Monte-Carlo Study of Bound States in Few-Nucleon System — Method of Continued Fractions —

by

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abstract

Monte-Carlo method has been widely applied to study of the nuclear many-body systems. There exist several methods of Monte-Carlo calculations: The variational Monte-Carlo method (VMC) and Green's function Monte-Carlo method (GFMC) are used to study of the ground state properties of light nuclei by using the realistic nuclear force, while the shell-model Monte-Carlo method (SMMC) and the quantum Monte-Carlo diagonalization (QMCD) are used for medium and heavy nuclei whose structure can be described by the shell-model. Except QMCD, the diagonalization method, all the Monte-Carlo methods are applicable to only the ground state of the system. This is because VMC is based on the variational principle, and GFMC and SMMC, on the imaginary-time evolution method.

The aim of the present paper is to propose a new type of Monte-Carlo method which enables us to calculate the excited state properties of the many-body system. It consists of the method of continued fractions (MCF) and Monte-Carlo random walk for the multi-dimensional integration. Convergence of MCF and its accuracy are studied in detail for the one-dimensional model. As an application to the realistic problem, we study the ground state of the ^{4}He nucleus by using the Volkov potential. It is shown that our results on the ground state are in good agreement with those of previous works in different formalisms in the four-body system. This would imply that the present method opens a new world in the study of the many-body nuclear system.

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1 Introduction

Nuclei are isolated system of an ensemble of many, but finite number of nucleons interacting with each other through the nuclear force, and reveals many different aspects of their structure from nuclei to nuclei. They are really quite interesting objects as the quantum many-body systems. Although at this point the nuclear system looks very similar to the atomic system, there are many different points: 1) Nuclear force is strong and short-range, while the Coulomb force is weak and long-range. 2) Nuclear force is dominantly two-body force, but three-body and many-body forces possibly exist, while the Coulomb force in atoms is two-body force. 3) The structure of nuclear force has not been understood very well, while the Coulomb force is well understood. 4) Nucleus has no massive center, while center of atomic mass is, in a good approximation, a nucleus. Due to these features, the nuclear physics provides many branches of its study in fundamental and phenomenological ways, i.e., nuclear force and few-body system, cluster-model, shell-model structure, collective motions, fission, exotic elements, meson-nuclear physics, quark-nuclear physics and so on, and has revealed many characteristic features that do not exist in atomic physics.

1.1 Background

From the fundamental points of view, the nuclear force is a kind of the effective interactions, which should be derived from the QCD theory, but is yet far from its goal. At present, two-body force has been rather understood theoretically and experimentally except for the short-range region, but our knowledge of many-body force is very limited, due to the experimental difficulties. Therefore, the study of many-body force is necessarily reduced to the study of the nuclear bound states and limited kinds of nuclear reactions. Furthermore, through the studies of complex nuclei, it has been clarified that the conventional two-body force is not attractive enough to reproduce the the binding energy of nuclei. This seems to require the many-body force. For this purpose, it is very important to find a way which enables us to treat the nuclear (few-body) system in exact ways. This opened the research field of the few-body system.

The standard methods to study the three- or four-nucleons systems were developed and now are known as the Faddeev and Faddeev-Yakubovsky (FY) equations, respectively. In FY method, the Hamiltonian and the wave function relevant to the system are decomposed into three subsystems. Generally, the maximum angular momentum of the subsystems is not limited, that is, it takes a value up to infinity. If it is allowed to treat the wave function with any values of angular momentum, this method, in principle, will give us exact results. Although,in the actual case, the maximum value of the angular momentum of the subsystem is obliged to be limited to any several units of $\hbar$, FY method gives highly accurate binding energy of the ground state of ^{4}He when we adopt the

realistic spin-dependent nuclear force with a hard core [1]. Convergence of the energy of the ground state of ^{4}He is slow, but it is achieved within the maximum angular momentum of $l^{\max} = 6$. In spite of this success, FY method requires us a complex decomposition of the wave function. Furthermore, for nuclei with mass number $A \geq 5$ the two-body force is not strong enough to reproduce the observed binding energy of nuclei. To include the three-body force in FY method, a special technique is also required. In this way, it seems not practical to extend the theory such as FY method to any complex nuclei. We must develop any methods which may work at least for light nuclei under the realistic nuclear force and possible many-body force, and also enables us to calculate the excited states as well as the ground state of nuclei. This would open a new sight to the nuclear physics 'far from stable line'.

On the other hand, from the phenomenological points of view, we have some reliable nuclear models, such as cluster-model, shell-model and collective model with phenomenological two-body force. (This is not the same as the two-body force in the nucleon-nucleon scattering.) Essential point in these is that the feature of the short-range and exchange force brings us various kinds of nuclear structure and excitation mode. This implies that we are required to treat the nuclear system much more in detail, which, we hope, will show new aspects of nuclear structure. As the number of nucleons N increases, the computational time grows up as $\mathcal{O}(M^{3N})$ where M is number of typical mesh points at each dimension. Therefore, the standard numerical integration method becomes almost impossible to carry out in many-body problems.

1.2 Monte-Carlo approach

Against the above situations, a stochastically numerical approach, Monte-Carlo method may overcome this difficulty under the recent development of the computer with high speed calculation and large capacity of memory. Monte-Carlo method has been widely applied even to the study of nuclear structure from light to heavy nuclei.

The recent methods applied to nuclear few-body systems are variational Monte-Carlo method (VMC) and Green's function Monte-Carlo method(GFMC). These have been developed mainly by J. Carlson *et al.* [2, 3, 4, 5]. The results for $A \leq 7$ nuclei are reviewed in Ref. [6]. VMC and GFMC have been applied to the study of the ground state properties of nuclei with mass number of $A \leq 7$ with realistic potential [6]. It is now well known that the three-body force is required to reproduce the observed binding energy of these nuclei. First of all, VMC was applied to study of the ground state properties of ^{3}H, ^{3}He and ^{4}He by taking into account three-body force [2] in addition to the Urbana v_{14} two-body force [7]. Here, the three-body force used is rather realistic force with two-pion-exchange and repulsive core. The calculated binding energies are in agreement with the observed data with accuracy of a few percent. In VMC, the variational principle

was applied to search the energy minimum for the trial wave function, in which Metropolis method is used to calculate the nuclear matrix elements. In recent study for light nuclei [6], GFMC was found to give the correct binding energy by using the Argonne v_{18} two-body force [8] and the Urbana IX three-body force [2]. GFMC uses a variational wave function obtained by VMC as a starting trial function, since the VMC trial function is already good approximate function of the eigen state. Then, the imaginary-time evolution $e^{-\tau H}$ is carried out by quantum Monte-Carlo random walk, where imaginary-time evolution operator i.e. Green's function is taken as random walk kernel, and it makes use of the property of diffusion equation. The operation of GFMC time evolution extracts the true ground state from the trial wave function. In light p-shell nuclei, $A = 5$ nuclei is unbound and $A = 6, 7$ nuclei have few excited unbound states with narrow width. The ground state of ^{6}He $(J^\pi; T) = (0^+; 1)$ can be regard as a bound state, since it has a mean life time 807ms, and its 1-st excited state $(0^+; 1)$ has a width of 113keV. The ground state of ^{6}Li $(1^+; 0)$ is stable, and the 1st-, 2nd-, and 3rd-excited states $(3^+; 0), (0^+; 1), (2^+; 0)$ have a width 24keV, 8.2eV, and 1.7MeV respectively. ^{6}Be $(0^+; 1)$ state has a width 92keV. Then, GFMC calculations were performed by assuming these state as bound states. Calculations for $A = 7$ nuclei were performed in a similar way. The results were shown to be generally in good agreement with experimental values. In particular, the binding energy of the ground states of ^{3}He, and ^{4}He were completely reproduced.

For p-shell nuclei, although the absolute values of the ground state energies are still underestimated, relative energy spacings of low-lying excited state with different spin-isospin quantum numbers from those of the ground state were reproduced. Difference of the absolute binding energies between the theory and experiment would be reduced to ambiguities in three-body force, because the difference is much smaller than the expectation value of three-body force. Even though GFMC seems, at a moment, to be a powerful tool for the study of the bound states of light nuclei, it is limited to the calculation of the ground state.

For the states of the medium and heavy nuclei which are regarded to be described by the shell-model, the Shell-Model Monte-Carlo (SMMC) was proposed by S. E. Koonin *et al* [9] and has been widely applied to the study of the ground states of *sd*-shell [10] and *fp*-shell nuclei [11, 12]. This method is a kind of thermal cooling for obtaining the exact ground state energy with a partition function $\hat{\mathrm{T}}\mathrm{r}[\exp(-\tau\hat{H})]$, $\hat{H}$ being the shell-model Hamiltonian, and is, in fact, the method with the same restriction as that of GFMC.

Nevertheless, it is possible to calculate the excited state properties by using the Monte-Carlo method. A possible way is to use Monte-Carlo method as an integration process or as to pick up an important part stochastically, but not to use projection $\exp(-\tau\hat{H})$ directly. This kind of method is the matrix diagonalization by the bases distributed with the quantum Monte-Carlo method, known as QMCD (Quantum Monte-Carlo Diagonalization) in the large scale shell-model calculation[13, 14, 15]. In shell-model calculation, the number of basis for valence-

nucleon in Hilbert space increases drastically. For example, the number of basis are up to $1.0 \times 10^5 \sim 2.0 \times 10^6$ for pf-shell of $A = 48$ nuclei in m-scheme [16]. QMCD can reduce number of basis drastically. The basis are generated stochastically by using auxiliary field Monte-Carlo technique as in SMMC, and only the important part of Hilbert space are picked up. Then the number of basis is reduced to $\sim 1.0 \times 10^3$ for ^{64}Ge nuclei, while the number of full m-scheme basis of $M = 0$ is 1,087,455,228 [15]. The Hamiltonian within the truncated space is diagonalized so that the energy spectra of the excited states are obtained. It is noticed that this method cannot be applied to light nuclei, because the effective nuclear force is assumed to non-singular, i.e., the force without hard core which the realistic force provides with.

1.3 A new approach of Monte-Carlo method

The purpose of the present paper is to propose a new Monte-Carlo method, as an attempt to study the excited states of light nuclei with realistic nuclear forces by Monte-Carlo method. We put the Method of Continued Fractions (MCF) as a central part in the new formalism. This method doesn't limit our calculation to the ground state properties of nuclei. MCF in nuclear physics was originally proposed by Sasakawa *et al.* [17] as a fast calculational method for evaluating the T-matrix elements for three-nucleon system. The wave functions of higher order defined in MCF are generated so as to be orthogonal to those of lower order. Then, the matrix elements calculated by these wave functions rapidly converge against iteration procedure. MCF is also applicable to the bound state problem with a little modification of the original method. It is noted that MCF method is also applicable to the study of the excited states by using the Monte-Carlo evaluation, because this method does not use projection procedure to the ground state component which is in contrast to GFMC. Moreover, this method, in principle, does not pose any restrictions on the starting trial wave function and also nuclear force to be used.

In this paper, we carry out a first try to apply MCF with Monte-Carlo calculation to the excited states of few-nucleon bound states. Our calculation is performed in the following points of view: 1) We carry out calculations by regarding the binding energy as a parameter, and determine the bound state energy by searching the parameters so as to make a expectation value of a certain operator which vanishes for the correct binding energy. 2) The integrations in MCF which include the free Green's function can be performed by the random walk of quantum Monte-Carlo technique. Therefore, we expect that our method will be a useful and powerful tool for studying few-nucleon system.

During the calculation, the wave functions of MCF are generated by using their orthogonality condition to those of lower order. This process is carried out by random walk of method. However, the random walk of points which have positive and negative signs meets what is called "sign problem". This problem

is deeply lying in quantum Monte-Carlo method, and induces large errors in the matrix elements calculated by these wave functions. To avoid this problem, we introduce the "multiple cancellation" method [18] in the random walk procedure.

As a test of our method, we adopt a simple one-dimensional potential model which produces three bound states. We calculate the bound state energies and shapes of wave function of three bound states. As a realistic example, we study $A = 4$ nuclei with Volkov potential [19]. We obtain successful results for both of the examples.

This paper is organized as follows. In section 2, we briefly review various Monte-Carlo methods mentioned above developed in nuclear physics. Then, in section 3 we give a formalism for the nuclear bound state problem by the method of continued fractions, and in section 4, show a method of Monte-Carlo random walk how to perform the calculations obeying method of continued fractions. In section 5, at first we apply the present method to one-dimensional problem and examine the convergence and accuracy of the calculated results. Next, we calculate the energy of the ground state of ^{4}He nucleus by adopting the Volkov potential and discuss our results by comparing with other works. Summary and conclusion are given section 6.

2 Brief review of various Monte-Carlo methods

We will briefly review various Monte-Carlo methods applied and developed in nuclear physics. There are different fields of nuclear physics where Monte-Carlo methods have been developed.

One is to study the few-nucleon system exactly with the realistic nuclear interactions. Variational Monte-Carlo (VMC) and Green's function Monte-Carlo (GFMC) belong to this field. These works have been developed by J. Carlson *et al.* in the study of $A \leq 7$ nuclei. VMC is most primitive application of Monte-Carlo method. It uses variational principle to obtain the ground state wave function in which Monte-Carlo method is applied for generating the weight by Metropolis random walk procedure. GFMC is a type of diffusive quantum Monte-Carlo method. Starting from a trial function, the ground state wave function is extracted by time evolution $e^{-\tau H}$. Obviously, these methods are restricted to the study of the ground state of the system.

