Extended Brueckner-Hartree-Fock theory with pionic correlation in finite nuclei

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Abstract. An extended Brueckner-Hartree-Fock (EBHF) theory is constructed for the description of nuclear structure in order to use a bare interaction among constituent particles. The nuclear interaction is characterized by the strong tensor force induced by pion exchange interaction. To handle the strong tensor force based on the single-particle picture, the Hartree-Fock variational model space is extended to include 2-particle 2-hole (2p-2h) states with all possible configurations, which are able to describe high momentum components originating from pseudo-scalar nature of the pion. We take a variational principle of the total energy in this extended model space. We obtain an equation for single-particle states in the Fermi sea with inclusion of the effect of the pion exchange and short-range repulsive interaction. We elucidate the nature of the EBHF theory by comparing with the Brueckner-Hartree-Fock (BHF) theory and the Feshbach projection operator method. The EBHF theory has a similar structure as the BHF theory except for the inclusion of the concept of the energy of the total system. The Feshbach projection operator method completely agrees with our framework when the P-space projection corresponds to the Hartree-Fock state and the Q-space projection corresponds to 2p-2h states with all possible configurations.

1. Introduction

One of the fundamental subjects of Nuclear Physics is to understand basic structure of nucleus, binding energy, magic number and saturation properties, etc., as a consequence of the interaction among constituent particles. The pion is the most important ingredient in nuclear physics as a mediator of the nuclear force, which is introduced by Yukawa[1]. The nuclear interaction is characterized by strong tensor interaction induced by the pion exchange interaction and short-range repulsion. It is well known that the deuteron has a bound state due to the tensor force. The binding energy is very tiny at 2.2 MeV, but this value is dynamically obtained by strong cancelation of large kinetic energy (20MeV) and large attraction due to the tensor interaction (17MeV) with small central attraction (5MeV). There is a strong correlation between tensor interaction and the kinetic energy. This is because the tensor interaction is accompanied by particle excitation in high momentum region. Since the tensor operator includes the spherical harmonics Y_2, it produces s- and d-wave mixing. Reflecting this mechanism d-wave contains high-momentum components and has a spatially compact distribution due to uncertainty principle. The amplitude of the wave functions are very small due to the short-range repulsive force in the region where the relative distance of the interacted pair becomes smaller than the nucleon size. As a consequence the matrix element of the tensor force has maximum value at around 1 fm. We have to take into account explicitly all these mechanisms in a theoretical framework. Furthermore, an *ab initio* variational calculation using the Green's Function Monte-Carlo method by the Argonne-Illinois group for light nuclei (A $\leq$ 12) shows that the pion plays an important role and the energy contribution of the pion exchange in the total two-body attractive force is about 80 %[2]. Due to pseudo-scalar nature of pion, strong tensor correlation is induced by the pion exchange interaction between an interacted pair. To take into account those correlations in a few-body system, it is essential to use the trial functions which depend explicitly on the relative coordinates of each nucleon pair, r_{ij}. This few-body technique is, however, hard to apply to medium and heavy nuclei, because the number of nuclear relative coordinates increases as A^2 and becomes tremendously large as the mass number A increases. It is therefore highly desirable to construct a theoretical framework for finite system with large mass numbers to treat explicitly the strong tensor and short-range repulsive interaction.

A very powerful method of treating the tensor correlation, which is called the tensor optimized shell model (TOSM), was developed based on the shell model framework by including 2p-2h states up to high momentum excitations for finite nuclei[3, 4]. This framework shows a good convergence of the tensor correlation with full tensor strengths by taking enough particle states in the 2p-2h space. In medium and heavy nuclei, a single-particle picture is a good approximation as a first step and we need to use a self-consistent field theoretical method based on the single-particle picture. It is therefore very interesting to construct the framework based on the Hartree-Fock theory and to extend the model space up to 2p-2h states with spatially compact configurations to treat the tensor correlation. In this talk we present the framework to handle the strong tensor and short-range repulsion in a convincing manner to the many-body problem for medium and heavy nuclei[5]. In this case, there are two difficult points to be solved when we construct a powerful framework for finite nuclei. First of all, a large model space is needed, because the tensor and short-range repulsion induce particle excitation in high momentum region. The second is that the single-particle wave functions in the Fermi sea should be self-consistently obtained by solving an appropriate equation. The second point is linked with the first one.

