QUANTUM MONTE CARLO DIAGONALIZATION METHOD FOR REALISTIC SHELL MODEL CALCULATIONS *

T. MIZUSAKI[a], M. HONMA[b] AND T. OTSUKA[a,c]

[a]Department of Physics, University of Tokyo, Hongo
Tokyo 113, Japan
[b]Center for Mathematical Sciences, University of Aizu
Tsuruga, Ikki-machi Aizu-Wakamatsu
Fukushima 965, Japan
[c]RIKEN, Hirosawa, Wako-shi
Saitama 351-01, Japan

(Received December 10, 1996)

A stochastic method for performing large-scale shell model calculations is presented, which utilizes the auxiliary field Monte Carlo technique and diagonalization method. This method overcomes the limitation of the conventional shell model diagonalization and can extremely widen the feasibility of shell model calculations with realistic interactions for spectroscopic study of nuclear structure.

PACS numbers: 21.60. Ka, 21.60. Cs, 24.10. Cn

One of the trends in theoretical nuclear structure physics is a stochastic approach for nuclear shell model which describes the dynamics of nucleons strongly interacting each other via residual two-body interaction. The conventional shell model diagonalization clearly meets the difficulty as the dimension of the Hilbert space increases, while, several stochastic approaches are proposed in order to overcome this limitation. For instance, Horoi *et al.* [1] proposed a truncation scheme with stochastic criteria for the conventional shell model diagonalization. Koonin and his collaborators [2] developed the Shell Model Monte Carlo (SMMC) method based on the auxiliary field Quantum Monte Carlo method, which turns out to be a powerful method to extend the feasibility of shell model calculation for ground state and finite temperature properties. However, this method is not free

* Presented at the XXXI Zakopane School of Physics, Zakopane, Poland, September 3–11, 1996.

of the sign-problem which is a generic problem in Quantum Monte Carlo method. Consequently it is not enough for investigating spectroscopic study of nuclear structure. In a glance, Quantum Monte Carlo method and exact diagonalization seems to be incompatible each other because they are based on completely different principles. However, we combine advantages both of methods and develop a new method called *Quantum Monte Carlo Diagonalization (QMCD) method* [3]-[6]. In this article, first we outline this new method and then present the feasibility of the large-scale shell model calculations by this method.

The ground state energy E_g can be written as

$$E_g = \lim_{\beta\to\infty} \frac{\langle\Psi| H e^{-\beta H} |\Psi\rangle}{\langle\Psi| e^{-\beta H} |\Psi\rangle} \tag{1}$$

where H is a Hamiltonian and $|\Psi\rangle$ is an arbitrary wave function which is not orthogonal to the ground state. The $e^{-\beta H}$ is a ground state projector with a sufficient large β and the ground state is expressed as,

$$|\Psi_g\rangle = \lim_{\beta\to\infty} e^{-\beta H} |\Psi\rangle . \tag{2}$$

In general, Hamiltonian consists of the one and two body interactions. The latter causes the difficulty in treating Quantum many-body problem. If we treat it as two-body interaction, exact diagonalization is inevitable and the ground state projection is often realized by the Lanczos method. In turn, if we can treat the Hamiltonian as an effective one-body interaction, there exist two approaches. One is a well-known mean-field approach. The other is an auxiliary field approach. The SMMC and QMCD methods utilize this auxiliary field approach, by which $e^{-\beta H}$ can be shown by the sum of the $e^{-\beta h(\sigma)}$ where $h(\sigma)$ is one-body Hamiltonian parameterized by the auxiliary field σ. In the SMMC method, the ground state energy is evaluated by the Monte Carlo integration over σ. As the action of $e^{-\beta h(\sigma)}$ to Slater determinant keeps form of Slater determinant, we can count the number of Slater determinant in the SMMC calculation. In the typical SMMC one [2], the ground state energy can be expressed by several thousand Slater determinants. In a sense, these Slater determinants can be considered to be potentially good basis for describing the ground state. Then, we proposed the diagonalization of the Hamiltonian evaluated by these Slater determinants [3]. For better efficiency of this method, we utilize a mean-field knowledge and consider stochastic methods and explicit treatment of symmetries. Details of the QMCD method are presented in Refs [3]-[6].

To what extend the QMCD method can describe exact wavefunctions is an important problem. We have examined the validity of the QMCD method for the shell model calculations of the sd-shell nuclei where the