The other is the shell-model study in the medium and heavy nuclei. Shell-Model Monte-Carlo (SMMC) and Quantum Monte-Carlo Diagonalization (QMCD) belong to this field. SMMC is also diffusive type of calculation as GFMC. The time evolution operator is expanded by Hubbard-Stratonovich (HS) transformation to rewrite the two-body operator into one-body operator form. The ground state energy is extracted by the time evolution. It is distinguished from the other methods, QMCD can evaluate the excited states properties. It requires diagonalization of Hamiltonian to calculate the eigen values. Monte-Carlo method is utilized only for choosing stochastically the basis of diagonalization. QMCD successfully reduces the number of basis.

2.1 Variational Monte-Carlo

VMC is a method of variational calculation for finding the minimum expectation value of Hamiltonian with varying parameters of a trial function $|\Psi_T\rangle$. Hence the accuracy of the solution depends on the functional form of the trial function to be adopted.

The simplest form of the trial function is Jastrow type $|\Psi_J\rangle$. It is constructed by shell-model wave function $|\Phi\rangle$ and the correlation functions f^c which depend only on the relative distance between nucleons and include variational parameters.

For s-shell nuclei, the spatial part of the trial function can be taken to be symmetric. It is expressed as,

$$|\Psi_J\rangle = \left[\prod_{i<j<k} f^c_{ijk}\right]\left[\prod_{i<j} f^c_{ij}\right]|\Phi_A(JMTT_3)\rangle \ . \tag{2.1}$$

Here f^c_{ij} and f^c_{ijk} are two- and three-body correlation functions, respectively, and the shell-model wave function is antisymmetrized as

$$|\Phi_3(\tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2})\rangle = \mathcal{A}|p\uparrow p\downarrow n\uparrow\rangle \quad \text{for } {}^3\text{He} \ , \tag{2.2}$$

and

$$|\Phi_4(0000)\rangle = \mathcal{A}|p\uparrow p\downarrow n\uparrow n\downarrow\rangle \quad \text{for } {}^4\text{He} \ , \tag{2.3}$$

where $\mathcal{A}$ is an antisymmetrizer.

For p-shell light nuclei ($A = 6, 7$), Jastrow type $|\Psi_J\rangle$ is also taken as

$$|\Psi_J\rangle = \mathcal{A}\left\{\left[\prod_{i<j<k} f^c_{ijk}\right]\left[\prod_{i<j} f^c_{ij}\right]|\Phi_A(JMTT_3)\rangle\right\} \ . \tag{2.4}$$

Here the different form of three-body correlation function f^c_{ijk} should be taken depending on whether the correlated nucleons i, j and k are in the same shell sss, or different shells ssp, spp, ppp (ppp is only for $A = 7$ nuclei). The shell-model wave function in Eq.(2.4) is constructed on the α particle i.e. ^{4}He nuclei and nucleon in p-shell. For example, the form of the wave function $|\Phi_6(JMTT_3)\rangle$ for $A = 6$ is as follows:

$$\begin{aligned}|\Phi_A(JMTT_3)\rangle = \mathcal{A}[\Psi_\alpha(00)\psi_p(r_{5,\alpha})\psi_p(r_{6,\alpha})] \times \\ \sum_{L,S}\beta_{JLS}\left[[Y_l(\Omega_{5,\alpha})Y_l(\Omega_{6,\alpha})]_L[\chi_5\chi_6]_S\right]_{JM} \times [\eta_5\eta_6]_{T,T_3} \ .\end{aligned} \tag{2.5}$$

Here χ_i and η_i denote spin and isospin function of i-th nucleon, respectively.

To improve the trial function furthermore, one must include correlation terms which include spin and isospin degrees of freedom. As a simple expression, the trial function is written as follows:

$$|\Psi_T\rangle = \left[\mathcal{S}\prod_{i<j<k} F_{ijk}\right]\left[\mathcal{S}\prod_{i<j} F_{ij}\right]|\Psi_J\rangle \ . \tag{2.6}$$

Here, $\mathcal{S}$ is symmetrizer and F_{ij} and F_{ijk} are correlation functions which include functions whose form is similar to the potential of two- and three-body, respectively.

Two-body correlation term F_{ij} reflects the short- and medium-range part of nuclei. A typical form of F_{ij} is parameterized as follows:

$$F_{ij} = \left[1 + \sum_{m=2,8} u_m(r_{ij})O^m_{ij}\right] \ . \tag{2.7}$$

It depends on the interaction between inter nucleon O^m_{ij},

$$O^m_{ij} = [1, \sigma_i\cdot\sigma_j, S_{ij}, (\boldsymbol{L}\cdot\boldsymbol{S})_{ij}]\otimes[1, \tau_i\cdot\tau_j] \ . \tag{2.8}$$

Here, the function u_{ij} in Eq.(2.7) also includes the variational parameters. and the dependence of u_{ij} upon the pair distance r_{ij} is obtained as a solution of Schrödinger-like equation in the various two-body channels.

In principle, the structure of the three-nucleon correlations F_{ijk} can be quite complicated. The most important correlation is of the three-body type like V_{ijk}, and it is assumed to be

$$F_{ijk} = 1 - \beta V_{ijk} \tag{2.9}$$

where β is a variational parameter.

Once the form of the trial function is fixed, we must carry out the parameter search of the trial function so as to make the expectation value of Hamiltonian minimum. In VMC calculation, we use Metropolis random walk method [20] to generate the distribution with a probability density $W(R)$. $W(R)$ is a positive definite weight function and, usually it is chosen as an absolute value of probability of the trial function,

$$W(R) = |\langle \Psi_T(R) | \Psi_T(R) \rangle| \ . \tag{2.10}$$

Here R represents the coordinates of all nucleon and sums over the spin and isospin degrees of freedom assume to be already done.

Once we obtained the optimum (approximately exact) eigen function, we can estimate the expectation values of any types of operators $\hat{O}$ as follows:

$$\langle \hat{O} \rangle = \frac{\int dR \langle \Psi_T(R) | \hat{O} | \Psi_T(R) \rangle}{\int dR \langle \Psi_T(R) | \Psi_T(R) \rangle} \approx \frac{\sum_i \langle \Psi_T(R_i) | \hat{O} | \Psi_T(R_i) \rangle / W(R_i)}{\sum_i \langle \Psi_T(R_i) | \Psi_T(R_i) \rangle / W(R_i)} \ . \tag{2.11}$$

Off-diagonal observables, such as momentum distributions, can be similarly evaluated. They simply require an additional integration variable corresponding to the off-diagonal displacement. Experimental quantities of interest include charge and magnetic form factors, sum rues, and so on.

Variational principle ensure that we can obtain the upper bound of binding energy for the ground state of Hamiltonian with varying the variational parameters in the trial function. Simultaneously, we can also obtain the ground state wave function with analytic functional form. However, it is obvious that the calculatable observables are restricted to the only ground state for given spin-isospin channel.

2.2 Green's function Monte-Carlo

Green's function Monte-Carlo (GFMC) is a diffusive method to project out the ground state of Hamiltonian with imaginary-time time evolution. Starting from a trial function $|\Psi_T\rangle$ which is not orthogonal to the ground state, the time developed wave function $|\Psi(\tau)\rangle$ converges into the ground state wave function $|\phi_0\rangle$:

$$|\Psi(\tau)\rangle = \lim_{\tau \to \infty} \exp(-\tau H) |\Psi_T\rangle$$

$$= \lim_{\tau\to\infty} \sum_n \exp(-\tau E_n)|\phi_n\rangle\langle\phi_n|\Psi_T\rangle$$
$$\Rightarrow \exp(-E_0\tau)|\phi_0\rangle \ . \tag{2.12}$$

The main task of GFMC is the iteration of infinitesimal time step $\Delta\tau$ until the wave function converges into the ground state,

$$|\Psi(\tau+\Delta\tau)\rangle = \exp(-\Delta\tau H)|\Psi(\tau)\rangle \ . \tag{2.13}$$

The infinitesimal time development is carried out with the propagator induced by imaginary time evolution operator $\exp(-\Delta\tau H)$.

At first, we consider a spin-isospin independent Hamiltonian with two-body central potential $V(r_{ij})$,

$$\begin{aligned} H &= T + V \\ &= -\frac{\hbar^2}{2m}\sum_{i=1}^{A} \nabla^2_{\boldsymbol{r}_i} + \sum_{i<j} V(r_{ij}) \ . \end{aligned} \tag{2.14}$$

Then the infinitesimal time $\Delta\tau$ propagator is written as follows:

$$\begin{aligned} \langle \boldsymbol{R}|\exp(-\Delta\tau H)|\boldsymbol{R}'\rangle &\equiv G(\boldsymbol{R},\boldsymbol{R}';\Delta\tau) \\ &= \langle \boldsymbol{R}|\exp(-\Delta\tau\{T+V\})|\boldsymbol{R}'\rangle \\ &\approx \langle \boldsymbol{R}|\exp(-\Delta T)|\boldsymbol{R}'\rangle\langle \boldsymbol{R}'|\exp(-\Delta V)|\boldsymbol{R}'\rangle \\ &= G_0(\boldsymbol{R}-\boldsymbol{R}')\exp(-\Delta V(\boldsymbol{R}')) \ . \end{aligned} \tag{2.15}$$

Here, $\boldsymbol{R}$ represent A-nucleon coordinates, $\boldsymbol{R}:\{\boldsymbol{r}_1,\boldsymbol{r}_2,\cdots,\boldsymbol{r}_A\}$, and $G_0(\boldsymbol{R}-\boldsymbol{R}')$ is the free one-body imaginary-time propagator, given by

$$G_0(\boldsymbol{R}-\boldsymbol{R}') = N_0 \prod_{i=1}^{A} \exp\left[-m\frac{(\boldsymbol{r}_i-\boldsymbol{r}_i')^2}{2\Delta\tau}\right] \ , \tag{2.16}$$

where N_0 is a normalization factor. This equation is valid for $\mathcal{O}(\Delta\tau^2)$. The infinitesimal time evolution is carried out by random walk form $\boldsymbol{R}'$ to $\boldsymbol{R}$ with the Gaussian probability distribution in Eq.(2.16). The potential term, $\exp(-\Delta V(\boldsymbol{R}'))$, is regarded as a "weight" at point $\boldsymbol{R}$. Therefore the imaginary-time evolution operator for τ is written as

$$\begin{aligned} \langle \boldsymbol{R}_M;\tau|\exp(-\tau H)|\boldsymbol{R}_0;0\rangle &= \langle \boldsymbol{R}_M;\tau|\exp(-\Delta\tau H)|\boldsymbol{R}_{M-1}\rangle\langle \boldsymbol{R}_{M-1}|\exp(-\Delta\tau H)|\boldsymbol{R}_{M-2}\rangle \times \\ &\quad \ldots \times \langle \boldsymbol{R}_1|\exp(-\Delta\tau H)|\boldsymbol{R}_0;0\rangle \\ &= \prod_{n=1}^{M} G(\boldsymbol{R}_n,\boldsymbol{R}_{n-1};\Delta\tau) \ , \end{aligned} \tag{2.17}$$

where $\boldsymbol{R}_n$ represents the coordinates at the time $\tau = n\Delta\tau$. Hence starting from a trial function $|\Psi_T(\boldsymbol{R}_0);0\rangle$, time developed wave function $|\Psi(\boldsymbol{R};\tau)\rangle$ is obtained

as

$$|\Psi(\boldsymbol{R});\tau\rangle = \int d\boldsymbol{R}_0 \cdots d\boldsymbol{R}_M G(\boldsymbol{R},\boldsymbol{R}_n;\Delta\tau) \prod_{n=1}^{M} G(\boldsymbol{R}_n,\boldsymbol{R}_{n-1};\Delta\tau)|\Psi_T(\boldsymbol{R}_0);0\rangle \ . \tag{2.18}$$

Integrations on $d\boldsymbol{R}_0 \cdots d\boldsymbol{R}_M$ are replaced by the Gaussian random walk in Eq.(2.16).

For more realistic case, Hamiltonian includes the spin-isospin dependence, non-local forces and three-nucleon potentials. Its random walk kernel from $\boldsymbol{R}$,χ to $\boldsymbol{R}'$,χ' becomes complicated form [6], and is approximated as follows:

$$\begin{aligned}\langle \boldsymbol{R}',\chi'|\exp(-H\Delta\tau)|\boldsymbol{R},\chi\rangle \equiv G(\boldsymbol{R}',\boldsymbol{R};\Delta\tau) \approx \left[\prod_{i=1,A} G_{0,i}(|\boldsymbol{r}_i - \boldsymbol{r}_i'|)\right] \\ \times \sum_{\chi_1,\chi_2} \langle\chi'|\left[1 - \frac{\Delta\tau}{2}\sum_{i<j<k} V_{ijk}(\boldsymbol{R}')\right]|\chi_1\rangle\langle\chi_1|\mathcal{S}\prod_{i<j}\left[\frac{g_{ij}(\boldsymbol{r}_{ij}',\boldsymbol{r}_{ij})}{g_{0,ij}(\boldsymbol{r}_{ij}',\boldsymbol{r}_{ij})}\right]|\chi_2\rangle \\ \times\langle\chi_2|\left[1 - \frac{\Delta\tau}{2}\sum_{i<j<k} V_{ijk}(\boldsymbol{R})\right]|\chi\rangle \ ,\end{aligned} \tag{2.19}$$

where χ represents the spin-isospin states with A-nucleons, $G_{0,i}$ and $g_{0.ij}$ are the free one- and two-body imaginary-time propagator, respectively. The free propagator are of a simple Gaussian form as,

$$G_{0,i} = \mathcal{N}_1 \exp\left[-m\frac{(\boldsymbol{r}_i' - \boldsymbol{r}_i)^2}{2\Delta\tau}\right] \ , \tag{2.20}$$

$$g_{0,ij} = \mathcal{N}_2 \exp\left[-m\frac{(\boldsymbol{r}_{ij}' - \boldsymbol{r}_{ij})^2}{4\Delta\tau}\right] \ , \tag{2.21}$$

with normalization factors $\mathcal{N}_i$.