We discuss the construction and the structure of the EBHF theory by comparing with the Brueckner-Hartree-Fock theory and the Feshbach projection operator method. Finally, we give the summary and outlook.

2. Extended Brueckner-Hartree-Fock theory

The pion exchange interaction is expressed in terms of the tensor and spin-spin central parts,

$$\frac{\vec{\sigma}_1 \cdot \vec{q}\vec{\sigma}_2 \cdot \vec{q}}{\vec{q}^2 + m_\pi^2} = \frac{1}{3} S_{12}(\hat{q}) \frac{\vec{q}^2}{\vec{q}^2 + m_\pi^2} + \frac{1}{3} \vec{\sigma}_1 \cdot \vec{\sigma}_2 \frac{\vec{q}^2}{\vec{q}^2 + m_\pi^2}. \tag{1}$$

There appears the tensor interaction due to the pion exchange interaction. Hence, it is fundamentally important to treat the tensor interaction in order to consider the effect of the role of pion in nuclei.

2.1. Tensor interaction

When two nucleons approach each other within a distance of the Compton wave length of the pion, they feel a strong tensor interaction from each other. The pion exchange interaction brings about spin and iso-spin flips of single-particle states of interacting nucleons, because it induces the tensor interaction, $S_{12} = [Y_2 \otimes [\vec{\sigma} \otimes \vec{\sigma}]_2]_0$, having $Y_2(\hat{q})$ spherical harmonics with rank 2. Since spin and iso-spin flipped states are already occupied by other nucleons in spin-saturated nuclear ground state $|0\rangle$ the interacted nucleons must jump into states above the Fermi level. In the spin saturated Hartree-Fock (HF) state the expectation value of the tensor operator becomes zero, $\langle 0|S_{12}|0\rangle = 0$. Hence, we have to extend the HF model space at least up to 2p-2h states with all possible configurations so as to express the effect of the tensor correlation. The total wave function is taken as

$$|\Psi\rangle = C_0|0\rangle + \sum_\alpha C_\alpha|2p-2h;\alpha\rangle, \tag{2}$$

where we take summation of all the possible 2p-2h configurations labeled, α, with higher pionic angular momentum $(0^- \otimes L^{(-1)^L})$ of exchange pion until energy convergence is achieved. The normalization condition of the total wave function is given by $\langle\Psi|\Psi\rangle = |C_0|^2 + \sum_\alpha |C_\alpha|^2 = 1$. Validity of this model space is checked by detailed comparison of the ground state of ^{4}He with the tensor-optimized shell model[4, 6] and the rigorous few-body model calculations[7]. Furthermore, the relativistic Brueckner-Hartree-Fock method takes 2p-2h space and its results show a good reproduction of the saturation property in nuclear matter[8]. For the total Hamiltonian we write in the creation and annihilation operator form,

$$\hat{H} = \sum_{ij}\langle i|T|j\rangle a_i^\dagger a_j + \frac{1}{2}\sum_{ijkl}\langle ij|V|kl\rangle a_i^\dagger a_j^\dagger a_l a_k, \tag{3}$$

and the total energy of the nuclear ground state is given by

$$\begin{aligned} E = C_0^* C_0\langle 0|\hat{H}|0\rangle &+ C_0^*\sum_\beta C_\beta\langle 0|\hat{H}|2p-2h;\beta\rangle + C_0\sum_\alpha C_\alpha^*\langle 2p-2h;\alpha|\hat{H}|0\rangle \\ &+ \sum_{\alpha\beta} C_\alpha^* C_\beta\langle 2p-2h;\alpha|\hat{H}|2p-2h;\beta\rangle. \end{aligned} \tag{4}$$

The guiding principle for the total wave function Ψ is to make the total energy minimization, $\delta\langle\Psi|\hat{H}|\Psi\rangle/\langle\Psi|\Psi\rangle = 0$. The variational condition for the amplitudes of 2p-2h states as a whole, C_α^*,

$$\frac{\partial}{\partial C_\alpha^*}\langle\Psi|\hat{H} - E|\Psi\rangle = 0. \tag{5}$$

