Antisymmetrized Molecular Dynamics with Coherent State Pions and Its Application to Excited Spectrum of $^{12}$C

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We introduce coherent state neutral pions into Antisymmetrized Molecular Dynamics. With the aid of coherent state technique, it becomes possible to calculate transition matrix elements of the pion field operator and to study excited states containing pions. For a large pion-nucleon coupling, $f_{\pi N} \gtrsim 1.6$, pions have a finite expectation value and cause a large energy gain in $^{12}$C. We discuss two aspects of pionic effects in spectroscopy, an $LS$-like interaction effect and the mixing of different nucleon parity states, which would modify low energy nuclear levels.

§1. Introduction

Nuclei have been basically understood as nucleon many-body systems in which nucleons move in a mean field and interact via small residual interactions. In shell models, each nucleon single particle wave function is assumed to have its own orbital angular momentum, spin and parity ($lj\pi$), provided that the spherically symmetric mean field consists of central and spin-orbit ($LS$) parts. This basic picture of nuclei has been successful in describing low-lying states of most of medium to heavy nuclei, although there are several exceptions, such as clustering states in light nuclei.

By contrast, the long-range part ($r \gtrsim 2$ fm) of the bare nucleon-nucleon potential is described by the one-pion exchange potential (OPEP), possessing a strong tensor part, which mixes different partial waves. This mixing is essential for the binding of deuterons, but makes it difficult to treat many-body systems exactly. Thus, this tensor force has been usually treated in the form of effective central and $LS$ forces in solving nuclear many-body problems, in spite of its importance in the bare nuclear force, with the hope that the explicit role of the tensor force is not large in nuclei. Actually, the first-order effects of the tensor force vanish in the Fermi gas state, due to cancellations in the $(2J + 1)$-weighted sum.

However, if pions have non-zero expectation values in nuclei or in nuclear matter, the cancellation is not complete, and hence in this case, the tensor force may play a dominant role. There have been many studies of the possibility of pion condensation in nuclear matter. For some time, it was considered that a strong nucleon-$\Delta$ short-range repulsion might suppress pion condensation, provided that the Landau-Migdal parameter displays “universality”, i.e. $g'_{N\Delta} = g'_{NN} \simeq 0.6$, and that it is density independent.1) Recent observations of non-quenching in the Gamow-Teller giant resonance sum rule2) have clarified that the short-range repulsion between nucleons
and $\Delta$ resonances is not very strong, specifically $g'_{N\Delta} < 0.25$.\textsuperscript{3)} This suggests that pion condensation may exist, at least in high-density nuclear matter. Also, in recent \textit{ab initio} calculations of light nuclei ($A \leq 12$) with realistic bare $NN$ potentials, it has been shown that the OPEP contribution is dominant in the total potential energy.\textsuperscript{4)} This result suggests that the cancellation that occurs in Fermi gas does not occur for actual nuclei and that it is necessary to consider the explicit role of pions more seriously.

With this background, pion condensation and the explicit role of the tensor force in nuclei have now attracted renewed interest. In a relativistic mean field framework, it has been demonstrated that neutral pions can condense in the surface region of nuclei, and that this condensation enhances the binding energy of $jj$ closed nuclei, such as $^{12}$C.\textsuperscript{5)} In their model, single particle states are first prepared with fixed $lj\pi$, and those states with the same $j$ mix, and thereby gain the potential energy from pions. This mixture also plays the role of an $LS$-like potential.\textsuperscript{6), 7)} Since pions mix single particle states of different parity (but the same $j$), the yrast single particle states (the lowest energy single particle states for given $j$, $s_{1/2}, p_{3/2}, d_{5/2}, f_{7/2}, g_{9/2}, h_{11/2}, i_{13/2}$) will have the largest energy gain. On the other hand, those states having smaller $j$ near the Fermi energy will be pushed up from the mixing with the lower energy single particle states. It is interesting that the last four yrast single particle states determine the nuclear magic numbers of 28, 50, 82 and 126. More recently, the Charge and Parity Projected Hartree-Fock (CPPHF) method has been developed in order to take account of the coupling of proton and neutron single particle states generated by OPEP.\textsuperscript{8)} It has been shown that the charge projection enhances the tensor contribution by approximately three times in the case of $^{4}$He nuclei.