g_{ij} is the exact imaginary-time propagator, and it is a matrix in the two-body spin-isospin space and must be calculated numerically. The propagator satisfies the time-evolution equation,

$$\langle\chi_{ij}'|\left[\frac{\partial}{\partial\tau} + H_{ij}\right] g_{ij}(\boldsymbol{r}',\boldsymbol{r};\tau)|\chi_{ij}\rangle = 0 \tag{2.22}$$

where

$$H_{ij} = -(1/m)\nabla_{ij}^2 + v_{ij} \tag{2.23}$$

and χ_{ij} and χ_{ij}' stands for two-nucleon spin-isospin states. The g_{ij} also satisfies a boundary condition,

$$\langle\chi_{ij}'|g_{ij}(\boldsymbol{r}',\boldsymbol{r};\tau=0)|\chi_{ij}\rangle = \delta(\boldsymbol{r}-\boldsymbol{r}')\delta_{\chi_{ij}',\chi_{ij}} \ . \tag{2.24}$$

Once the infinitesimal time-evolution propagator $G(\boldsymbol{R},\boldsymbol{R}';\Delta\tau)$ is obtained, the time evolution is carried out in a similarly way to Eq.(2.18). Since the wave functions are vectors and propagator are matrices in spin-isospin space. In principle,

any set of paths can be taken to calculate the matrix elements or expectation values. However it is useful to perform the importance sampling to minimize the variance of calculation rather than taking "any" set of paths. The importance sampling is an acceleration technique to generate the configuration $\boldsymbol{R}$ into the importance function (weight) $I(\boldsymbol{R})$. Usually, the importance function is taken as probability density of the trial function with the sum of spin-isospin degrees of freedom,

$$I[\Psi_T(\boldsymbol{R}), \Psi(\boldsymbol{R},\tau)] = \left|\sum_\chi \langle\Psi_T(\boldsymbol{R})|\chi\rangle\langle\chi|\Psi(\boldsymbol{R};\tau)\rangle\right| + \epsilon \sum_\chi \left|\langle\Psi_T(\boldsymbol{R})|\chi\rangle\langle\chi|\Psi(\boldsymbol{R};\tau)\rangle\right| \tag{2.25}$$

where ϵ is a small positive coefficient. The second term ensures that all paths are allowed to take positive probability. The expectation values can be obtained similarly as in Eq. (2.11), and is evaluated between the trial function $|\Psi_T\rangle$ and time developed wave function with GFMC manner $|\Psi(\boldsymbol{R}_i;\tau)\rangle$ as

$$\langle\hat{O}\rangle \approx \frac{\sum_i \langle\Psi_T(\boldsymbol{R}_i)|\hat{O}|\Psi(\boldsymbol{R}_i;\tau)\rangle / I[\Psi_T(\boldsymbol{R}), \Psi(\boldsymbol{R},\tau)]}{\sum_i \langle\Psi_T(\boldsymbol{R}_i)|\Psi(\boldsymbol{R}_i;\tau)\rangle / I[\Psi_T(\boldsymbol{R}), \Psi(\boldsymbol{R},\tau)]} \,. \tag{2.26}$$

The matrix element in Eq. (2.26) is a "mixed" estimate. It is of the form,

$$\langle\hat{O}\rangle_{\rm mix} = \frac{\langle\Psi_T|\hat{O}\exp(-H\tau)|\Psi_T\rangle}{\langle\Psi_T|\exp(-H\tau)|\Psi_T\rangle} \,. \tag{2.27}$$

The value $\langle\hat{O}\rangle_{\rm mix}$ is the matrix element of the trial function and the true ground state obtained by GFMC calculation. The mixed estimate is sufficient to evaluate the ground state energy, since the Hamiltonian commutes with the propagator. Indeed, an upper bound to the true ground-state energy E_0 is obtained for any value of τ,

$$\langle H\rangle_{\rm mix} = \frac{\langle\Psi_T|\exp(-H\tau/2)H\exp(-H\tau/2)|\Psi_T\rangle}{\langle\Psi_T|\exp(-H\tau/2)\exp(-H\tau/2)|\Psi_T\rangle} \geq E_0 \,. \tag{2.28}$$

Of course, the actual convergence of calculation depends on the accuracy of the trial function $|\Psi_T\rangle$ and the structure of the spectrum of the Hamiltonian. The knowledge of the spectrum tells us that we can proceed the calculation only for a finite τ in light nuclei. For quantities other than the energy, one typically estimates the true ground-state expectation value by extrapolating from the mixed and variational estimates,

$$\langle\hat{O}\rangle \approx 2\langle\hat{O}\rangle_{\rm mix} - \frac{\langle\Psi_T|\hat{O}|\Psi_T\rangle}{\langle\Psi_T|\Psi_T\rangle} \,. \tag{2.29}$$

However, for momentum-dependent operators $\hat{O}$, the statistical fluctuations associated with this estimate can be quite large.

VMC provides upper bound of the energy and the approximately true wave function for the ground state. GFMC makes use of this wave function as a trial function. After time evolution according above description, the true ground state wave function is extracted out from the trial function due to $\exp(-\tau H)$. Therefore, GFMC calculation is also restricted to the ground state properties.

2.3 Shell-model Monte-Carlo

The medium and heavy nuclei are well described by the shell-model picture. Usually, the shell-model wave function is constructed by valence nucleon and hole in medium and heavy nuclei. However, the number of basis which is required for full diagonalization of the Hamiltonian increases so fast. Because the total number of states is 2^m with $m = 12$, 24,40 in the p-, sd- and pf-shells, respectively. It is obvious that a problem of this magnitude lies beyond the capability of computers at the present time. In this limitation, the traditional approach to circumvent it is *ad hoc* truncation on the number of basis. However, since the residual interaction is strong enough, calculations of this nature can be unreliable and significant re normalizations of the residual interaction and transition operators are required.

The Shell-model Monte-Carlo (SMMC) which was proposed by S. E. Koonin *et al.* [9] and has been developed to study the ground states of sd-shell [10] and fp-shell [11, 12] nuclei. This method can derive the exact ground state energy of the nuclear shell-model Hamiltonian. SMMC is a method of Monte-Carlo evaluation of the canonical expectation value of a operator $\hat{O}$ with finite temperature $1/\tau$ as

$$\langle \hat{O} \rangle = \frac{\hat{\mathrm{Tr}}[\hat{O}\exp(-\tau\hat{H})]}{\hat{\mathrm{Tr}}[\exp(-\tau\hat{H})]} \,. \tag{2.30}$$

Here, $\hat{\mathrm{Tr}}[\exp(-\tau\hat{H})]$ is the canonical partition function for fixed number of nucleons.

Suppose that the Hamiltonian is written in terms of "convenient" one-body operators $\hat{O}_\alpha$, as follows:

$$\hat{H} = \sum_\alpha \epsilon_\alpha \hat{O}_\alpha + \frac{1}{2}\sum_\alpha V_\alpha \hat{O}_\alpha^2 \,. \tag{2.31}$$

We can expand the time evolution operator by Hubbard-Stratonovich transformation [21]. Here, the Hamiltonian doesn't include the three-body or many-body potentials. The two-body potential term, $\frac{1}{2}\sum_\alpha V_\alpha \hat{O}_\alpha^2$, is obtained by the decomposition method from the original shell-model potential [9]. Although, any types of potentials can be used, the repulsive potential induces "sign problem" for $\hat{\mathrm{Tr}}[\exp(-\tau\hat{H})]$ which will be used as weight function [11].

The time evolution operator $\exp(-\tau\hat{H})$ is expressed by a product of the propagator with time slice so $\Delta\tau$,

$$\hat{U}(\tau) \equiv \exp(-\tau\hat{H}) = \left[\exp(-\Delta\tau\hat{H})\right]^{N_t} \,, \tag{2.32}$$

where $\tau = N_t \Delta\tau$. The infinitesimal time evolution operator $\exp(-\Delta\tau\hat{H})$ contains the two-body operator in $\hat{H}$. This fact makes it difficult to evaluate the time evolution operator. Fortunately, by applying the HS transformation with the auxiliary field $\sigma_{\alpha n}$, we can express the infinitesimal time evolution operator in the form which contains only one-body operator, shown as

$$\exp(-\Delta\tau\hat{H}) \simeq \int_{-\infty}^{\infty} \prod_{\alpha} d\sigma_{\alpha n} \left(\frac{\Delta\tau|V_\alpha|}{2\pi}\right)^{\frac{1}{2}} \times \exp\left\{-\Delta\tau\left(\sum_{\alpha}\frac{1}{2}|V_\alpha\sigma_{\alpha n}^2| + \epsilon_\alpha\hat{O}_\alpha + s_\alpha V_\alpha\sigma_{\alpha n}\hat{O}_\alpha\right)\right\} \quad (2.33)$$

Here, s_α is related with the sign of the potential in the original Hamiltonian, and it takes

$$s_\alpha = \pm 1 \text{ for } V_\alpha < 0 \ , \quad \text{and} \quad s_\alpha = \pm 1 \text{ for } V_\alpha > 0 \ .$$

Finally, the imaginary time evolution operator $\hat{U}(\tau)$ is given as an integral of the functional of the one-body operator $\hat{h}_\sigma(\tau_{t_n})$ in auxiliary field $\{\sigma\}$:

$$\hat{U}(\tau) = \left[\exp(-\Delta\tau\hat{H})\right]^{N_t} \simeq \int \mathcal{D}^{N_t}[\sigma] G(\sigma) \exp[-\Delta\tau h_\sigma(\tau_{N_t})] \cdots \exp[-\Delta\tau h_\sigma(\tau_1)] \ , \quad (2.34)$$

with

$$\mathcal{D}^{N_t}[\sigma] = \prod_{n=1}^{N_t} \prod_{\alpha} d\sigma_{\alpha n} \left(\frac{\Delta\tau|V_\alpha|}{2\pi}\right)^{\frac{1}{2}} \ , \quad (2.35)$$

where the Gaussian measure of auxiliary field is given by

$$G(\sigma) = \exp\left(-\sum_{\alpha n}\frac{1}{2}|V_\alpha|\sigma_{\alpha n}^2\right) \ , \quad (2.36)$$

and, one-body operator $\hat{h}_\sigma(\tau_{t_n})$,

$$\hat{h}_\sigma(\tau_{t_n}) = \sum_{\alpha}(\epsilon_\alpha + s_\alpha V_\alpha\sigma_{\alpha n})\hat{O}_\alpha \ . \quad (2.37)$$

The HS transformation enables us to calculate easily the weight function $\zeta(\sigma)$,

$$\zeta(\sigma) \equiv \hat{\mathrm{Tr}}[\hat{U}_\sigma(\tau)] \ . \quad (2.38)$$

For a set of auxiliary field $\{\sigma\}$, the calculation of the matrix element (2.30) is carried out by the integration for auxiliary fields $\{\sigma\}$:

$$\langle\hat{O}\rangle = \frac{\int \mathcal{D}[\sigma] G(\sigma)\langle\hat{O}(\sigma)\rangle\zeta(\sigma)}{\int \mathcal{D}[\sigma] G(\sigma)\zeta(\sigma)} \quad (2.39)$$

In order to evaluate Eq.(2.39) by Monte-Carlo method, we need the weight function W_σ to generate $\{\sigma\}$. The weight function W_σ must be normalized and chosen positive definite. Then we choose it as follows:

$$W_\sigma = |G(\sigma)\zeta(\sigma)| \ . \tag{2.40}$$

To generate $\{\sigma\}$ with the weight W_σ, the Metropolis random walk method [20] is most appropriate.

In thermal approach, we can calculate only the expectation values on the ground states. It is due to imaginary-time evolution $\exp(-\tau\hat{H})$ in the partition function.

2.4 Quantum Monte-Carlo diagonalization

SMMC successfully calculate the expectation value on the ground state in nuclear shell-model nuclear. It uses thermal approach which includes $\exp(-\tau\hat{H})$ in its partition function. This term strongly project out the ground state component for large τ, hence this projection, as similar to GFMC, prevents us to study the excited state of Hamiltonian.

The excited state properties may be studied by the non-projection method. Diagonalization of Hamiltonian is one of the most plausible ways. Quantum Monte-Carlo Diagonalization (QMCD) is the diagonalization method to study the excited state of the shell-model Hamiltonian in medium or heavy nuclear physics.

As discussed before, it needs a huge number of basis for full diagonalization of the Hamiltonian. QMCD reduces number of basis by using a stochastic method. QMCD base states are generated with auxiliary field Monte-Carlo technique as SMMC. The imaginary-time evolution operator is expressed as a product of N_t-times sliced evolution operator:

$$\exp(-\tau\hat{H}) = \prod_{n=1}^{N_t} \exp(-\Delta\tau\hat{H})^{N_t} \ , \tag{2.41}$$

where $\Delta\tau = \tau/N_t$ and H is a shell-model Hamiltonian which consists of the one- and two-body operators as follows:

$$\hat{H} = \sum_{\alpha=1} \hat{O} + \frac{1}{2}\sum_{\alpha} \hat{O}^2 \ . \tag{2.42}$$

For small time-step evolution $\exp(-\Delta\tau\hat{H})$, we use the Hubbard-Stratonovich transformation to convert the "two-body" Hamiltonian into the effective "one-body" form in a similar way to SMMC,

$$\exp(-\Delta\tau\hat{H}) \simeq \int_{-\infty}^{\infty} \prod_{\alpha} d\sigma_{\alpha n} \left(\frac{\Delta\tau|V_\alpha|}{2\pi}\right)^{\frac{1}{2}}$$

$$\times \exp\left\{-\Delta\tau\left(\sum_\alpha \frac{1}{2}|V_\alpha \sigma_{\alpha n}^2| + \epsilon_\alpha \hat{O}_\alpha + s_\alpha V_\alpha \sigma_{\alpha n}\hat{O}_\alpha\right)\right\} \quad .(2.43)$$

If we have performed the integration on the auxiliary field $\{\sigma_{\alpha n}\}$ completely, the time evolution operator $\exp(-\tau\hat{H})$ projects out the ground state component in the trial function. Therefore, in QMCD, instead of the integration for $\{\sigma_{\alpha n}\}$, we regard $\{\sigma_{\alpha n}\}$ as parameters of basis,

$$|\Phi(\sigma)\rangle \propto \prod_{n=1}^{N_t} \exp(-\Delta\tau h(\sigma_n))|\Psi_0\rangle \ . \tag{2.44}$$

Here, $h(\sigma_n)$ is the one-body operator obtained by the HS transformation,

$$h(\sigma_n) = \sum_\alpha (\epsilon_\alpha + s_\alpha V_\alpha \sigma_{\alpha n}\hat{O}_\alpha) \ , \tag{2.45}$$

and $|\Psi_0\rangle$ is a trial function. The Hamiltonian is diagonalized in the Hilbert space spanned by these basis $|\Phi(\sigma)\rangle$.

