$ orbits are 15.1, 2.6, 0.8, and 5.5, respectively, for low-lying states. We can see that more than six nucleons are excited from the $(f_{7/2})^{16}\ (p_{3/2})^8$ configuration, and that even $f_{7/2}$ is active. One sees that all these four orbits are mixed. Because of the huge basis dimension mentioned before, the conventional shell-model diagonalization is impossible.

The QMCD method can generate, in principle, all basis states which are needed to describe the exact eigenstate. It is free of the assumption of some specific collective coordinates as in the usual generator coordinate method. In addition, we can take into account various states around many different local energy minima, which is difficult in variational approaches with multi-Slater determinants or multi-HFB states.

In summary, it has been shown that large-scale realistic shell-model calculations can be carried out by the QMCD method. The QMCD method has been improved considerably with respect to (1) the sampling of auxiliary fields based on the local energy minima, (2) the selection of dominant fields, and (3) the explicit implementation of kinematic symmetry requirements. Several low-lying states of large systems have been described in terms of small numbers of QMCD basis states with the accuracy of several hundred keV in total energies. The accuracy of excitation energies and $E2$ transition matrix elements is much better. Such capability of describing low-lying states is the major advantage of the present method over the SMMC method. The present results demonstrate that the shell-model calculations with full valence shell configurations have become feasible by the QMCD method, shading light upon the structure of nuclei even beyond the pf shell with more direct relation to the effective nucleon-nucleon interaction. The minus-sign problem seems to be absent in the QMCD method, and, hence, any effective two-body interaction can be used as it is.

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[1] E. Caurier, A. P. Zuker, A. Poves, and G. Martinez-Pinedo, Phys. Rev. C **50**, 225 (1994).
[2] S. E. Koonin, D. J. Dean, and K. Langanke, Phys. Rep. (to be published).
[3] K. Langanke, D. J. Dean, P. B. Radha, Y. Alhassid, and S. E. Koonin, Phys. Rev. C **52**, 718 (1995).
[4] D. J. Dean, S. E. Koonin, K. Langanke, P. B. Radha, and Y. Alhassid, Phys. Rev. Lett. **74**, 2909 (1995).
[5] M. Honma, T. Mizusaki, and T. Otsuka, Phys. Rev. Lett. **75**, 1284 (1995).
[6] T. Mizusaki, M. Honma, and T. Otsuka, Phys. Rev. C **53**, 2786 (1996).
[7] P. J. Ennis *et al.*, Nucl. Phys. **A535**, 392 (1991).
[8] J. Hubbard, Phys. Lett. **3**, 77 (1959); R. D. Stratonovich, Dokl. Akad. Nauk SSSR **115**, 1907 (1957) [Sov. Phys. Dokl. **2**, 416 (1958)].
[9] M. Suzuki, Commun. Math. Phys. **51**, 183 (1976).
[10] B. A. Brown and B. H. Wildenthal, Annu. Rev. Nucl. Sci. **38**, 29 (1988).
[11] A. Poves and A. Zuker, Phys. Rep. **70**, 235 (1981).
[12] W. A. Richter, M. G. van der Merwe, R. E. Julies, and B. A. Brown, Nucl. Phys. **A523**, 325 (1991).
[13] W. E. Ormand and B. A. Brown, Phys. Rev. C **52**, 2455 (1995).