At this stage, it is desirable to extend the scope of the pion and tensor force study from the ground state and single particle states to nuclear excited level spectroscopy with specified $J^\pi$, which would yield more information concerning wave functions. Specifically, we are more interested in constructing a framework in which explicit pionic degrees of freedom are incorporated, rather than introducing a tensor interaction, since we believe that it is more fundamental to describe nuclear many-body systems with pions.

In this work, we introduce coherent state pions\textsuperscript{9)} into Antisymmetrized Molecular Dynamics (AMD)\textsuperscript{10), 11)} and discuss pionic effects on the excited states of $^{12}$C. Pion coherent states enable us to calculate the matrix elements of the pion operator with different states as well as the expectation value with a given state. In AMD, the nuclear wave function is represented by the Slater determinant of nucleon Gaussian wave packets, which is wide enough to describe clustering states as well as shell model states. By using the product of the nucleon AMD state and the pion coherent state, we can evaluate the transition matrix elements of the Hamiltonian operator containing nucleon and pion operators. Therefore, it becomes possible to project the wave function to the eigenstate of a given $J^\pi$ and to diagonalize the Hamiltonian matrix consisting of wave functions with different nucleon and pion configurations.
§2. AMD with coherent state pions

The nucleon-pion basis state is assumed to be given by the product of the nucleon AMD state\cite{10,11} and the pionic coherent state:\cite{9}

\[ |\Psi(Z, f)\rangle = |\Psi_{\text{AMD}}(Z)\rangle \otimes |\Phi_\pi(f)\rangle . \] (2.1)

The AMD wave function takes the form of the Slater determinant of nucleon Gaussian wave packets,

\[ |\Psi_{\text{AMD}}(Z)\rangle = A \prod_i |\psi_{z_i}\rangle |\chi_{i}^r \chi_{i}^T\rangle , \quad (Z = \{z_i ; i = 1, 2, \cdots A\}) \] (2.2)

\[ \langle r | \psi_z \rangle = \left(\frac{2\nu}{\pi}\right)^{3/4} \exp \left[ -\nu(r - z/\sqrt{\nu})^2 + z^2/2 \right] , \] (2.3)

where \( |\chi_{i}^r \chi_{i}^T\rangle \) represents spin-isospin wave function. The pion coherent state introduced by Amado et al.\cite{9} is represented as

\[ |\Phi_\pi(f)\rangle = \exp \left[ \int df (k) \hat{a}^\dagger(k) \right] |0\rangle . \] (2.4)

By defining the commutation relation of the annihilation and creation operators, \( \hat{a}(k) \) and \( \hat{a}^\dagger(k') \), as [\( \hat{a}(k), \hat{a}^\dagger(k') \)] = \( \delta(k - k') \), we can show that the above pion coherent state is an eigenstate of the positive frequency operator \( \hat{\phi}^+(r, t) \):

\[ \hat{\phi}^+(r, t) = \int \frac{hc \, dk}{\sqrt{(2\pi)^3 2\omega_k / c}} \hat{a}(k)e^{ik\cdot r - i\omega_k t} , \] (2.5)

\[ \hat{\phi}^+(r, t)|\Phi_\pi(f)\rangle = \varphi_f(r, t)|\Phi_\pi(f)\rangle , \] (2.6)

\[ \varphi_f(r, t) = \int \frac{hc \, dk}{\sqrt{(2\pi)^3 2\omega_k / c}} f(k)e^{ik\cdot r - i\omega_k t} . \] (2.7)