We take into account the effect of the two-pion exchange (iterative one-pion exchange) in the intermediate interaction range by using the variational method in this extended model space including 2p-2h states with all the possible configurations. This is a very important point of our method. Due to this method we can obtain the wave function including high-momentum components with pionic correlation. The amplitudes of 2p-2h states with all the possible configurations are decided by the variational condition (5),

$$C_\beta = \sum_\alpha \langle\beta|\frac{1}{E-\hat{H}}|\alpha\rangle\langle\alpha|\hat{H}|0\rangle C_0, \tag{6}$$

where we have introduced an abbreviation of expressing 2p-2h states as $|2p-2h;\alpha\rangle = |\alpha\rangle$ for the later use. As the next step in the many-body theory based on the single-particle picture mentioned in the introduction, we take the variation with respect to the single-particle wave function in the Fermi sea. The tensor and the short-range repulsive force have an effect on those single-particle states through the extended model space of 2p-2h states. They should be decided so as to make the total energy of the system minimized under the condition of orthonormalization $\langle i|j\rangle = \delta_{ij}$,

$$\frac{\partial}{\partial\psi_i^*(\vec{x})}\Big\{\langle\Psi|\hat{H}|\Psi\rangle - \sum_{ij}\varepsilon_{ij}\langle\psi_i|\psi_j\rangle\Big\} = 0. \tag{7}$$

This variational condition leads to the equation of motion for single-particle states in the Fermi sea. We call this an extended Brueckner-Hartree-Fock equation,

$$\begin{aligned} T\psi_i(\vec{x}) &+ \sum_j \int d^3x \psi_j^*(\vec{x}) V(\vec{x}-\vec{x}^{'})[\psi_i \otimes \psi_j]_{\mathcal{A}}(\vec{x},\vec{x}^{'}) \\ &+ C_0^* \sum_\alpha C_\alpha \frac{\partial}{\partial \psi_i^*(\vec{x})} \langle 0|\hat{H}|\alpha\rangle + \sum_{\alpha\beta} C_\alpha^* C_\beta \frac{\partial}{\partial \psi_i^*(\vec{x})} \langle \alpha|\tilde{H}|\beta\rangle = \varepsilon_i \psi_i(\vec{x}). \end{aligned} \tag{8}$$

Here, we use the relation $\langle\alpha|\hat{H}|\beta\rangle = \langle 0|\hat{H}|0\rangle + \langle\alpha|\tilde{H}|\beta\rangle$ and the normalization condition of the total wave function. The first line of the equation corresponds to the HF equation. The effect of the tensor correlation is included in the single-particle states in the Fermi sea through the second line of the equation. Equations (6) and (8) should be solved iteratively until self-consistency for the wave function and the energy is achieved. We obtain the equation that connects straightforwardly between nuclear structure and bare interaction among the constituent particles.

2.2. Short-range repulsion

We take a method for treating the short-range repulsion in order to describe quantitatively nuclear many-body system without seeking the origin of this force in this stage. In finite nuclear system we should try to express the short-range behaviour of the relative wave function to a certain extent in terms of 2p-2h configurations as the case of the tensor interaction. Considering the extreme short-ranged nature, we use a suitable method which is developed by Jastrow[9] or the unitary correlation operator method by Feldmeier[10]. In these methods the correlated wave function can be obtained by multiplying a trial wave function with a certain correlation function $\prod_{ij} f(r_{ij})$. This correlation function $f(r_{ij})$ is zero at the small relative distance and gradually approaches unity at the healing distance. The form of the correlation function is decided by energy minimization. We have to treat regorously the short-range repulsive correlation, because it affects the amount of the tensor matrix element. In the previous subsection of the EBHF formulation, we use the correlated wave functions or correlated operators.