The actual calculation is proceeded as follows. Starting from the trial function $|\Psi_0\rangle$, we calculate the initial energy E_0 as

$$E_0 = \frac{\langle\Psi_0|H|\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle} \ . \tag{2.46}$$

The following procedure is iterated until the ground state energy E converges. We generate auxiliary fields $\{\sigma\}$ in a stochastic way and calculate a time developed wave function $|\Phi(\sigma)\rangle$ as Eq.(2.44). A new basis $|\Phi'(\sigma')\rangle$ is determined so as to be ortho-normal to all other basis $\{\Phi\}$. We diagonalize the Hamiltonian with these basis plus a new set of basis $|\Phi(\sigma')\rangle$. Then we obtain the eigen values and functions. Adding a new basis, in principle, reduces the ground state energy. If the new basis is chosen well in Hilbert space, energy difference ΔE between with and without the new basis becomes large. When ΔE is small, the new basis $|\Phi'\rangle$ is discarded.

3 Method of continued fractions

Method of continued fractions (MCF) has been developed as an efficient method to study scattering problems for atomic physics and three-body system of nuclear physics. Lately, this method is improved to study the bound state problem. It enables us to calculate quickly the binding energies and the wave functions of the bound states. We briefly review the method of continued fractions.

3.1 Modified Green's function approach

The Schrödinger equation of multi-nucleon system can be written as

$$(H_0 + V)|\phi\rangle = E|\phi\rangle \tag{3.1}$$

Here, H_0 is a kinetic energy operator and V is nuclear potential between nucleons. For the bound state, Eq.(3.1) can be written as

$$|\phi\rangle = G_0(E)V|\phi\rangle \tag{3.2}$$

where $G_0(E)$ is a free Green's function,

$$G_0(E) = \frac{1}{E - H_0} \ . \tag{3.3}$$

There are two ways to perform the calculation using continued fractions form of the bound state problem. The one is to introduce modified potential approach (MCFV) [22] and the other is modified Green's function approach (MCFG) [23]. Both methods are equally useful in general. In this work, we use the MCFG approach, which is easy to implement in Monte-Carlo evaluation, while the original formalism in [23] was developed in the first approach. In this section, we will show the idea of modified Green's function of MCFG.

We introduce arbitrary functions $|F_0\rangle$ and $|f\rangle$ which are non-orthogonal to the bound state wave function $|\phi\rangle$ and possess the same symmetry as $|\phi\rangle$.

First of all, we start the calculation from $|F_0\rangle$, and define a new function $|F_1\rangle$ as

$$|F_1\rangle \equiv G_0(E)V|F_0\rangle \ , \tag{3.4}$$

and modified Green's function $G_1(E)$ as

$$G_1(E) \equiv G_0(E) - \frac{|F_1\rangle\langle f|}{\langle f|V|F_0\rangle} \ . \tag{3.5}$$

$G_1(E)$ is chosen so as to operate on only the space which is orthogonal to $V|F_0\rangle$ as

$$\begin{aligned} G_1(E)V|F_0\rangle &= \left(G_0(E) - \frac{|F_1\rangle\langle f|}{\langle f|V|F_0\rangle}\right) V|F_0\rangle \\ &= |F_1\rangle - |F_1\rangle \\ &= 0 \ . \end{aligned} \tag{3.6}$$

Eliminating $G_0(E)$ from Eq.(3.2) with aid of Eq.(3.5), the bound state wave function $|\phi\rangle$ is written as follows:

$$|\phi\rangle = G_1(E)V|\phi\rangle + |F_1\rangle\frac{\langle f|V|\phi\rangle}{\langle f|V|F_0\rangle} . \tag{3.7}$$

In the next step, we introduce the second order wave function $|F_2\rangle$ as

$$|F_2\rangle \equiv G_1(E)V|F_1\rangle , \tag{3.8}$$

and also a modified Green's function as

$$G_2(E) \equiv G_1(E) - \frac{|F_2\rangle\langle f|}{\langle f|V|F_1\rangle} . \tag{3.9}$$

Now the second order Green's function $G_2(E)$ is orthogonal to both $V|F_0\rangle$ and $V|F_1\rangle$:

$$G_2(E)V|F_0\rangle = G_2(E)V|F_1\rangle = 0 . \tag{3.10}$$

Therefore, the bound state wave function is written as

$$|\phi\rangle = G_2(E)V|\phi\rangle + \sum_{i=1,2}|F_i\rangle\frac{\langle f|V|\phi\rangle}{\langle f|V|F_{i-1}\rangle} . \tag{3.11}$$

By this modification of Green's function, the wave function can be expressed by a sum of orthogonal basis $|F_i\rangle$. The modified Green's function always operates on the space which is orthogonal to the lower order wave functions. Therefore, the higher order modified Green's function is expected to become smaller, and the iteration procedure may converge quickly.

In general, the modified Green's functions and the wave functions are defined as following iteration procedure,

$$|F_{i+1}\rangle \equiv G_i(E)V|F_i\rangle , \tag{3.12}$$

and

$$G_i(E) \equiv G_{i-1}(E) - \frac{|F_i\rangle\langle f|}{\langle f|V|F_{i-1}\rangle} , \tag{3.13}$$

where $G_i(E)$ satisfies the following orthogonality relation,

$$G_i(E)V|F_j\rangle = 0 \qquad (i > j) . \tag{3.14}$$

Finally, the bound state wave function is expressed in terms of the MCF wave functions as

$$|\phi\rangle = \sum_{i=1}^{\infty}|F_i\rangle\frac{\langle f|V|\phi\rangle}{\langle f|V|F_{i-1}\rangle} . \tag{3.15}$$

3.2 A new equation for the bound state problem and its solution

In this section, we show how the bound state energy can be obtained by using the iteration formula in the previous section.

Eq.(3.2) is rewritten as

$$\begin{aligned}|\phi\rangle &= \left(G_1(E) + \frac{|F_1\rangle\langle f|}{\langle f|V|F_0\rangle}\right) V|\phi\rangle \\ &= \frac{1}{1-G_1(E)V}|F_1\rangle\frac{\langle f|V|\phi\rangle}{\langle f|V|F_0\rangle} \\ &= |\phi_1\rangle\frac{\langle f|V|\phi\rangle}{\langle f|V|F_0\rangle}\end{aligned} \tag{3.16}$$

where we define $|\phi_1\rangle$ as

$$|\phi_1\rangle \equiv \frac{1}{1-G_1(E)V}|F_1\rangle \ . \tag{3.17}$$

Multiplying $\langle f|V$ to Eq.(3.16) from left, we obtain the following condition for determining the eigen value E and the wave function of the bound state,

$$\langle f|V|\phi\rangle = \frac{\langle f|V|\phi_1\rangle}{\langle f|V|F_0\rangle}\langle f|V|\phi\rangle \ . \tag{3.18}$$

Therefore, the bound state condition is equivalent to the equation,

$$\langle f|V|F_0\rangle - \langle f|V|\phi_1\rangle = 0 \ . \tag{3.19}$$

In order to solve this equation, we have to obtain $|\phi_1\rangle$. This can be done by MCFG iteration formula in the previous section. We define the i-th order wave function $|\phi_i\rangle$ as

$$|\phi_i\rangle \equiv \frac{1}{1-G_i(E)V}|F_i\rangle \ . \tag{3.20}$$

We can rewrite Eq.(3.20) as

$$|\phi_i\rangle = |F_i\rangle + G_i(E)V|\phi_i\rangle \ . \tag{3.21}$$

We substitute Eq.(3.13) into Eq.(3.21), and obtain

$$|\phi_i\rangle = |F_i\rangle + \left(G_{i+1}(E) + \frac{|F_{i+1}\rangle\langle f|}{\langle f|V|F_i\rangle}\right) V|\phi_i\rangle \ , \tag{3.22}$$

which is reduced to the equation:

$$|\phi_i\rangle = |F_i\rangle + |\phi_{i+1}\rangle\frac{\langle f|V|\phi_i\rangle}{\langle f|V|F_i\rangle} \ . \tag{3.23}$$

Here we use an orthogonal relation of Green's function as

$$\begin{aligned}\frac{1}{1-G_{i+1}(E)V}|F_i\rangle &= [1+G_{i+1}(E)V+\cdots]|F_i\rangle \\ &= |F_i\rangle \end{aligned} \tag{3.24}$$

We multiply $\langle f|V$ form left to Eq.(3.23), and obtain

$$\langle f|V|\phi_i\rangle = \frac{\langle f|V|F_i\rangle^2}{\langle f|V|F_i\rangle - \langle f|V|\phi_{i+1}\rangle} \ . \tag{3.25}$$

The above formula is explicitly written for $i=1$ as

$$\begin{aligned}\langle f|V|\phi_1\rangle &= \frac{\langle f|V|F_1\rangle^2}{\langle f|V|F_1\rangle - \langle f|V|\phi_2\rangle} \\ &= \frac{\langle f|V|F_1\rangle^2}{\langle f|V|F_2\rangle - \dfrac{\langle f|V|F_2\rangle^2}{\langle f|V|F_2\rangle - \langle f|V|\phi_3\rangle}} \\ &= \cfrac{\langle f|V|F_1\rangle^2}{\langle f|V|F_2\rangle - \cfrac{\langle f|V|F_2\rangle^2}{\langle f|V|F_2\rangle - \cfrac{\langle f|V|F_3\rangle^2}{\langle f|V|F_3\rangle - \ddots}}} \ .\end{aligned} \tag{3.26}$$

As a result, the bound state condition Eq.(3.19) can be also written as the form of continued fractions:

$$\begin{aligned}\langle f|V|F_0\rangle - \langle f|V|\phi_1\rangle &= x_0 - \cfrac{x_1^2}{x_1 - \cfrac{x_2^2}{x_2 - \cfrac{x_3^2}{x_3 - \ddots}}} \\ &\equiv \Omega(E) \ ,\end{aligned} \tag{3.27}$$

where the matrix elements x_i are defined as

$$x_i \equiv \langle f|V|F_i\rangle \ . \tag{3.28}$$

The condition $\Omega(E)=0$ is equivalent to the original Schrödinger equation for bound state Eq.(3.1) and determines the bound state energy.

In the iteration procedure, the Green's function project the states which is orthogonal to the lower order wave functions, as Eq.(3.14). We expect that x_i becomes smaller for higher i. Since this method is not restricted on the ground state, we can use the continued fractions form to study the excited state. Here, it is noticed again that we must adopt trial function $|F_0\rangle$ and $|f\rangle$, which are not orthogonal to the eigen function.

3.3 Wave function of the bound state

Once the eigen energy is determined, the bound state wave function is determined simultaneously from Eq(3.16) as

$$\begin{aligned} |\phi\rangle &= |\phi_1\rangle \frac{\langle f|V|\phi\rangle}{x_0} \\ &= \mathcal{N}|\phi_1\rangle \ , \end{aligned} \tag{3.29}$$

where $\mathcal{N}$ is a normalization constant. Using Eq.(3.23) and Eq.(3.25), we can express the state $|\phi\rangle$ as

$$\begin{aligned} |\phi\rangle &= \mathcal{N}|\phi_1\rangle \\ &= \mathcal{N}\left[\, |F_1\rangle + |\phi_2\rangle \frac{\langle f|V|\phi_1\rangle}{\langle f|V|F_1\rangle}\right] \\ &= \mathcal{N}\left[\, |F_1\rangle + |\phi_2\rangle \frac{\langle f|V|F_1\rangle}{\langle f|V|F_1\rangle - \langle f|V|\phi_2\rangle}\right] . \end{aligned} \tag{3.30}$$

Further, by using Eq.(3.23) and Eq.(3.25) iteratively, we obtain the bound state wave function $|\phi\rangle$ as follows:

$$|\phi\rangle = \mathcal{N}\left[\, |F_1\rangle + y_1|F_2\rangle + y_1y_2|F_3\rangle + y_1y_2y_3|F_4\rangle + \cdots\right] \tag{3.31}$$

where y_i is given by the following continued fraction series:

$$\begin{aligned} y_i &\equiv \frac{x_i}{x_i - \langle f|V|\phi_{i+1}\rangle} \\ &= \cfrac{x_i}{x_i - \cfrac{x_{i+1}^2}{x_{i+1} - \cfrac{x_{i+2}^2}{x_{i+2} - \ddots}}} \ . \end{aligned} \tag{3.32}$$

4 Continued fractions and Monte-Carlo method

In order to solve the bound state problem in the previous section, we start from a trial function $|F_0\rangle$, and generate MCF wave functions $|F_i\rangle$ by the iteration formula (3.12) and the modified Green's functions $G_i(E)$ by the iteration formula (3.13). Since both $G_i(E)$ and $|F_i\rangle$ are given by the iteration formula, and moreover the form of $G_i(E)$ is separable,

$$G_i(E) = G_{i-1}(E) - \frac{|F_i\rangle\langle f|}{x_i} , \tag{4.1}$$

the original form of MCF is not suitable for Monte-Carlo evaluation. Hence, we modify the iteration formula (3.12) by using the orthogonality (3.14) as follows:

$$\begin{aligned} |F_{i+1}\rangle &= G_i(E)V|F_i\rangle \\ &= G_0(E)V\left[|F_i\rangle - |F_{i-1}\rangle\frac{x_i}{x_{i-1}}\right] . \end{aligned} \tag{4.2}$$

Advantage of this formula is that a higher order wave function $|F_{i+1}\rangle$ is always given by the free Green's function $G_0(E)$ which has a simple analytical form. Because we know the technique of random walk used in Green's function Monte-Carlo, the distribution according to the free Green's function $G_0(E)$ is easily obtained. In this work, we will show the coordinate space representation for random walk formula.