Since the bra state is an eigenstate of the negative frequency operator, \( \hat{\phi}^-(r, t) \), and the pion operator is given by the sum of \( \hat{\phi}^+(r, t) \) and \( \hat{\phi}^-(r, t) \), we can easily calculate the transition matrix elements of the pion operator as

\[ \hat{\phi}(r, t) = \hat{\phi}^+(r, t) + \hat{\phi}^-(r, t) , \quad \hat{\phi}^-(r, t) = \left(\hat{\phi}^+(r, t)\right)^\dagger , \] (2.8)

\[ \langle \Phi_\pi(f)|\hat{\phi}(r, t)|\Phi_\pi(g)\rangle = N_\pi(f, g) \times (\overline{\varphi}_f(r, t) + \varphi_g(r, t)) , \] (2.9)

\[ N_\pi(f, g) \equiv \langle \Phi_\pi(f)|\Phi_\pi(g)\rangle = \exp \left[ \int dk\overline{f}(k)g(k) \right] . \] (2.10)

Now, we consider the following Hamiltonian of an \( N \)-body nucleon and pion system containing the second quantized pion operator \( \hat{\phi} \) in the axial vector \( P \)-wave pion-nucleon coupling:

\[ H = \sum_{i=1}^{N} \frac{p_{i}^2}{2m} + \sum_{i<j} V(r_{ij}) + \frac{1}{2hc} \int dr \left[ \nabla \hat{\phi}(r) \cdot \nabla \hat{\phi}(r) + \mu^2 \hat{\phi}^2(r) \right] \]

\[ + \sum_{i=1}^{N} \frac{f_\pi N}{\mu_\pi} \tau_0 \left( \sigma_i \cdot \nabla_i \right) \hat{\phi}(r_i) , \] (2.11)
where $\mu_\pi = m_\pi c / \hbar$, and we have omitted the time dependence in the pion part.

The matrix elements of this Hamiltonian are evaluated as

$$H = \frac{\langle \Psi(Z, f)|\hat{H}|\Psi'(Z', g) \rangle}{\langle \Psi(Z, f)|\Psi'(Z', g) \rangle} = H_N(Z, Z') + H_\pi(\vec{f}, g) + H_{\pi N}(\bar{Z}, \bar{Z}'; \vec{f}, g), \quad (2.12)$$

$$H_\pi(\vec{f}, g) = \int \frac{dr}{2\hbar c} \left\{ \{ \nabla (\varphi_f(r) + \varphi_g(r)) \}^2 + \mu_\pi^2 \{ \varphi_f(r) + \varphi_g(r) \}^2 \right\}, \quad (2.13)$$

$$H_{\pi N}(\bar{Z}, \bar{Z}'; \vec{f}, g) = \frac{f_{\pi N}}{\mu_\pi} \int d\mathbf{r} \mathbf{S}(\mathbf{r}) \cdot \nabla (\varphi_f(\mathbf{r}) + \varphi_g(\mathbf{r})), \quad (2.14)$$

$$S(\mathbf{r}) = \frac{\langle \Psi_{AMD}(\bar{Z})| \sum_i \sigma_{i0i} \delta(\mathbf{r} - \mathbf{r}_i) |\Psi_{AMD}(\bar{Z}') \rangle}{\langle \Psi_{AMD}(\bar{Z})|\Psi_{AMD}(\bar{Z}') \rangle}. \quad (2.15)$$

Here $H_N$ is the usual AMD Hamiltonian matrix element, including the $NN$ interaction.

In the actual calculation, we expand the pion eigenfunction $\varphi(r)$ in local Gaussians, whose centers and amplitudes are the variation parameters. Thus, we can apply the cooling equations for these pion parameters and nucleon phase space parameters $z_i$. We make the non-relativistic approximation in the calculation of the pionic state norm,

$$N_\pi(\vec{f}, g) \simeq \exp \left[ \frac{2m_\pi c^2}{\hbar^3 c^3} \int d\mathbf{r} \varphi_f(\mathbf{r}) \varphi_g(\mathbf{r}) \right]. \quad (2.16)$$

The Hamiltonian given in Eq. (2.11), with the pion-nucleon $P$-wave interaction, is the simplest one. In addition to the coupling with charged pions, higher dimensional terms such as the pion-nucleon $S$-wave interaction coming from the $\bar{N}\phi^2N$ coupling, would have significant contributions when pions have large expectation values. Charged pions should yield similar energy gains to neutral pions, but the coherent state treatment of charged pions mixes different charge states, and this charge mixing may lead to serious problems in the analysis of excited levels. In order to overcome this problem, it is necessary to perform a coupled-channel calculation of different nucleon and pion charge states or to perform an isospin projection.\textsuperscript{12} These are beyond the scope of this paper, and will be discussed elsewhere. On the other hand, higher-dimensional terms, such as that of the pion-nucleon $S$-wave interaction, are not expected to yield large contributions to the energy, since the number of pions is approximately 0.1 in $^{12}\text{C}$ nuclei within the present framework as is shown below.

