The study of light nuclei with the Brueckner-AMD

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Abstract. We propose a new approach of the Brueckner-AMD that makes the antisymmetrized molecular dynamics (AMD) calculations possible with realistic nuclear forces. In this method, we solve the Bethe-Goldstone equation and calculate the $G$-matrix for every nucleon pair described by wave packets of AMD. In addition, we perform the spin and parity projection correctly using the two-body correlators derived from the solutions of the Bethe-Goldstone equation. We report the results of applications to light nuclei with the Brueckner-AMD plus the spin and parity projection.

1. Introduction
Recent developments of the cluster model based on the antisymmetrized molecular dynamics (AMD) [1] have led to success in reproducing the various kinds of cluster structure in excited states, in addition to the shell model structure in the ground and low-lying states, without any assumption concerning cluster configurations. However, up to this time, the AMD studies have been carried out without detailed investigations of the relationship to realistic nuclear forces. So, recently, we proposed a framework of the Brueckner-AMD to calculate the $G$-matrix for AMD and demonstrated its applicability to some light nuclei [2].

The application of the Brueckner theory to the cluster model had been tried in association with the appearance of alpha-clustering in $^8$Be and $^{12}$C by Bando et al. [3] An important aspect of their approach is that the molecular orbits are constructed as single-particle orbits, however, it is difficult to construct molecular orbits for various kinds of cluster configurations. This problem of single-particle orbits in the cluster model can be easily solved in AMD, because the AMD wave functions are obtained from a Slater determinant of single-particle wave packets and its single-particle orbits can be defined with the AMD-Hartree-Fock method [2,4]. In our framework, the $G$-matrix and the single-particle energies are determined self-consistently and each position of the single-particle wave packets are determined variationally with the frictional cooling method [1], therefore, in a sense, the determination of the $G$-matrix and single-particle orbits in AMD can be performed “double self-consistently”. This is the reason that we call the present method “Brueckner-AMD”.

In general, however, the AMD wave functions don’t have spin and parity ($J^\pi$) as good quantum numbers. Therefore, it is necessary to perform the projection to the spin and parity eigenstates, where one needs to make a liner combination of space-inversed and rotated AMD Slater determinants [1]. For this purpose, we introduce a new definition of the $G$-matrix for different configurations in bra and ket states because the $G$-matrix in the Brueckner-AMD is defined in only one configuration corresponding to a single Slater determinant. In our calculation, we employ the method of the two-body correlators based on the Bethe-Goldstone equation [3].
In the next section, the framework of the Brueckner-AMD plus the spin and parity projection is explained. In the third section, we report the application of this framework and its results to p-shell nuclei. In the final section, we summarize this paper and refer to our future works.

2. Framework

2.1. The AMD wave function

The AMD wave function $|\Phi\rangle$ is represented as a Slater determinant of the single-particle wave functions $|\phi_i\rangle = |\vec{Z}_i\rangle \cdot |\chi_i\rangle$ where $|\vec{Z}_i\rangle$ is a spatial part and $|\chi_i\rangle$ is a spin-isospin part. The spatial part has the form of a Gaussian wave packet:

$$
\langle \vec{r} | \vec{Z}_i \rangle = \left( \frac{2\nu}{\pi} \right)^{3/4} \exp \left[ -\nu \left( \vec{r} - \frac{\vec{Z}_i}{\sqrt{\nu}} \right)^2 + \frac{\vec{Z}_i^2}{2} \right],
$$

where $\vec{Z}_i$ represents the wave-packet position of nucleon in the phase space and the complex variational parameters of molecular dynamics. We assume that the spin-isospin part is a spin-charge fixed state, $p\uparrow$, $p\downarrow$, $n\uparrow$, or $n\downarrow$.