However it should be noticed that the iteration formula (4.2) is not simply related to the diffusion equation,

$$|\phi\rangle = G_0(E)V|\phi\rangle . \tag{4.3}$$

The diffusion equation guarantees that the wave function obtained by iteration of Eq.(4.3) converges into the ground state, iteration being carried out by random walk $G_0(E)$ with the weight V. The difference between MCF iteration formula (4.2) and diffusion equation (4.3) is in wave functions obtained by iteration, since Eq.(4.2) can be regarded as

$$|\psi_1\rangle = G_0(E)V|\psi_0\rangle , \tag{4.4}$$

where $|\psi_1\rangle$ and $|\psi_0\rangle$ correspond to $|F_{i+1}\rangle$ and $[|F_i\rangle - \frac{x_i}{x_{i-1}}|F_{i-1}\rangle]$, respectively. Therefore we can not use naive procedure as the diffusion equation.

In addition, $|\psi_0\rangle$ is given by a subtracted form of the wave functions, $[|F_i\rangle - |F_{i-1}\rangle\frac{x_i}{x_{i-1}}]$, so that the sampling with positive and negative points causes the problem in the iteration procedure of MCF. This problem will be solved by using the multiple cancellation [18], which will be discussed later on.

4.1 Free Green's function in dimensionless coordinate

We consider the random walk by free Green's function $G_0(E)$ in configuration space. N-body Schrödinger equation for the bound state in the coordinate space $\boldsymbol{x}_i$:$(i = 1, \cdots, N)$ is written as

$$\left[-\sum_{i=1}^{N} \frac{1}{2m_i} \nabla^2_{\boldsymbol{x}_i} + V(\boldsymbol{x}_1, \cdots, \boldsymbol{x}_N)\right] \Psi(\boldsymbol{x}_1, \cdots, \boldsymbol{x}_N) = -B\Psi(\boldsymbol{x}_1, \cdots, \boldsymbol{x}_N) \ , \quad (4.5)$$

where B is the binding energy of the system. By separating out the center of mass coordinate, we rewrite the equation in terms of the relative coordinate $\boldsymbol{r}_i$ and reduced masses μ_i:$(i = 1, \cdots, N-1)$ as

$$\left[-\sum_{i=1}^{N-1} \frac{1}{2\mu_i} \nabla^2_{\boldsymbol{r}_i} + V(\boldsymbol{r}_1, \cdots, \boldsymbol{r}_{N-1})\right] \phi(\boldsymbol{r}_1, \cdots, \boldsymbol{r}_N) = -B\phi(\boldsymbol{r}_1, \cdots, \boldsymbol{r}_{N-1}) \ , \quad (4.6)$$

where the potential V is as function of only the relative coordinate $\boldsymbol{r}_i$. Then we denote $V(\boldsymbol{x}_1, \cdots, \boldsymbol{x}_N)$ as $V(\boldsymbol{r}_1, \cdots, \boldsymbol{r}_{N-1})$. We introduce the dimensionless coordinates as

$$\boldsymbol{z}_i = \sqrt{2\mu_i B/\hbar^2}\boldsymbol{r}_i \quad (4.7)$$

$$W(\boldsymbol{z}_1, \cdots, \boldsymbol{z}_{N-1}) = -V(\boldsymbol{r}_1, \cdots, \boldsymbol{r}_{N-1})/B \ , \quad (4.8)$$

The Schrödinger equation (4.6) reads as

$$\left(-\sum_{i=1}^{N-1} \nabla^2_{\boldsymbol{z}_i} + 1\right) \phi(\boldsymbol{z}_1, \cdots, \boldsymbol{z}_{N-1}) = W(\boldsymbol{z}_1, \cdots, \boldsymbol{z}_{N-1})\phi(\boldsymbol{z}_1, \cdots, \boldsymbol{z}_{N-1}) \ . \quad (4.9)$$

To solve Eq.(4.9), we define a free Green's function $G_0(R, R')$ which satisfies the equation,

$$(-\nabla^2 + 1)G_0(R, R') = \delta(R, R') \quad (4.10)$$

where R denotes $3(N-1)$ coordinates i.e. $R = \{\boldsymbol{z}_1, \cdots, \boldsymbol{z}_{N-1}\}$. It is noticed that the energy dependence of $G_0(R, R')$ is included in the dimensionless coordinates $\boldsymbol{r}_i$ and dimensionless potentials W.

Hence the Schrödinger equation (4.9) is expressed as an integral equation:

$$\phi(R) = \int G_0(R, R')W(R')\phi(R')dR' \ . \quad (4.11)$$

In MCF calculation, a wave function $|F_i\rangle$ is generated by Eq.(4.2) expressed properly in terms of the corresponding dimensionless quantities.

4.2 Random walk with free Green's function

We consider to apply the random walk with free Green's function $G_0(R, R')$ to the integration of non-diffusion type:

$$\psi_1(R) = \int G_0(R, R')W(R')\psi_0(R')dR' \ . \tag{4.12}$$

For simplicity, we assume that wave functions $\psi_1(R)$ and $\psi_0(R)$, and potential $W(R)$ are positive definite. Notice that positive sign of $W(R)$ stands for the attractive potential. The general case will be discussed in the next subsection.

Since the free Green's function $G_0(R, R')$ is normalized as

$$\int G_0(R, R')dR' = \int G_0(R, R')dR = 1 \ , \tag{4.13}$$

$G_0(R, R')$ can be regarded as a probability function of the random numbers distributed according to $G_0(R, R')$. The algorithm of random walk with $G_0(R, R')$ is provided by M. H. Kalos [24] (see Appendix A. for detail). The ground state wave function is obtained by the iteration of Eq.(4.11) with random walk method [24] using the feature of the diffusion equation.

Now, we consider the mechanism of random walk in Eq.(4.12). The function $\psi_1(R)$ generated by integration of Eq.(4.12) is represented by distribution of points $\{R_{0,i}\}$ using the probability of the functional form ψ_0 and the weights $\{W_{0,i}\}$ as

$$\begin{aligned} \psi_1(R) &= \int G_0(R, R')W(R')\psi_0(R')dR' \\ &= \sum_{i=1}^{N} W_{0,i}G_0(R, R_{0,i}) \ , \end{aligned} \tag{4.14}$$

where N is a number of sampling points.

We assume that $\psi_1(R)$ is represented by the points $\{R_{1,j}\}$ and the weights $\{W_{1,j}\}$. Then integration of an arbitrary function $F(R)$ is represented as

$$\int F(R)\psi_1(R)dR = \sum_{j}^{N} W_{1,j}F(R_{1,j}) \ . \tag{4.15}$$

The question is how $\{R_{1,j}\}$ and $\{W_{1,j}\}$ in Eq.(4.15) are generated from $\{R_{0,j}\}$ and $\{W_{0,j}\}$.

From Eq.(4.12), the integration in Eq.(4.15) is rewritten as

$$\int F(R)\psi_1(R)dR = \int F(R)\sum_{i}^{N} W_{0,i}G_0(R, R_{0,i})dR \ . \tag{4.16}$$

The right hand side of Eq.(4.16) is rewritten as

$$\int F(R)\sum_i^N W_{0,i}G_0(R,R_{0,i})dR = \int F(R)\sum_i^N W_{0,i}G_0(R,R_{0,i})\frac{G_0(R,X)}{G_0(R,X)}dR$$
$$= \int F(R)\sum_i^N W_{0,i}\frac{G_0(R,R_{0,i})}{G_0(R,X)}G_0(R,X)dR$$
$$\equiv \int A(R,X)G_0(R,X)dR\ . \tag{4.17}$$

where X can be an arbitrary value in $3(N-1)$ dimensional space. We assume that $G_0(R,R')$ satisfies the hyperspherical boundary condition,

$$G_0(R,R') = 0 \quad : \quad R,R' \to \infty\ . \tag{4.18}$$

This means that $G_0(R,R')$ is a function of only a variable $|R-R'|$. Hence we define a vector $\mathcal{R}$ in the $3(N-1)$ hyperspherical coordinate as $\mathcal{R} \equiv R - X$, and rewrite the free Green's function as

$$G_0(R,X)dR = G_0(\mathcal{R})d\mathcal{R}\ . \tag{4.19}$$

We can generate the random number $\mathcal{R}$ with probability of $G_0(\mathcal{R})$ by using GFMC random walk technique in [24]. The integration including $G_0(R,X)$ is carried out with the set of random numbers $\{\mathcal{R}_j\}$ generated by $G_0(\mathcal{R})$ as follows:

$$\int A(R,X)G_0(R,X)dR = \int A(X+\mathcal{R},X)G_0(X+\mathcal{R},X)d\mathcal{R}$$
$$= \int A(X+\mathcal{R},X)G_0(\mathcal{R})d\mathcal{R}$$
$$= \sum_j^N \frac{1}{N}A(X+\mathcal{R}_j,X)\ . \tag{4.20}$$

Therefore the right hand side of Eq.(4.17) is rewrite as follows:

$$\int A(R,X)G_0(R,X)dR = \int F(R)\sum_i^N W_{0,i}\frac{G_0(R,R_{0,i})}{G_0(R,X)}G_0(R,X)dR$$
$$= \sum_j^N \frac{1}{N}F(X+\mathcal{R}_j)\sum_i^N W_{0,i}\frac{G_0(X+\mathcal{R}_j,R_{0,i})}{G_0(X+\mathcal{R}_j,X)}$$
$$= \sum_j^N F(X+\mathcal{R}_j)\frac{\sum_i W_{0,i}G_0(X+\mathcal{R}_j,R_{0,i})}{NG_0(X+\mathcal{R}_j,X)}\ . \tag{4.21}$$

We notice that Eq.(4.21) holds for any values of X. Therefore, we replace X in $F(X+\mathcal{R}_j)$, $G_0(X+\mathcal{R}_j,X)$ and $G_0(X+\mathcal{R}_j,R_{0,i})$ by

$$X = R_{0,j} \quad (j=1,\cdots,N)\ , \tag{4.22}$$

and finally obtain,

$$\begin{aligned}\int F(R)\psi_1(R)dR &= \sum_j^N F(X+\mathcal{R}_j)\frac{\sum_i W_{0,i}G_0(X+\mathcal{R}_j,R_{0,i})}{NG_0(X+\mathcal{R}_j,X)} \\ &= \sum_j^N F(R_{0,j}+\mathcal{R}_j)\frac{\sum_i W_{0,i}G_0(R_{0,j}+\mathcal{R}_j,R_{0,i})}{NG_0(R_{0,j}+\mathcal{R}_j,R_{0,j})} \\ &\equiv \sum_j^N F(R_{1,j})W_{1,j} \ . \end{aligned} \tag{4.23}$$

Here, $\{R_{1,j}\}$ and $\{W_{1,j}\}$ are defined as

$$R_{1,j} \equiv R_{0,j}+\mathcal{R}_j \tag{4.24}$$

$$W_{1,j} \equiv \frac{\sum_i W_{0,i}G_0(R_{0,j}+\mathcal{R}_j,R_{0,i})}{NG_0(R_{0,j}+\mathcal{R}_j,R_{0,j})} \ . \tag{4.25}$$

By comparing Eq.(4.15) with Eq.(4.23), we can regard $\psi_1(R)$ as the distribution of the points $\{R_{1,j}\}$ which are generated by the points $\{R_{0,j}\}$ and random numbers $\{\mathcal{R}_j\}$ with probability of $G_0(\mathcal{R})$ and each point has the weight $W_{1,j}$ as Eq.(4.25). From this reading, the integration (4.12) is carried by using random walk form $\{R_{0,j}\}$ to $\{R_{1,j}\}$ with probability of $G_0(\mathcal{R})$.

We mention difference between our random walk method and the diffusion equation method. In the diffusion equation, a weight of new point $W_{1,i}$ is taken to be the same value as that of old point $W_{0,i}$, so that the component of the ground state in the trial function is extracted during the iteration. In contrast, in our method for Eq.(4.12), a weight $W_{1,i}$ of new point $R_{1,i}$ is generated by using all the other old points $\{R_{0,i}\}$ in the random walk. For non-diffusion type integration formula like Eq.(4.2), weights of new points must be generated by using our method, otherwise the ground state component is enhanced in the iteration. For study of the excited state calculation, it should be kept in mind.

4.3 Multiple cancellation

If $\psi_0(R)$ and $W(R)$ are not positive definite, we must add the sign $s_{0,j}$ to the weight $W_{0,j}$ as

$$W_{0,j} \Rightarrow s_{0,j}W_{0,j} \ . \tag{4.26}$$

Similarly, $W_{1,j}$ should include the sign

$$W_{1,j} \Rightarrow s_{1,j}W_{1,j} = \frac{\sum_i s_{0,i}W_{0,i}G_0(R_{0,j}+\mathcal{R}_j,R_{0,i})}{NG_0(R_{0,j}+\mathcal{R}_j,R_{0,j})} \ . \tag{4.27}$$

This is required, since a potential term $W(R)$ is not positive definite.