§3. An example of application — $^{12}\text{C}$ nucleus

We have applied the AMD with coherent state pions to the study of $^{12}\text{C}$ nuclei. In the ground state of $^{12}\text{C}$, nucleons occupy the single particle states $0s_{1/2}$ and $0p_{3/2}$, both of which are yrast single particle states. For this reason, the pionic effects are expected to be large. While the $3\alpha$ cluster model generally describes the excited levels of this nucleus very well, the predicted energy of the first excited state ($2^+_1$) is too low. Since the “spin-orbit” splitting of the $0p_{3/2}$ and $0p_{1/2}$ single particle
states is responsible to the $0^+_1$-$2^+_1$ level spacing, the pionic effect to push up the $0p_{1/2}$ level may appear as the increase of $E^*(2^+_1)$ in $^{12}$C. It would be also interesting to study unnatural parity levels, such as $0^-, 1^+, 2^-, \cdots$, whose excitation energies might decrease due to the coupling to the natural parity nucleon state with the $0^-$ pionic state.

In this paper, we apply the simplest model of AMD with coherent state pions as a first step. We present the results with projection after variation (PAV). In this analysis, we first construct the intrinsic state by using the cooling variational method for the parametrized wave function Eq. (2.1), and the projection to a specified $J^\pi$ has been carried out from a prepared intrinsic state. We find that the effects of the parity projection before variation in the $^{12}$C nuclei are not large when pions are included explicitly, while it has been found to be important for spectroscopic studies of light nuclei without pions.$^{5,11}$ In the cooling stage of the intrinsic energy, the imaginary part of $\varphi_f(\mathbf{r})$ is a redundant degree of freedom, as is clear from Eqs. (2.13) and (2.14) with $\varphi_f = \varphi_g$. Therefore we cannot control the imaginary part, which is given randomly in the initial state of variation. Thus we have restricted the pion eigenfunction $\varphi(\mathbf{r})$ to be real. We find that there are many local minima, especially for small values of $f_{\pi N}$. For this reason, we have selected the lowest energy wave functions from several candidates obtained from different random seeds. Since we do not take account of the isospin projection, which enhances the tensor force effect by approximately a factor of three, we use a larger value of $f_{\pi N}$ in the range $1 \leq f_{\pi N} \lesssim \sqrt{3}$. For finite nuclei, we use the scaled coupling constant $f^{(A)}_{\pi N} = \sqrt{(A-1)/Af_{\pi N}}$ in order to approximately include the effects of the Fock (exchange) term of OPEP, which requires quantum corrections in a field description.

As the effective nucleon-nucleon interaction, we start from Brink-Boeker$^{13}$ type two range Gaussian interactions, which approximately reproduces the binding energies of $^4$He and $^{16}$O (28.4 and 128.9 MeV, BBO1$^{14}$) or the binding energy of $^4$He and nuclear matter saturation (28.1 MeV and $E/A = -16.8$ MeV at $\rho = 0.165$ fm$^{-3}$, BBO2). Since the potential energy from pions is very large, it would be important for the nucleon-nucleon interaction to have the saturation property in order to avoid collapsing. The interaction range is chosen to be shorter than that of, for example, the Volkov interaction.$^{15}$ When we include pions, we employ the nucleon-nucleon interaction BBO$\pi$, which is obtained by slightly modifying BBO2 to reproduce the ground state energy and the first excited state energy of $^{12}$C. The parameter values for these interactions are listed in Table I.