2.2. The $G$-matrix in AMD

In order to apply the Brueckner-Hartree-Fock to AMD, we construct the orthonormal single-particle orbits $|f_\alpha\rangle$ with the AMD-Hartree-Fock method [2,4]. In this case, $|f_\alpha\rangle$ is the eigenstates of the overlap matrix $B_{ij} \equiv \langle \phi_i | \phi_j \rangle$. When calculating the $G$-matrix, $\hat{G}$, we use the Bethe-Goldstone equation:

$$
\hat{G} = \hat{v} + \hat{v} \varepsilon_\alpha + \varepsilon_\beta - (\hat{t}_\alpha + \hat{t}_\beta) \hat{G},
$$

$$
\varepsilon_\alpha = \langle f_\alpha | \hat{t} | f_\alpha \rangle + \sum_\gamma \langle f_\alpha f_\gamma | \hat{G} | A \{ f_\alpha f_\gamma \} \rangle,
$$

where the reference space $P$ is composed of the occupied states $\{ f_\alpha \}$, and therefore the Pauli projection operator, $Q = 1 - P$, is expressed as $1 - \sum_{\alpha<\beta} |f_\alpha f_\beta\rangle \langle f_\alpha f_\beta|$. The way to solve the Eq.(2) including treatment of the Pauli projection operator is explained in Ref.[2] following the prescription formulated by Bando et al. [3], and the single-particle energies $\varepsilon_\alpha$ and the $G$-matrix elements are determined self-consistently.

2.3. The spin and parity projection

The parity-projected state $|\Phi^\pm\rangle$ is expressed as a linear combination of two Slater determinants:

$$
|\Phi^\pm\rangle = \frac{1}{\sqrt{2}} \left( 1 \pm P \right) |\Phi\rangle,
$$

where $P$ is the space-inversion operator which operates on the spatial coordinates of each nucleon, and therefore, makes the single-particle wave functions $|\phi_i\rangle = |\vec{Z}_i\rangle \cdot |\chi_i\rangle$ change into $|\vec{Z}_i\rangle \cdot |\chi_i\rangle$. Furthermore, the spin- and parity-projected state $|\Phi^\pm_{MK}\rangle$ is expressed as

$$
|\Phi^\pm_{MK}\rangle = \frac{2J + 1}{8\pi^2} \int d\Omega \ D^J_{MK}(\Omega) \ \hat{R}(\Omega) \ |\Phi^\pm\rangle,
$$

where $D^J_{MK}(\Omega)$ is the Wigner D-function and $\hat{R}(\Omega)$ is the rotational operator which makes the spatial and spin-isospin coordinates rotated by the Euler angles $\Omega$. And then, The energy
expectation value of \(| \Phi_{MK}^{J \pm} \rangle \) is given by

\[
\langle \hat{H}_{K'K}^{J \pm} \rangle \equiv \frac{\langle \Phi_{MK}^{J \pm} | \hat{H} | \Phi_{MK}^{J \pm} \rangle}{\langle \Phi_{MK}^{J \pm} | \Phi_{MK}^{J \pm} \rangle} = \frac{\int d\Omega D_{K'K}^{J \pm}(\Omega) \left\{ \langle \Phi^{R} | \hat{H} | \Phi^{\prime} \rangle \pm \langle \Phi^{P} | \hat{H} | \Phi^{\prime} \rangle \right\}}{\int d\Omega D_{K'K}^{J \pm}(\Omega) \left\{ \langle \Phi^{R} | \Phi^{\prime} \rangle \pm \langle \Phi^{P} | \Phi^{\prime} \rangle \right\}},
\]

(6)

where \(| \Phi^{(P)} \rangle \equiv (P) \hat{R}(\Omega) | \Phi \rangle \).

2.4. The G-matrix in the spin and parity projection
In the spin and parity projection, as seen previously, we need the G-matrix element for different configurations in bra and ket states: \( \langle \Phi^{(a)} | \hat{G} | \Phi^{(b)} \rangle \). Therefore, we pay attention to the fact that the G-matrix can be represented with the two-body correlator \( \hat{F}_{ij} \) [3] based on the Bethe-Goldstone equation as:

\[
\psi_{ij} = \varphi_{ij} + \frac{Q}{\varepsilon_i + \varepsilon_j - (\hat{t}_i + \hat{t}_j)} \hat{G} \cdot \varphi_{ij} \equiv \hat{F}_{ij} \cdot \varphi_{ij} \quad (\hat{v} \cdot \psi_{ij} = \hat{G} \cdot \varphi_{ij}),
\]