A higher order wave function $|F_{i+1}\rangle$ is generated by Eq.(4.2). Since Eq.(4.27) shows that a weight of a new point is generated by taking into account of all the

other weights and signs of old points, the points which have positive and negative signs are canceled according to weigh counting in Eq.(4.27). If we carried out the random walk for points of positive signs and negative signs independently, the weights of each points grow up and destructive interference of these wave functions induces large errors in the matrix elements x_{i+1} calculated with wave function $|F_{i+1}\rangle$. In this way, Eq.(4.27) play a important and critical role of this random walk procedure.

The weight cancellation of Eq.(4.27) can be regard as a sort of "multiple cancellation" by J. B. Anderson *et al.* [18]. Multiple cancellation method has been applied to, developed in the atomic physics, and provided very accurate results for the two- and three-electron bound system. Since our random walk method is the same procedure of multiple cancellation, the validity of our method may be confirmed.

4.4 Improvement of the accuracy

In MCF calculation, a higher order wave function is generated with $G_0(E)V$ random walk as

$$|F_{i+1}\rangle = G_0(E)V\left[|F_i\rangle - \frac{x_i}{x_{i-1}}|F_{i-1}\rangle\right]. \tag{4.28}$$

A subtraction procedure on the right hand side of is carried out by "multiple cancellation", as shown previously. However, the first large error in generating $|F_2\rangle$ is due to a large large cancellation between wave functions. In order to improve accuracy of calculation, we modify the equation for $|F_2\rangle$ into the analytic form of subtraction as

$$\begin{aligned}
|F_2\rangle &= G_0(E)V\left[|F_1\rangle - \frac{x_1}{x_0}|F_0\rangle\right] \\
&= G_0(E)V\left[G_0(E)V|F_0\rangle - \frac{x_1}{x_0}|F_0\rangle\right] \\
&= G_0(E)VG_0(E)\left[V|F_0\rangle - \frac{x_1}{x_0}G_0(E)^{-1}|F_0\rangle\right] \\
&= G_0(E)VG_0(E)\left[V - \frac{x_1}{x_0}G_0(E)^{-1}\right]|F_0\rangle\ .
\end{aligned} \tag{4.29}$$

Since $|F_0\rangle$ is analytic and known function, the operation $\left[V - \frac{x_1}{x_0}G_0(E)^{-1}\right]$ can be carried out as analytic calculation. Then the accuracy of $|F_2\rangle$ is improved.

5 Applications to the bound state problems

The procedure in our method is summarized in order.

1. Assume an appropriate form of the trial function and determine its parameters by variational method or numerical fitting.
2. Distribute the points by Metropolis method according to the probability of absolute value of the trial function $|F_0\rangle$.
3. Calculate a matrix element $\langle f|V|F_i\rangle$ by $|F_i\rangle$.
4. Generate $|F_{i+1}\rangle$ by random walk $G_0(E)$.
5. Iterate steps 3 and 4 until the x_i and $\Omega(E)$ converge.

Binding energy $B(=-E)$ is determined by searching the energy which satisfies the condition $\Omega(E)=0$.

5.1 One-dimensional model

As a simplest example, we studied 1-dimensional potential model. In the 1-dimensional problem, we can use other accurate numerical methods such as Simpson integration method, and test our method by comparing with them.

We solve the 1-dimensional Schrödinger equation as follows:

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\phi(x)+V(x)\phi(x)=-B\phi(x)\ , \tag{5.1}$$

where $B(=-E)$ is the binding energy and nucleon mass m is fixed as $m=$ 940MeV. $V(x)$ is chosen as follows:

$$V(x)=V_0\exp(-\mu x) \tag{5.2}$$

with

$$V_0=-69.3(\text{MeV})\ ,\ \mu=140(\text{MeV}\ )\ . \tag{5.3}$$

The potential is assumed to be of the simple exponential type so as to produce three bound states (-38.7, -10.6 and -2.01 MeV). The binding energy of the 2nd-excited state is very small, and is compared with the deuteron binding energy (≈ -2 MeV). Since this model is 1-dimensional and doesn't contain any other degrees of freedom (spin and isospin), the wave function of the bound states are classified by their parity. The ground and the 2nd-excited states are even parity states, and the 1st-excited state is odd parity state. Usefulness of our method will be examined for the 2nd-excited state, with the same symmetry as the ground state.

In order to use random walk with a free Green's function $G_0(E)$, we transform the Schrödinger equation (5.1) into an equation with dimensionless variable z as follows:

$$\left[-\frac{d^2}{dz^2}+1\right]\phi(z) = W(z)\phi(z) \tag{5.4}$$

with

$$z = \sqrt{2mB/\hbar^2}x \ , \ W(z) = -V(z)/B \ . \tag{5.5}$$

The Green's function for Eq.(5.4) satisfies the equation,

$$(-\frac{d^2}{dz^2}+1)G_0(z,z') = \delta(z-z'). \tag{5.6}$$

Then, the wave function $\psi(z)$ satisfies the integral equation,

$$\phi(z) = \int dz' G_0(z,z')W(z')\phi(z') \ . \tag{5.7}$$

The free Green's function $G_0(z,z')$ with boundary condition, $G_0 \to 0$ for $z \to \pm\infty$, is given by

$$G_0(z,z') = \frac{1}{2}\exp(-|z-z'|). \tag{5.8}$$

Therefore, the algorithm to generate z' from z according to the random walk kernel G_0 is simply given by

$$z = z' + \log\xi \cdot (\text{random sign}). \tag{5.9}$$

Here, ξ is an equidistributed random number in $(0,1)$, and "random sign" means to take $+$ or $-$ sign randomly.

We take a Gaussian form as a trial function for the even-parity states, and a Gaussian form multiplied by an odd parity term for the odd parity states,

$$|F_0\rangle = \frac{1}{\sqrt{b\sqrt{\pi}}}\exp(-\frac{x^2}{2b^2}) \ , \text{ for even parity,} \tag{5.10}$$

$$= \sqrt{\frac{2}{b\sqrt{\pi}}}\frac{x}{b}\exp(-\frac{x^2}{2b^2}) \ , \text{ for odd parity.} \tag{5.11}$$

We assume $b = 3$(fm) for the ground and the 1st-excited state, and $b = 10$(fm) for the 2nd-excited state.

In the Monte-Carlo calculation, number of sampling points we used is 20,000, 70,000 and 100,000 for the ground, the 1st- and the 2nd-excited state, respectively. The excited states need more points than the ground state. The initial distribution of points with the probability $|F_0\rangle$ is generated by Metropolis method [20]. Typically number of thermalization step is $1,000$.

The convergence of x_i defined in Eq.(3.28) against the iteration steps is shown in Fig. 1, 2, and 3, for the ground, the 1st- and the 2nd-excited states, respectively. In the case of the ground state energy, numerical values of x_i are given in Table 1. Since $G_i(E)$ is generated so as to be orthogonal to the lower order term $V|F_j\rangle$ $(i > j)$, x_i decreases quickly after a few times of iterations. The ground and the 1st-excited states are the lowest states with positive and negative parity, respectively, and x_i converges with 3 times of iteration. For the 2nd-excited state, x_i converges after 6 times of iteration. Since we used a simple Gaussian form as the trial function for the 2nd-excited state which should have nodes, the convergence of x_i for the 2nd-excited state is more slowly than for the ground and the 1st-excited states.

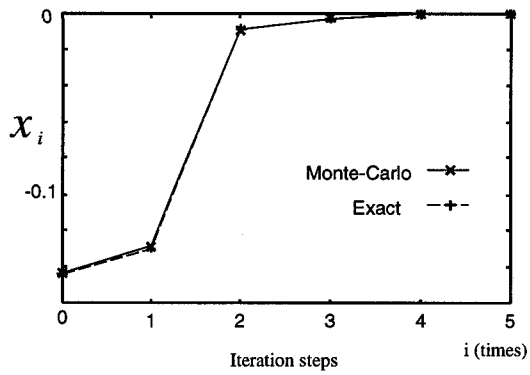

Figure 1: x_i versus iteration steps i at the ground state energy (-38.7MeV). "$\times$" are obtained by Monte-Carlo method, while points "+" are obtained by numerically exact method. The vertical axis is in unit of MeV. Lines are for eye-guide

Convergence of $\Omega(E)$ against iteration steps is shown in Figs. 4, 5, and 6, and it is very similar to the convergence of x_i.

The values of $\Omega(E)$ calculated by Monte-Carlo method fluctuate due to its sampling errors. Therefore, we performed calculations of $\Omega(E)$ several times with different sets of random numbers. The energies of bound states are determined by averaging of these calculated results. The errors are estimated by the standard deviation. We assumed a linear or a quadratic function for $\Omega(E)$, which is determined by the least square search for the calculated values of $\Omega(E)$ against discrete values of E, and determine the energy of bound state from the condition $\Omega(E) = 0$. As a result, we obtain the energies of three bound states and their errors, which are in a good agreement with exact ones. In Table 2, the eigen energies obtained by our Monte-Carlo method are compared with those by the numerically 'exact' method. Our method is found to give a good agreement with

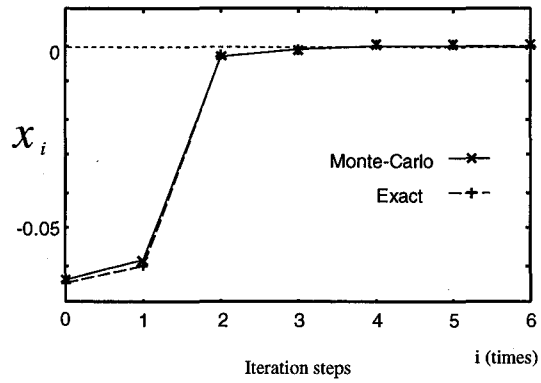

Figure 2: x_i versus iteration steps i at the 1st-excited energy (-10.6MeV). See the caption of Fig. 1.

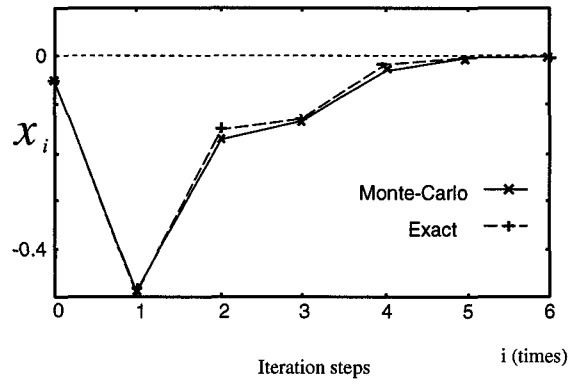

Figure 3: x_i versus iteration steps i at the 2nd-excited energy (-2.01 MeV). See the caption of Fig. 1.

	x_i	
i	'exact'	our Monte-Carlo
1	-1.44×10^{-1}	-1.44×10^{-1}
2	-1.30×10^{-1}	-1.29×10^{-1}
3	-8.33×10^{-3}	-8.97×10^{-3}
4	-2.50×10^{-3}	-2.62×10^{-3}
5	-6.29×10^{-5}	-1.25×10^{-4}
6	-9.34×10^{-6}	-1.20×10^{-5}

Table 1: Comparison of x_i between numerically 'exact' calculation and Monte-Carlo method for the ground state energy (-38.7MeV).

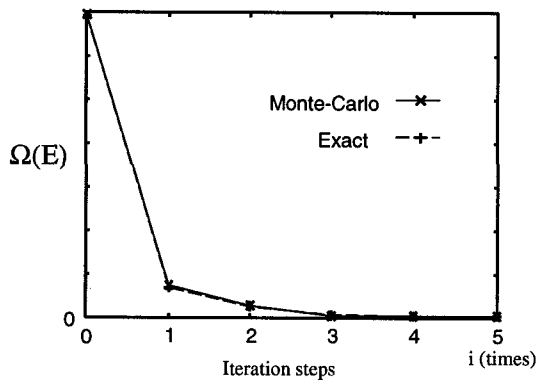

Figure 4: Convergence of $\Omega(E)$ versus iteration steps i at the ground state energy with arbitrary scale. "$\times$" (the solid line) are obtained by Monte-Carlo method, "+" (the dashed line) are obtained by numerically 'exact' method.

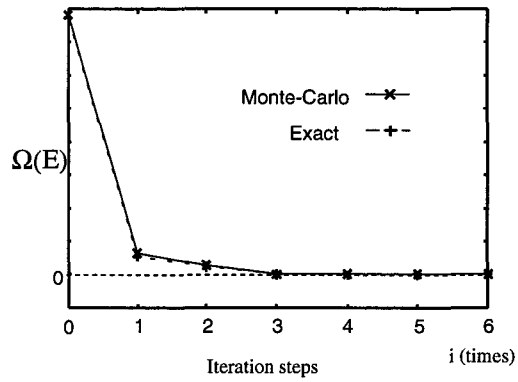

Figure 5: Convergence of $\Omega(E)$ versus iteration steps i at the 1st-excited state energy (-10.6MeV). See the caption of Fig. 4.

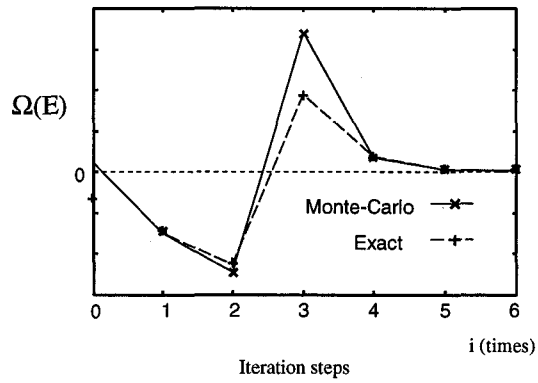

Figure 6: Convergence of $\Omega(E)$ versus iteration steps i at the 2nd-excited state energy (-2.01MeV). See the caption of Fig. 4.

the exact method. Therefore, it is shown that our method works for excited state even though we use Monte-Carlo method.

state	'exact'	Monte-Carlo	N
ground	-38.7	-38.8 ± 0.1	20,000
1st-excited	-10.6	-10.6 ± 0.1	70,000
2nd-excited	-2.01	-2.03 ± 0.14	100,000

Table 2: Eigen values (MeV) for the ground, the 1st-, and the 2nd-excited states by Monte-Carlo method are compared with those by the numerically 'exact' method. N is number of sampling points.