3. Structure of the theory

We would like to discuss the structure of the EBHF theory by comparing with the Brueckner-Hartree-Fock (BHF) theory. We substitute the expression of 2p-2h amplitudes (6) in the EBHF equation (8). We obtain an effective Hamiltonian and take the expectation value of the HF states, $|0\rangle = \prod_i^{occ.} a_i^\dagger|\mathrm{vac}\rangle$, as follows,

$$\langle 0|\hat{H}_{eff}|0\rangle = |C_0|^2\langle 0|\hat{T}+\hat{V}|0\rangle - |C_0|^2 \sum_{\alpha\beta} \langle 0|\hat{V}|\alpha\rangle\langle\alpha|\frac{1}{\hat{H}-E}|\beta\rangle\langle\beta|\hat{V}|0\rangle. \tag{9}$$

The energy denominator which is an important part in this framework is written by

$$\langle\alpha|\hat{H}|\beta\rangle - E = \hat{e} + \langle\alpha|\tilde{H}|\beta\rangle + \langle 0|\hat{H}|0\rangle - E. \tag{10}$$

Here, $\hat{e}$ denotes 2p-2h energies.

3.1. Comparison with the Brueckner-Hartree-Fock theory

The BHF theory is based on the two-body scattering with the Pauli principle in self-consistent uniform potential $\hat{U}$[11]. This self-consistent potential is formed from the reaction matrix, G, obtained by solving the following 2-body equation,

$$G = V - V\frac{Q}{\hat{e}}G = V - V\Big(\frac{Q}{\hat{e}} - \frac{Q}{\hat{e}}V\frac{Q}{\hat{e}} + \cdots\Big)V = V - V\frac{Q}{\hat{e}+V}V. \tag{11}$$

Here, the energy denominator, $\hat{e} = \hat{T} + \hat{U} - \varepsilon_{h1} - \varepsilon_{h2}$, represents 2 particle-energies minus 2 hole-energies, $\hat{e}|\alpha\rangle = (\varepsilon_{p1} + \varepsilon_{p2} - \varepsilon_{h1} - \varepsilon_{h2})|\alpha\rangle$. An interacted pair must jump above the Fermi surface and the intermediate states are 2p-2h states. The iteration process for the G-matrix is to repeat scattering many times within 2p-2h states. This G-matrix is considered to be the 2-body effective interaction in the HF-space. We write the expectation value of the HF states in the following form,

$$\langle 0|T + G|0\rangle = \langle 0|T + V|0\rangle - \sum_{\alpha\beta}\langle 0|V|\alpha\rangle\langle\alpha|\frac{1}{\hat{e} + V}|\beta\rangle\langle\beta|V|0\rangle. \tag{12}$$

Comparing (9) with (12), both have similar structures except for the coefficient $|C_0|^2$ and the energy denominator (10). The difference of the total energy, E, and the HF energy appears in the denominator of EBHF theory as shown as the last two terms in (10) is a very important term. This is because this part expresses the particle excitation in high momentum region induced by the strong tensor and short-range repulsion. The concept of the total energy E appears in the EBHF theory, because this theory handles the fully many-body system by using the variational method.

3.2. Comparison with the Feshbach projection operator method

It is very interesting to compare the EBHF theory with the Feshbach projection operator method[12]. We introduce the projection operator P and Q, where $P^2 = P$, $Q^2 = Q$ and $PQ = 0$ under the condition $P + Q = 1$. From the many-body Schroedinger equation,

$$H\Psi = E\Psi, \tag{13}$$

we can derive an effective Hamiltonian for the $P\Psi$ state using the properties of the projection operators,

$$(PHP - PHQ\frac{1}{QHQ - E}QHP)\Psi = EP\Psi. \tag{14}$$

We should identify P-projection as $|0\rangle\langle 0|$ and Q-projection as 2p-2h states $\sum_\alpha |\alpha\rangle\langle\alpha|$, namely, $P|\Psi\rangle = C_0|0\rangle$ and $Q|\Psi\rangle = \sum_\alpha C_\alpha|\alpha\rangle$, we then obtain the effective Hamiltonian for HF state, $|0\rangle$. The matrix element by HF state is given as

$$\begin{aligned}\langle 0|H_{eff}|0\rangle &= \langle\Psi|PHP|\Psi\rangle - \langle\Psi|PHQ\frac{1}{QHQ - E}QHP|\Psi\rangle \\ &= |C_0|^2\langle 0|H|0\rangle - |C_0|^2\sum_{\alpha\beta}\langle 0|V|\alpha\rangle\langle\alpha|\frac{1}{H - E}|\beta\rangle\langle\beta|V|0\rangle.\end{aligned} \tag{15}$$

If we take the energy variation of HF energy, $\langle 0|H_{eff}|0\rangle$, with respect to the single-particle states ψ_i^* in the Fermi sea leads to precisely the EBHF equation (8). Hence, both the effective Hamiltonians agree completely with each other. The normalization requires the contribution of the Q-space wave function. This means that the HF state alone is not normalized to unity.