In Fig. 1, we plot the intrinsic state energy as a function of the pion number

| Table I. Volkov and Brink-Boeker-Okabe interaction parameters. The central interactions are given as the form $V = \sum_{i=1}^2 v_i \exp(-r^2/\mu_i^2)(1 - M_i - M_i P_\sigma P_\tau)$. |
|-----------------|-------|-------|-------|-------|
|                 | $\mu_1$ (fm) | $v_1$ (MeV) | $M_1$ | $\mu_2$ (fm) | $v_2$ (MeV) | $M_2$ | $f_{\pi N}$ |
| Volkov          | 1.6   | -83.34 | 0.575 | 0.82  | 144.86 | 0.575 | 0          |
| BBO$^{14}$      | 1.2   | -253.798 | 0.2186 | 0.6 | 924.631 | -1.551 | 0          |
| BBO2            | 1.2   | -258.3 | 0.25  | 0.6 | 950.00 | -1.658 | 0          |
| BBO$\pi$        | 1.2   | -258.0 | 0.25  | 0.6 | 950.00 | -1.658 | 1.63       |
Fig. 1. Intrinsic energy of $^{12}$C as a function of the pion number expectation value, $n_\pi$. Results with $f_{\pi N} = 1.0, 1.2, 1.4, 1.5, 1.6, 1.7$ and $1.8$ are shown. The dots indicate the energy minimum for $f_{\pi N} \gtrsim 1.6$.

Fig. 2. Composition of the pionic energies for $f_{\pi N} = 1.63$. The thick solid, long-dashed, and short-dashed curves show total, nucleonic, and pionic energies, respectively. For the pionic energy, the kinetic and interaction energy contributions are also plotted by the thin solid lines. The dots indicate the minimum points of $E_{\text{tot}}, E_\pi$, and $E(0^+)$. 

At small values of $f_{\pi N}$ close to one, the pure nucleon state is energetically favored.

expectation value,

$$n_\pi = \frac{\langle \Phi_\pi(f) | \int dk \hat{a}^\dagger(k) \hat{a}(k) | \Phi_\pi(f) \rangle}{\langle \Phi_\pi(f) | \Phi_\pi(f) \rangle} \approx \frac{2m_\pi c^2}{\hbar^3 c^3} \int dr \varphi_f(r) \varphi_f(r). \quad (3.1)$$
When we increase $f_{\pi N}$, the pion-nucleon interaction gives a very large binding, and the optimal state has a finite number of pions for $f_{\pi N} \gtrsim 1.6$. The total pionic energy amounts to approximately $-90$ MeV in the case $f_{\pi N} = 1.63$, as shown in Fig. 2. In well-developed pionic states, the nucleus loses energy in the nucleon part, $H_{NN}$, instead of gaining pion-nucleon interaction energy efficiently. This feature is similar to that in the case of pion condensation in high density nuclear matter.\textsuperscript{16)

In the upper panel of Fig. 3, we show the results for the total energy after the $J^\pi$ projection from the cooled intrinsic wave functions under the $n_{\pi}$ constraint. The minima for all the $J^\pi$ states are at finite $n_{\pi}$ when we adopt $f_{\pi N} = 1.63$. It is interesting that natural parity states favor smaller $n_{\pi}$, and unnatural parity states favor larger $n_{\pi}$.

Fig. 3. Pion number dependence of the total energy (top), energy difference from $0^+_1$ state (middle), and the nucleonic abnormal parity probability (bottom) for $^{12}$C. The dots indicate the energy minimum points for each $J^\pi$. 

Cal. Exp.
A finite number of pions is expected to act as an $LS$-like interaction and to increase the excitation energy of $2^+_1$. In the middle panel of Fig. 3, we plot the energy difference $E(J^+ - E(0^+_1)$ as a function of $n_\pi$ for $f_{\pi N} = 1.63$. At $n_\pi = 0$, where the present model is equivalent to the normal AMD, the $2^+_1$ state has a small excitation energy, which is a feature of $\alpha$-cluster models. Near $n_\pi \approx 0.05$, the energy difference starts to increase for the $2^+_1$ state. This increase of the energy difference for $n_\pi > 0.1$ is not a consequence of the nuclear shrinkage, but a result of a pionic $LS$-like effect. Actually, we find that the calculated rms radius grows for $n_\pi \gtrsim 0.07$.