Once we obtain the bound state energies, the eigen functions are given by MCF wave functions $|F_i\rangle$ and matrix elements x_i. MCF wave functions $|F_i\rangle$ are shown in Figs. 7, 8, and 9, for the ground, the 1st-, and the 2nd-excited state, respectively. As the iteration step i increases, $|F_i\rangle$ become smaller due to orthogonality of $G_i(E)$ to $V|F_i\rangle$ given in Eq.(3.14).

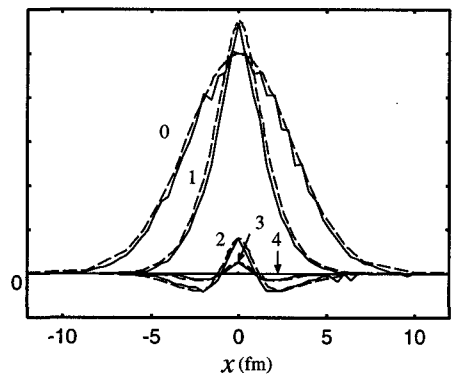

Figure 7: The wave function of MCF, $|F_i\rangle$, for the ground state. The solid lines are obtained by Monte-Carlo method and the dashed lines are obtained by numerical exact method. Numbers in $(0 \sim 4)$ specify the wave functions $|F_i\rangle$. Normalization of wave functions obtained by Monte-Carlo method is adjusted to the exact ones.

The wave functions for the ground, the 1st-, and the 2nd-excited states are shown in Figs. 10, 11, and 12, respectively. The wave functions are in good agreements with the exact results even for the 2nd-excited state. This results show that our method is useful to study the excited states.

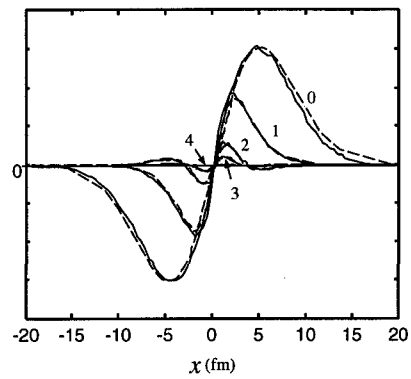

Figure 8: The wave function of MCF $|F_i\rangle$ for the 1st-excited state. See the caption of Fig. 7.

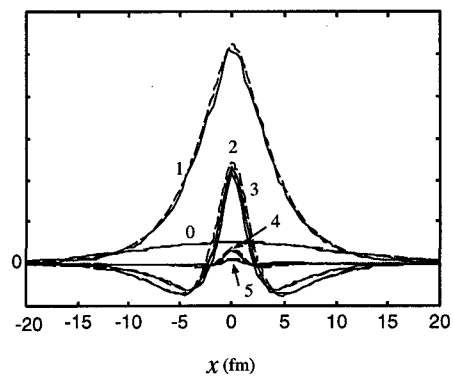

Figure 9: The wave function of MCF $|F_i\rangle$ for the 2nd-excited state. See the caption of Fig. 7.

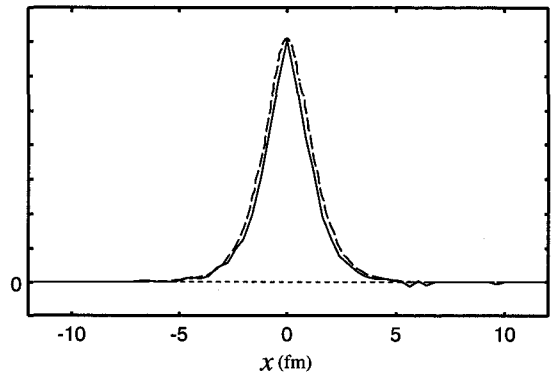

Figure 10: The eigen function for the ground state. The solid line is obtained by Monte-Carlo method. The dashed line is obtained by numerical exact method. Normalization of wave function obtained by Monte-Carlo method is adjusted to the exact ones.

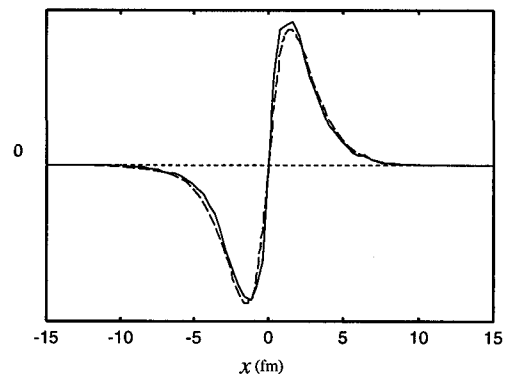

Figure 11: The eigen function for the 1st-excited state. See the caption of Fig. 10.

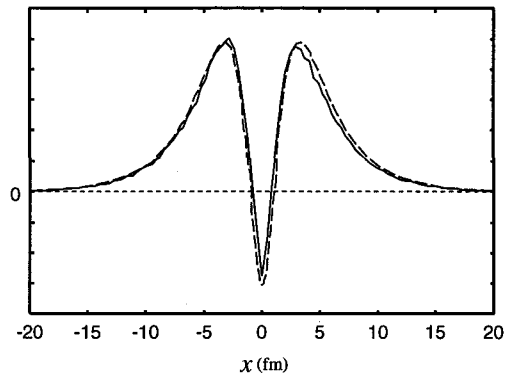

Figure 12: The eigen function for the 2nd-excited state. See the caption of Fig. 10.

5.2 Realistic four-body bound system in the three-dimensional space

As a realistic example, we study a 4-nucleon bound state in the 3-dimensional space. The Schrödinger equation for 4-nucleon system is written as

$$-\sum_{i=1}^{4}\frac{\hbar^2}{2m_i}\nabla_{x_i}^2|\phi\rangle+\sum_{i<j}^{4}V_{ij}|\phi\rangle=-B|\phi\rangle\ . \tag{5.12}$$

We can separate the center of mass motion by introducing the relative coordinates. We take Jaccobi coordinate system for this purpose, and remove the center of mass coordinate from Eq.(5.12). We obtain 9-dimensional Schrödinger equation as follows:

$$-\sum_{k=1}^{3}\frac{\hbar^2}{2\mu_k}\nabla_{r_k}^2|\phi\rangle+\sum_{i<j}^{4}V_{ij}|\phi\rangle=-B|\phi\rangle \tag{5.13}$$

Here, $\boldsymbol{r}_k$ are Jaccobi coordinates defined as

$$\begin{cases}\boldsymbol{r}_1 &= \boldsymbol{x}_2-\boldsymbol{x}_1\ ,\\ \boldsymbol{r}_2 &= \boldsymbol{x}_3-(\boldsymbol{x}_1+\boldsymbol{x}_2)/2\ ,\\ \boldsymbol{r}_3 &= \boldsymbol{x}_4-(\boldsymbol{x}_1+\boldsymbol{x}_2+\boldsymbol{x}_3)/3\ ,\end{cases}$$

and μ_k are reduced masses relevant to the coordinate system $\boldsymbol{r}_k$,

$$\begin{cases}\mu_1 &= m/2\ ,\\ \mu_2 &= 2m/3\ ,\\ \mu_3 &= 3m/4\ .\end{cases}$$

Here, we adopt the Volkov potential, with a repulsive short-range potential and an attractive long-range central potential [19],

$$V_{ij} = V_1 \exp(-\mu_1 r_{ij}^2) + V_2 \exp(-\mu_2 r_{ij}^2) \ , \tag{5.14}$$

with

$$\begin{cases} V_1 = -83.34(\mathrm{MeV}) \ , & \mu_1 = 1.60^{-2}(\mathrm{fm}^{-2}) \ , \\ V_2 = 144.86(\mathrm{MeV}) \ , & \mu_2 = 0.82^{-2}(\mathrm{fm}^{-2}) \ . \end{cases}$$

The ground state energy of ^{4}He has been studied by various methods: Faddeev-Yakubovsky (FY) method gives -30.27(MeV), which is calculated by taking into account only S-wave component in FY wave functions [1]. The result obtained by Stochastic Variational Method (SVM) is -30.42(MeV) [25], and, by Hyperspherical Harmonics (HH), -30.39(MeV) [26]. Although, this potential gives over binding for the ground state energy of ^{4}He and is not best potential model to describe systematically the nuclear bound state energies, it is a good example to examine our method in the 4-body system.

The free Green's function in dimensionless coordinates is expressed as

$$G_0(R, R') = \frac{1}{2(2\pi)^4} \frac{1}{\mathcal{R}^4} \left(1 + \frac{6}{\mathcal{R}} + \frac{15}{\mathcal{R}^2} + \frac{15}{\mathcal{R}^3}\right) \exp(-\mathcal{R}) \ , \tag{5.15}$$

where $\mathcal{R} \equiv |R - R'|$ is relative distance in the 9-dimensional space. As the dimensionality increases, the Green's function becomes singular at $\mathcal{R} = 0$. While it is difficult to treat the singularity of Green's function in the conventional integration method, the random walk used in this work inverts the Green's function explicitly and we can obtain numerically stable results. A standard method to generate points with probability $G_0(\mathcal{R})$ is given in Appendix A.

The ground state of ^{4}He is expected to be spatially symmetric and anti-symmetric in spin-isospin space. Then we use a trial function $|F_0\rangle$ given by a product of Gaussian wave function $|\varphi_s\rangle$ with correlation function $g(r)$, and the spin-isospin function $|\Xi\rangle$, as

$$|F_0\rangle = \mathcal{N} \prod_{i<j} g(r_{ij}) |\varphi_s\rangle |\Xi\rangle \ , \tag{5.16}$$

with

$$|\varphi_s\rangle = \prod_{i<j} \exp(-r_{ij}^2/2b^2) \ , \tag{5.17}$$

where b is a size parameter. We used the following form of correlation function $g(r)$,

$$g(r_{ij}) = [1 - \alpha \exp(-r_{ij}^2/a)]^2 \tag{5.18}$$

with

$$\alpha = 0.11 \ , \ a = 0.5(\mathrm{fm}^2) \ .$$

The parameter of correlation function is determined to simulate the wave function of two nucleon bound state with Volkov potential. The size parameter b of Gaussian wave function in Eq.(5.17) is chosen so as to give a minimum to the expectation value of the energy by variational calculation. For the other trial function $\langle f|$, we assume the same functional form as $|F_i\rangle$, and take a slightly larger value of size parameter b,

$$b = 3.0(\text{fm}): \text{ for } |F_0\rangle \tag{5.19}$$

$$= 4.5(\text{fm}): \text{ for } \langle f| \ . \tag{5.20}$$

Since Volkov potential is central potential with no exchange terms, we can take anti-symmetric spin-isospin wave function $|\Xi\rangle$ with $S = 0$ and $T = 0$, which will not change during iteration steps of MCF. Here, the spin-isospin function $|\Xi\rangle$ for $S = 0$, $T = 0$ is defined as

$$|\Xi\rangle = \frac{1}{\sqrt{2}}\{[[\chi_1 \otimes \chi_2]_0 \otimes [\chi_3 \otimes \chi_4]_0]_0 \ [[\eta_1 \otimes \eta_2]_1 \otimes [\eta_3 \otimes \eta_4]_1]_0 + [[\chi_1 \otimes \chi_2]_1 \otimes [\chi_3 \otimes \chi_4]_1]_0 \ [[\eta_1 \otimes \eta_2]_0 \otimes [\eta_3 \otimes \eta_4]_0]_0\} \ , \tag{5.21}$$

where χ_i and η_i are spin and isospin function of particle i, respectively.

Convergence of x_i is shown in Fig. 13 which shows three-times of iteration is enough in this problem. Similarly, the $\Omega(E)$ also converges quickly as shown in Fig. 14. Here, we take $N = 200,000$ sampling points.

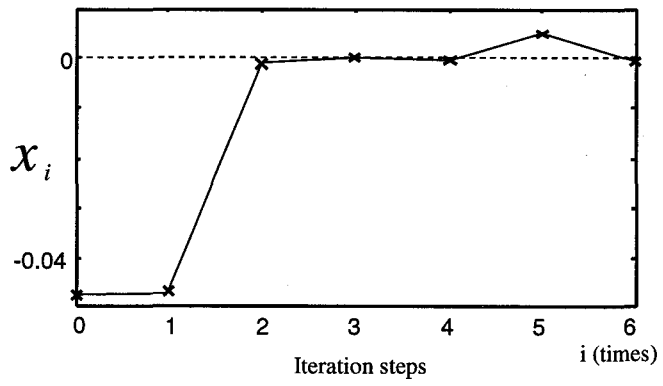

Figure 13: Convergence of x_i versus iteration steps i at $B = 30$MeV.

The bound state energy and its uncertainty are estimated in the same way as 1-dimensional case. We assume a linear function for fitting, as shown in Fig. 15. As a result, we obtain $E = -29.88 \pm 0.59$ MeV. Our results of binding energy of ^{4}He is in good agreement with the results of the other methods within uncertainties, shown in Table 3. Typical time of calculation is one hour for each energy point with 200,000 sampling points and 6-times of iterations.