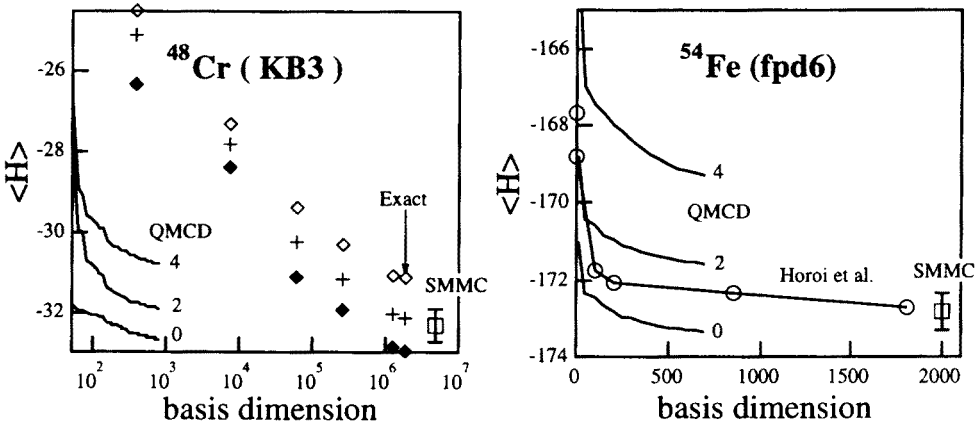

Fig. 1. Energies of lowest three states of ^{48}Cr and ^{54}Fe plotted as a function of the basis dimension. The results of the QMCD method are plotted by lines, In the left figure, the results of the QMCD method are compared to those of the exact and truncated shell model calculations. In the right figure, the results of the QMCD method are compared to those of the stochastic truncation method which are shown by symbols and lines. The SMMC results are also shown by open square with an error bar.

exact solutions are known. This has been reported in Ref. [5], and is not reported here. Instead, we then proceed to full pf shell calculations, which is a crossover region between the conventional shell model diagonalization and the QMCD calculation. The largest calculation [7] which has been carried out by the conventional shell model diagonalization is for ^{48}Cr with the KB3 interaction [8]. Figure 1 shows the energies of several low-lying states obtained by the QMCD method, conventional shell model diagonalization [7], and the SMMC method [2]. In the results of conventional shell model diagonalization, different dimensions mean the different truncation schemes. The maximum number of particles allowed to jump from the $f_{7/2}$ orbit to the remaining ones, denoted t, is given in each truncation differently. In this figure results for t=0,1,2,3,5 are shown as well as the exact result (*i.e.* t=8). The SMMC result corresponds to the finite temperature T=0.5MeV, and is plotted near the exact results since we cannot define the dimension for the SMMC calculations. We can see that the QMCD method gives energies with rather good quality by taking only 600 basis states.

Next we compare the QMCD method to other stochastic methods for ^{54}Fe nuclei. Although there is no exact calculation for this nuclei, two stochastic methods evaluated the ground state energy of ^{54}Fe nuclei with

the FPD6 interaction [9]. One is a method proposed by Horoi *et al.* [1]. They truncate the shell model basis based on the unperturbed energies of the basis states and on the constancy of their spreading widths. Consequently the JT dimensions of the order of a few times 10^6 are reduced to a few times 10^3. The other is the SMMC method. As a realistic interaction includes both good and bad parts for sign-problem, we need an extrapolation method for extracting physical quantities. In this case, the estimated ground state energy is shown within a certain error bar [2]. Note that the QMCD method is free of sign-problem, it can handle any realistic interaction without any problem. We also evaluate the same nuclei with the same interaction by the QMCD method. In the present calculation, the M-projected QMCD basis is utilized [4]. Fig.1 shows the results of above three methods. As the lowest energy of the deformed Hatree Fock method in the same shell model configuration is -167.622 MeV, above three methods are found to include certain correlations for the ground state. However, in the view of variation principle, the QMCD method offers the best value among them. Furthermore, one sees that the QMCD method can describe excited states too. Although we do not mention in this short article, we can evaluate the B(E2), Q moment and so on. As the application of the present QMCD method, the results of Ge and Mn nuclei were presented in my talk, but these issues will be reported in the forthcoming paper.

In summary, we present the QMCD method, which is a diagonalization method by the bases generated by the auxiliary field Monte Carlo method. It is reported that the present QMCD method is superior to other stochastic methods. The present method is useful for the large-scale shell model calculations and will be contributed for analysis of experimental data from recent high sensitivity gamma ray detectors.

REFERENCES

[1] M.Horoi, B.A.Brown, V.Zelevinsky, *Phys. Rev.* **C50**, R2274 (1994).

[2] S.E. Koonin, D.J. Dean, K. Langanke, to be published in *Phys. Rep.*; W.E. Ormand, *et al.*, *Phys. Rev.* **C49**, 1422 (1994); C.W. Johnson *et al.*, *Phys. Rev. Lett.* **69** (1992) 3147; K. Langanke, D.J. Dean, P.B. Radha, Y. Alhassid, S.E. Koonin, *Phys. Rev.* **C52**, 718 (1995).

[3] M.Honma, T.Mizusaki, T.Otsuka, *Phys. Rev. Lett.* **75**, 1284 (1995).

[4] T. Mizusaki, M. Honma, T. Otsuka, *Phys. Rev.* **C53**, 2786 (1996).

[5] Otsuka, M. Honma, T. Mizusaki, Proceedings of the Workshop on Comtemporary Nuclear Shell model, 29-30 April, 1996, Drexel University, USA, to be published in *Lecture Notes in Physics*, Springer-Verlag.

[6] M. Honma, T. Mizusaki, T. Otsuka, *Phys. Rev. Lett.* **77**, 3315 (1996).

[7] E. Caurier, A.P. Zuker, A. Poves, G. Martinez-Pinedo, *Phys. Rev.* **C50**, 225 (1994); Private communication with Poves.

[8] A. Poves, A. Zuker, *Phys. Rep.* **70**, 235 (1981).

[9] W.A. Richter, M.G. van der Merwe R.E. Julies, B.A. Brown, *Nucl. Phys.* **A523**, 325 (1991)