(7)

and then

\[
\langle \varphi_{ij} | \hat{v} | \psi_{ij} \rangle = \langle \varphi_{ij} | \hat{G} | \varphi_{ij} \rangle = \langle \varphi_{ij} | \hat{F}_{ij} | \varphi_{ij} \rangle,
\]

(8)

where \( \psi_{ij} \) is the solution of the Bethe-Goldstone equation and \( \varphi_{ij} \) is the two-body wave function of the reference space, in this case, by the AMD wave function. The two-body correlators \( \hat{F}_{ij} \) are represented by \( \psi_{ij}/\varphi_{ij} \) and the two-body G-matrix elements can be defined as

\[
\langle \phi_{i}^{(a)} \phi_{j}^{(a)} | \hat{G} | \mathcal{A} \{ \phi_{k}^{(b)} \phi_{l}^{(b)} \} \rangle \equiv \frac{1}{2} \langle \phi_{i}^{(a)} \phi_{j}^{(a)} | \hat{F}_{ij}^{(a)} \hat{F}_{kl}^{(b)} | \mathcal{A} \{ \phi_{k}^{(b)} \phi_{l}^{(b)} \} \rangle,
\]

(9)

where \( \phi_{i}^{(a)} \) and \( \hat{F}_{ij}^{(a)} \) are the single-particle wave functions and the two-body correlators derived from the reference space \( \{ \Phi^{(a)} \} \).

2.5. Energy variations in the Brueckner-AMD
We apply the frictional cooling method [1] in molecular dynamics to determine \( \bar{Z}_i \). The equation of frictional cooling method is

\[
\frac{d\bar{Z}_i}{dt} = -\frac{\partial \mathcal{H}}{\partial \bar{Z}_i}, \quad \frac{d\bar{Z}_i}{dt} = -\frac{\partial \mathcal{H}}{\partial \bar{Z}_i}, \quad \mathcal{H} = \frac{\langle \Phi | \hat{H} | \Phi \rangle}{\langle \Phi | \Phi \rangle}.
\]

(10)

The frictional cooling method is also applicable to the projected state. In this case, the projection is performed at each time step in frictional cooling, and therefore, such a calculation is called the energy variation after the projection. Its advantage is that the energy variation is carried out with the orthogonality for other quantum states kept and, in general, we can obtain better solutions than the case of the projection after energy variation and no projection.

3. Results and Discussion
We apply the Brueckner-AMD method to various light nuclei with \( A \leq 12 \). In these calculations, we use the Argonne \( v8'(AV8') \) [5] as the realistic nuclear force and switch off Coulomb interactions. We perform the energy variation after the projection (VAP) for the parity but the projection after the energy variation (PAV) for the total spin. In the spin projection, we
choose a $K$ quantum number for each spin and parity that make the energy expectation value \( \langle \hat{H}_{KK}^{I\pm} \rangle \) minimum.

In this paper, we present the results of some $p$-shell nuclei, $^7\text{Li}$, $^8\text{Be}$, $^9\text{Be}$, $^{10}\text{Be}$, and $^{12}\text{C}$. In the calculation of $^9\text{Be}$, we investigate not only the lowest-energy negative-parity solution corresponding to the ground state but also the positive parity solution representing a kind of excited state with VAP for the parity. The Gaussian width parameter $b$ of the wave packets [ $\nu = 1/2b^2$ in Eq.(1) ] is the optimised value, $b=1.55$ fm, for the positive parity state of $^8\text{Be}$ obtained with VAP for the parity.

3.1. Intrinsic structure

The intrinsic densities obtained with VAP for the parity are shown in Figure 1. We present not only matter densities but also proton and neutron ones. In these figures, $X$, $Y$, $Z$ axes are chosen so as to be $\langle \sum_i x_i^2 \rangle \geq \langle \sum_i y_i^2 \rangle \geq \langle \sum_i z_i^2 \rangle$ and $\langle \sum_i x_i y_i \rangle = \langle \sum_i y_i z_i \rangle = \langle \sum_i z_i x_i \rangle = 0$ using the diagonalization of the matrix: $I_{pq} = \langle \sum_i r_i^p r_i^q \rangle$, where $r^p$ and $r^q$ mean $x$, $y$, and $z$ in the space-fixed frame, and the densities in the X-Y plane are shown.