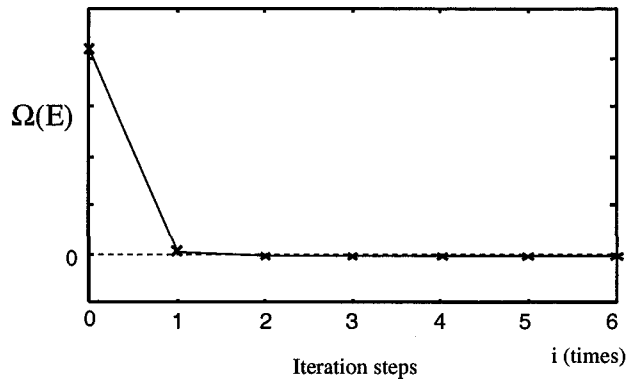

Figure 14: Convergence of $\Omega(E)$ versus iteration steps i at B =30MeV.

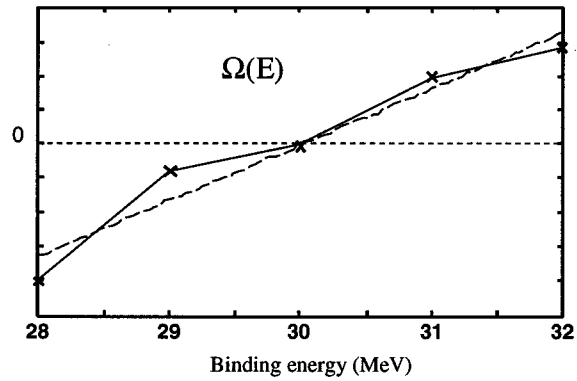

Figure 15: Energy ($B = -E$) dependence of $\Omega(E)$. "$\times$" (solid line) is obtained by Monte-Carlo method, and dashed line is obtained by fitting.

Method	Energy (MeV)
Faddeev-Yakubovsky [1]	-30.27
HH [26]	-30.39
SVM [25]	-30.42
MCF with MC	-29.88 ± 0.59

Table 3: The bound state energy of ^{4}He

6 Summary and Discussion

Monte-Carlo method is expected to be a useful tool for investigating the problem of the bound states in the many-body nucleon system because of its simple treatment and good efficiency in the higher dimensional integration. The previous Monte-Carlo methods were, however, restricted to apply on the ground state problem. In this work, we proposed a new method to investigate bound states of a few nucleon system, not only the ground state but also the excited states.

We used a method of continued fractions. Advantages of this method is that this method can be applied to the excited state and the continued fraction series converges quickly. The original formula of continued fraction is modified into a useful form for the Monte Carlo integration. The random work integration is used to calculate the continued fraction series. The higher order wave function in the continued fraction series should satisfy the orthogonality relation to the wave functions of lower order. Therefore, the treatment of the sign problem is much more important, and a naive important sampling technique cannot be applied in this method, in contrast to the GFMC. The former problem is solved by introducing the multiple cancellation mechanism, which occupies the most of computational time.

Our method was examined in the 1-dimensional problem. We demonstrated that our method works for the binding energy and wave function of the ground, the 1st- and the 2nd-excited states. In the 4-nucleon bound state problem in the 3-dimensional space, we obtained the ground state energy with a good agreement with the other methods. These facts suggest that our method can be one of the powerful tools to investigate the few-nucleon bound state problems.

Application of this method to few-nucleon systems with the realistic nuclear potential including exchange terms is one of the future problems. Here, we have to deal with coupled channel problem on various spin-isospin components to satisfy the exchange symmetry of the total wave function, and to take into account of the state dependence and repulsive core of the nuclear potential. It would be necessary to take into account the correlation of nucleons in the trial function as far as possible. The wave function obtained by the variational or the other method should be used as a trial function at the starting point in our procedure. This will also help to accelerate convergence of the continued fraction series. It could be important to maintain the correct symmetry of wave function in the intermediate step. In the realistic case with many channel coupled, we have to implement an efficient method to take into account the symmetry of wave functions.

Another challenging problem will be to apply the method to the continuum state. It should be possible to study the narrow resonance just above the threshold of the breakup.

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Appendix

A Random walk in the configuration space

We consider to generate the random number according to M-dimensional free Green's function $G_0(R, R')$. Here R denotes M-dimensional coordinates $R\{z_1, z_2, \cdots, z_M\}$.

We assume that R is dimensionless coordinates and the Schrödinger equation is written as

$$(-\nabla_R^2 + 1)\phi(R) = W(R)\phi(R) \ . \tag{A.1}$$

We define the free Green's function $G_0(R, R')$ as

$$(-\nabla_R^2 + 1)G_0(R, R') = \delta(R - R') \ , \tag{A.2}$$

which is normalized as

$$\int G_0(R, R')dR = \int G_0(R, R')dR' = 1 \ . \tag{A.3}$$

Eq.(A.1) is converted to the integral equation using free Green's function $G_0(R, R')$,

$$\phi(R) = \int dR' G_0(R, R')W(R')\phi(R') \ . \tag{A.4}$$

Here, we assumed that $G_0(R, R')$ provides the hyperspherical boundary condition with $G_0 \to 0$ as $R \to \infty$. An explicit form of $G_0(R, R')$ is given as

$$G_0(R, R') = \frac{1}{(2\pi)^{\frac{M}{2}}} K_{\frac{M}{2}-1}(|R - R'|)/|R - R'|^{\frac{M}{2}-1} \ , \tag{A.5}$$

where $K_\nu(z)$ is a Modified Bessel function of the order ν. Since the free Green's function depends only on the absolute value of relative coordinate $\mathcal{R} \equiv |R - R'|$, we can work on the hyper-spherical coordinate $\mathcal{R}$ in order to carry out the integration,

$$d^M R = \mathcal{R}^{M-1} d\mathcal{R} d\Omega \ . \tag{A.6}$$

Hence, an integration which includes Green's function becomes as follows:

$$\begin{aligned} G_0(R, R')d^M R &= G_0(\mathcal{R})\mathcal{R}^{M-1} d\mathcal{R} d\Omega \\ &= \frac{1}{(2\pi)^{\frac{M}{2}}} K_{\frac{M}{2}-1}(\mathcal{R})\mathcal{R}^{-\frac{M}{2}+1}\mathcal{R}^{M-1} d\mathcal{R} d\Omega \ . \end{aligned} \tag{A.7}$$

Right hand side of Eq.(A.7) can be separated as

$$\mathcal{N}_\Omega P_\mathcal{R}(\mathcal{R}) d\mathcal{R} d\Omega \tag{A.8}$$

where $P_{\mathcal{R}}(\mathcal{R})$ is defined as

$$P_{\mathcal{R}}(\mathcal{R}) \equiv \frac{2^{\frac{M}{2}-1}\Gamma(\frac{M-1}{2})}{\Gamma(\frac{1}{2})\Gamma(M-1)}\mathcal{R}^{\frac{M}{2}}K_{\frac{M}{2}-1}(\mathcal{R}) \ , \tag{A.9}$$

which is normalized as

$$\int P_{\mathcal{R}}(\mathcal{R})d\mathcal{R} = 1 \ . \tag{A.10}$$

$\mathcal{N}_\Omega$ is defined as

$$\mathcal{N}_\Omega \equiv \frac{1}{(2\pi)^{\frac{M}{2}}}\frac{\Gamma(\frac{1}{2})\Gamma(M-1)}{2^{\frac{M}{2}-1}\Gamma(\frac{M-1}{2})} \ . \tag{A.11}$$

The random number according to the weight of $P_{\mathcal{R}}(\mathcal{R})$ is generated by the following algorithm. We generate u and v using $M+1$ random numbers $(\xi_0, \xi_1, \cdots, \xi_M)$ equidistributed in the range $(0,1)$,

$$u = -\ln(\xi_1 \times \cdots \times \xi_M) \ , \tag{A.12}$$

$$v = (1 - \xi_0^{\frac{2}{M-1}})^{\frac{1}{2}} \ . \tag{A.13}$$

Then the distribution of $\mathcal{R}$ with $P_{\mathcal{R}}(\mathcal{R})$ is obtained as

$$\mathcal{R} = u \cdot v \ . \tag{A.14}$$

Isotropic components of a unit vector $\hat{\Omega}$ in M-dimension, $\omega_1, \cdots, \omega_M$ is generated by the random numbers $(\zeta_1 \cdots \zeta_M)$ with the M-dimensional Gaussian distribution,

$$\exp(-\zeta_1^2 - \zeta_2^2 - \cdots - \zeta_M^2) \ , \tag{A.15}$$

then each ω_i is given as

$$\omega_i = \zeta_i \ (\sum_j \zeta_j^2)^{-\frac{1}{2}} \ . \tag{A.16}$$

To summarize, the algorithm to generate the random number according to the free Green's function $G_0(\mathcal{R})$ is that $\mathcal{R}$ is generated by the probability $P_{\mathcal{R}}(\mathcal{R})$, and its direction is determined by $\{\omega_i\}$.

The proof of Eqs.(A.12) - (A.14):

The proof of the algorithm Eqs.(A.12) - (A.14) is as follows. First of all, we define η_i and u using $(0,1)$ random numbers ξ_i as

$$\eta_i \equiv -\ln \xi_i \ : \ \xi_i \in (0,1), \tag{A.17}$$

$$u \equiv -\sum_{i=1}^{n} \ln \xi_i = \sum_{i=1}^{n} \eta_i. \tag{A.18}$$

We consider the probability distribution function (p.d.f.) of η, $A(\eta)$ as

$$A(\eta)d\eta = d\xi \ . \tag{A.19}$$

From Eq.(A.17), we obtain $A(\eta)$ as

$$A(\eta) = \frac{d\xi}{d\eta} = e^{-\eta} \ . \tag{A.20}$$

Since u is defined as Eq.(A.18), the p.d.f. of u, $B_n(u)$ for $n = 1$ is obviously given as

$$B_1(u) = A(\eta) = e^{-\eta} = e^u \ . \tag{A.21}$$

Here, we assume that x and y are random numbers in the range $(0, \infty)$ distributed as $f(x)$ and $g(y)$, respectively, and define valuables z and w as

$$z \equiv x + y \ , \text{ and } w \equiv xy \ . \tag{A.22}$$

Then the probability distribution function (p.d.f.) of z and w are given by $h(z)$ and $j(w)$, respectively,

$$h(z) = \int_0^z f(x)g(z-x)dx, \tag{A.23}$$

and

$$j(w) = \int_0^\infty f(x)g(w/x)dx. \tag{A.24}$$

For $n = 2$, we use Eq.(A.23) and obtain

$$\begin{aligned} B_2(u) &= \int_0^u B_1(x)B_1(u-x)dx \\ &= \int_0^u e^x e^{u-x} dx \\ &= ue^u \ . \end{aligned} \tag{A.25}$$

Hence we use Eq.(A.23) up to $n = M$ iteratively and obtain $B_M(u)$ as

$$B_M(u) = \frac{u^{M-1}}{(M-1)!} e^u \ . \tag{A.26}$$

Next, we consider the p.d.f. of v, $C(v)$ as

$$C(v)dv = -d\xi. \tag{A.27}$$

From Eq.(A.13), v is inverted as

$$\xi = (1-v^2)^{\frac{M-1}{2}} \ . \tag{A.28}$$

Hence we obtain $C(v)$ as

$$\begin{aligned} C(v) &= -\frac{d\xi}{dv} \\ &= \frac{M-1}{2} 2v(1-v^2)^{(M-3)/2} \\ &= v(M-1)(1-v^2)^{(M-3)/2} \ . \end{aligned} \tag{A.29}$$

Since $\mathcal{R}$ is defined as in Eq.(A.14), we use Eq.(A.26), Eq.(A.29) and Eq.(A.24), finally the p.d.f. for $\mathcal{R}$, $P_{\mathcal{R}}(\mathcal{R})$ is obtained as follows:

$$\begin{aligned} P_{\mathcal{R}}(\mathcal{R}) &= \int_0^1 C(v) B_M(\mathcal{R}/v) dv/v \\ &= \int_0^1 v(M-1)(1-v^2)^{(M-3)/2} \left(\frac{\mathcal{R}}{v}\right)^{M-1} \frac{1}{(M-1)!} e^{-\frac{\mathcal{R}}{v}} dv/v \\ &= \frac{\mathcal{R}^{M-1}}{(M-2)!} \int_0^1 (\frac{1}{v^2} - 1)^{(M-3)/2} v^{-2} e^{-\frac{\mathcal{R}}{v}} dv \ . \end{aligned} \tag{A.30}$$

We changed a variable as $t = \frac{1}{v}$, hence $P_{\mathcal{R}}(\mathcal{R})$ is given as

$$P_{\mathcal{R}}(\mathcal{R}) = \frac{\mathcal{R}^{M-1}}{(M-2)!} \int_1^\infty (t^2-1)^{(M-3)/2} e^{-t\mathcal{R}} dt \ . \tag{A.31}$$

Using the integral representation of modified Bessel function,

$$K_\nu(z) = \frac{\pi^{\frac{1}{2}}}{(\nu - \frac{1}{2})!} \left(\frac{z}{2}\right)^\nu \int_1^\infty (t^2-1)^{\nu - \frac{1}{2}} e^{-tz} dt, \tag{A.32}$$

with

$$\nu = \frac{M}{2} - 1 \ , \tag{A.33}$$

we obtain the functional form of $P_{\mathcal{R}}(\mathcal{R})$ as follows:

$$P_{\mathcal{R}}(\mathcal{R}) = \frac{2^{\frac{M}{2}-1}\Gamma(\frac{M-1}{2})}{\Gamma(\frac{1}{2})\Gamma(M-1)} \mathcal{R}^{\frac{M}{2}} K_{\frac{M}{2}-1}(\mathcal{R}) \ . \tag{A.34}$$

Therefore, the algorithm of Eqs.(A.12) - (A.14) gives the expected distribution.

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