In contrast to the positive parity rotational states, the energy differences for the $0^-_1$ and $1^+_1$ states decrease as the pion number increases. This is due to the coupling to the nucleonic abnormal parity states as

$$|\Psi(0^-)\rangle = |\Psi_N(0^-)\rangle + |\Psi_N(0^+)\rangle \otimes |\Phi_\pi(0^-)\rangle,$$  \hspace{1cm} (3.2)

for the $0^-$ state. In order to demonstrate this point, we show the nucleonic abnormal parity probability $P_N^{\text{Abn}}$ in the bottom panel of Fig. 3. At $n_\pi = 0$, all the states should be described purely in a nucleonic state ($P_N^{\text{Abn}} = 0$), but the probability increases to approximately 5% and 3% at the projected energy minima for $0^-$ and $1^+$ states, respectively. Other rotational levels are also predicted to contain an abnormal nucleonic parity component of approximately 1%. If these are true, it may be interesting to observe a pion knock-out reaction, which leaves the nucleus in unnatural parity states.

The ground state and the first $2^+$ state energy can be reproduced in AMD without pion effects when we adopt strong $LS$ interactions, but the wave functions in these two descriptions are very different. In Table II, we compare the energy components for $^{12}\text{C}$ levels in AMD employing the Volkov interaction with a strong $LS$ interaction ($V_{LS} = 1800 \text{ MeV}$) and in the present model with a moderate $LS$ interaction ($V_{LS} = 900 \text{ MeV}$). The difference in energy between $0^+$ and $2^+$ states results mainly from the $LS$ interaction in the case without pions, while the pionic energy is the main source of the energy difference when pions are included. In addition, it is interesting that the $LS$ interaction acts in the opposite manner: The $LS$ interaction is more attractive for $0^+$ without pions, but it is weakly repulsive for

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$0^+$ with pions.

§4. Summary

In this paper, we have developed a new framework to include pionic degrees of freedom in nuclear many-body systems, Antisymmetrized Molecular Dynamics (AMD) with coherent state pions. Compared to the mean field treatment of pions, the present model has the merit that it allows us to evaluate the transition matrix elements of the pion-nucleon coupling term containing the second quantized pion operator $\hat{\phi}$. This enables us to calculate the excitation energies for specified $J^\pi$ with explicit pion degrees of freedom by using the parity and angular momentum projection from the intrinsic state. It is also interesting that the pion coherent state has a non-trivial norm, and the pionic state overlap $\langle \Phi_\pi(f) | \Phi_\pi(g) \rangle$ reduces the total state overlap, $\langle \Psi(Z,f) | \Psi(Z',g) \rangle$.

We have applied this model to the study of $^{12}$C structure. The $LS$-like effects of pions can be seen in the increase of the $2^+_1$ state excitation energy. It is also suggested that the explicit pionic state $|\Psi_N(0^+)\rangle \otimes |\Phi_\pi(0^-)\rangle$ can admix into the $0^-$ state, giving a contribution of approximately 5% in the case $f_{\pi N} = 1.63$.

In order to obtain firm conclusions concerning explicit pionic effects in nuclear structure, further theoretical and experimental developments are needed. First, charged pions should be included in the framework. Combined with the charge (isospin) projection, the inclusion of pions is expected to enhance the tensor effect by a factor of three. We have simulated this enhancement by increasing the pion-nucleon coupling, $f_{\pi N}$, but the proton-neutron charge exchange may lead to non-trivial effects which cannot be mimicked by increasing $f_{\pi N}$. Next, we should treat the exchange term (Fock term) and the zero range ($\delta$ type) part of the OPEP in a manner that is more reliable than simply scaling the coupling constant by a factor of $\sqrt{(A-1)/A}$. Including the Landau-Migdal interaction may be an efficient way to solve this problem. The extension of the wave function is also an important possibility to consider. Since we have assumed that the total wave function is a product of the nucleonic state and pionic coherent state, the nucleonic part of the wave function is the same for the zero and one pion states. Thus the nucleonic part of the wave function has to contain both the $T = 0$ and $T = 1$ states. This may lead to an underestimate of the binding energy. Works on these topics are in progress.

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