4. Summary and outlook

A nuclear many-body theory, which is called extended Brueckner-Hartree-Fock (EBHF) theory, has been presented to understand the nuclear structure as a consequence of the bare interaction among constituent particles. The nuclear force is characterized by the strong tensor and the short-range repulsive forces. The fact that the tensor matrix element of the spin-saturated HF state vanishes forces us to extend the ground state HF wave function. We therefore take the HF + 2p-2h states with all possible configurations as the variational model space for medium and heavy nuclear system in a consistent manner of the single-particle picture. We take the variational method and obtain a total wave function including the high-momentum components originated from the pseudo-scalar nature of pion. We obtain the EBHF equation for the single-particle states in the Fermi sea under the influence of the Q-space (2p-2h) wave function. We have compared the EBHF equation with the BHF theory and the Feshbach projection operator method. The EBHF equation and the BHF theory has the same structure. There is the concept of the total energy in the energy denominator of the EBHF because of full consistency of many-body system. The energy difference between the HF and the total energy in the energy denominator of EBHF theory contains high-momentum components due to the tensor and short-range repulsive correlation. This is the reason why we would like to call the present framework as an extended Brueckner-Hartree-Fock theory. The coefficient $|C_0|^2$ appears in the EBHF theory, which means that the normalization condition of the HF state (P-space) is not normalized to 1, because of $|C_0|^2 \neq 1$.

Finally, we would like to mention our outlook and why we have constructed the present framework. The pseudo-scalar nature of pion, which emerges as the Nambu-Goldstone boson, originates from spontaneous chiral symmetry breaking[13]. The chiral symmetry is known to be the most important symmetry in hadron physics and the hadron mass generation is described clearly in the Nambu-Jona-Lasinio model with fermion fields[13]. The pion plays an important role in both nuclear and hadron physics. To handle the nature of pion is a key to make connection between nuclear and hadron physics governed by the strong force which has the fundamental principles in QCD. To understand nuclear structure on the same footing as hadron physics, we need the framework to understand the nuclear many-body system starting from bare interaction among the constituent particles instead of the nuclear force obtained phenomenologically from the phase-shift analysis of nucleon-nucleon scattering data. Recently, the specific characteristics of the nuclear force can be reproduced numerically by the Lattice QCD calculations[14], though the pion mass is still large. For this purpose, proper treatment of the pion based on the field theoretical method is essential.

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References
[1] Yukawa H 1935 *Proc. Phys. - Math. Soc. Jpn.* **17** 48
[2] Pieper S C and Wiringa R B 2001 *Annu. Rev. Nucl. Part. Sci.* **51** 53
[3] Myo T, Sugimoto S, Katō K, Toki H and Ikeda K 2007 *Prog. Theor. Phys.* **117** 257
[4] Myo T, Toki H and Ikeda K 2009 *Prog. Theor. Phys.* **121** 511
[5] Ogawa Y and Toki H 2011 *Ann. Phys.* **326** 2039
[6] Horii K, Toki H, Myo T and Ikeda K 2011 Tensor-optimized few-body model for s-shell nuclei *Preprint* arXive:1105.1420
[7] Kamada H *et al.,* 2001 *Phys. Rev.* C **64** 044001
[8] Brockmann R and Machleidt R 1990 *Phys. Rev.* C **42** 1965
[9] Jastrow R, 1955 *Phys. Rev.* **98** 1497
[10] Feldmeier H, Neff T, Roth R and Schnack J 1998 *Nucl. Phys.* A **632** 61
[11] Brueckner K A and Levinson C A 1955 *Phys. Rev.* **97** 1344
[12] Feshbach H 1962 *Ann. Phys.* **19** 287
[13] Nambu Y and Jona-Lasinio G 1961 *Phys. Rev.* **122** 345; Nambu Y and Jona-Lasinio G 196 *ibid.* **124** 246
[14] Aoki S, Hatsuda T and Ishii N 2010 *Prog. Theor. Phys.* **123** 89