These results with the Brueckner-AMD present the interesting features of clustering and molecular orbital structures, based on the realistic nuclear force (AV8'). The density of $^8\text{Be}$ shows the well-known alpha-alpha structure. Also, the density of $^7\text{Li}$ seems to be the triton-alpha structure judging from the proton and neutron density. In the lowest-energy negative-parity solution of $^9\text{Be}$ corresponding to the ground state, the valence neutron of alpha-alpha
Figure 2. The low-lying energy spectra of the experiment and the theoretical calculations for \(p\)-shell nuclei. The detailed explanations are in text.

shows the density distribution of a molecular orbit corresponding to the \(\pi\)-orbit. On the other hand, in the positive-parity solution representing an excited state of \(^9\)Be, its density distribution corresponds to a \(\sigma\)-orbit. However, the density of \(^{12}\)C shows the 3\(\alpha\) structure contrary to the well-known picture described by the shell model in the low-excitation energy region.

3.2. Energy spectra

We evaluate the energy spectra for each nucleus using the projection of the states obtained with VAP for the parity to each spin eigenstate. In these calculations, we adopt the proper body-fixed frame to the spin projection, where \(X\), \(Y\), \(Z\) axes are chosen so as to be \(\langle \sum_i z_i^2 \rangle \geq \langle \sum_i y_i^2 \rangle \geq \langle \sum_i x_i^2 \rangle\) and \(\langle \sum_i x_i y_i \rangle = \langle \sum_i y_i z_i \rangle = \langle \sum_i z_i x_i \rangle = 0\) with diagonalizing the previous mentioned matrix: \(I_{pq} = \langle \sum_i r_i^p r_i^q \rangle\).
The excitation energies for each spin and parity state are displayed in Figure 2, where the energies of the spin and parity state corresponding to the experimental ground state are normalized as zero energy and the values beside the line of zero energy express the binding energies of the ground state. For comparison with our results (B-AMD), we refer to the results of theoretical ab initio calculations using AV8′ not including genuine three-body forces, Green’s function Monte Carlo (GFMC) [6] and no-core shell model (NCSM) [7], in Figure 2. In the case of the positive parity states of $^9\text{Be}$, however, we refer to GFMC calculations [8] using Argonne v18 (AV18) instead of AV8′. It needs to be noted that these ab initio calculations without genuine three-body forces cannot reproduce the experimental binding energies of the ground state and some excitation energies correctly.

Our results with the Brueckner-AMD plus the spin and parity projection agree well with the experimental data and the ab initio calculations for the excitation energies of $^7\text{Li}$ and $^8\text{Be}$. However, in our results of $^9\text{Be}$, the $3/2^-$ and $1/2^-$ states are inverted and the $5/2^+$ and $3/2^+$ states are almost degenerated. In addition, in our calculations, each magnitude of the binding energy for the ground state is smaller than the value indicated by the ab initio calculations. Therefore, we consider that the calculation of VAP for the parity is not sufficient and it necessary to perform the variation for each spin and parity state correctly, that is to say, VAP for each spin and parity. Furthermore, reflecting that the binding energy of α-particle obtained with this framework is -24.7 MeV and the binding energy of $^8\text{Be}$: -44.0 MeV, don’t reach that of two α-particles, it may also be necessary to perform GCM for inter-cluster motion.

4. Summary and Future works
We proposed the framework of the Brueckner-AMD where the Brueckner theory is applied to AMD and introduced the G-matrix in the spin and parity projection using the two-body correlators based on the solutions of the Bethe-Goldstone equation. We applied the framework of the Brueckner-AMD plus VAP for the parity and PAV for the total spin to $p$-shell nuclei. As a result, we obtained good solutions for $^7\text{Li}$ and $^8\text{Be}$ but our results in $^9\text{Be}$ contradicted the experimental data and the ab initio calculations. In future works, in order to discuss and investigate nuclear structures of light nuclei more quantitatively, we will perform the Brueckner-AMD plus VAP for each spin and parity. In addition, we will expand this framework to the Brueckner-AMD plus GCM and introduce genuine three-body forces.

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