

δ -pairing forces and collective pairing vibrations

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Abstract. The collective pairing Hamiltonian is obtained in the framework of the generator coordinate method in the Gaussian overlap approximation with a slightly modified BCS function used as a generator function. The collective variable α , measuring the monopole moment of the pairing field, and the gauge transformation angle ϕ are chosen as generator coordinates. The vibrational ground states are calculated by diagonalisation of the collective pairing Hamiltonian in the harmonic-oscillator basis.

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1 Introduction

The collective pairing Hamiltonian was originally introduced in ref. [1], where the intrinsic deformation of the pairing field α , related to the BCS gap parameter Δ , and the gauge transformation angle ϕ were used as collective variables. The pairing Hamiltonian was then derived in the framework of the cranking approximation. A more general method which determines the wave functions and the collective Hamiltonian is the Generator Coordinate Method (GCM). The GCM derivation of the collective Hamiltonian with the BCS functions as the generator functions were already performed in refs. [2–4], where the Gaussian Overlap Approximation (GOA) of the generator wave functions was used. The collective pairing Schrödinger equation was constructed using the single-particle plus monopole pairing Hamiltonian.

The aim of this paper is to derive collective vibrations of the pairing field in the GCM + GOA approach for the Hamiltonian based on the single-particle Nilsson potential [5] and the δ -pairing interaction [6–8]. The latter requires introducing a suitable collective variable different from the monopole pairing gap used in [2]. Here we have used the same generator coordinate $\alpha = \sum u_k v_k$ as in ref. [1], which, as suggested in ref. [9], is a natural choice for this type of collective motion.

The paper is organized as follows: In sect. 2 we discuss the properties of the δ -pairing interaction. In sect. 3 the collective coordinates and the form of the collective pairing Hamiltonian are introduced. The formulae for the GCM + GOA mass parameters are compared to the cranking ones. The method of diagonalising the collective pairing Hamiltonian is described in sect. 4. Section 5

contains numerical results and sect. 6 conclusions. In appendix A we discuss the multipole expansion of the δ force and demonstrate the validity of our choice of α as the collective coordinate.

2 δ -pairing forces

The nuclear mean-field Hamiltonian with the residual pairing interaction can be written as

$$\hat{H} = \hat{H}_{\text{s.p.}} + \hat{H}_{\text{pair}}, \quad (1)$$

where

$$\hat{H}_{\text{s.p.}} = \sum_{k>0} \langle k | \hat{h} | k \rangle (c_k^\dagger c_k + c_{\bar{k}}^\dagger c_{\bar{k}}), \quad (2)$$

$$\hat{H}_{\text{pair}} = - \sum_{k,l>0} V_{k\bar{k}l\bar{l}} c_k^\dagger c_{\bar{k}}^\dagger c_l c_{\bar{l}}. \quad (3)$$

The summation runs over the eigenstates $|k\rangle$ of the single-particle Hamiltonian \hat{h} . The antisymmetrized matrix element of the pairing interaction $V_{k\bar{k}l\bar{l}}$ in the pairing Hamiltonian (3) is given by the following expression:

$$\begin{aligned} V_{k\bar{k}l\bar{l}} = & \int d^3 r_1 d^3 r_2 \sum_{\sigma_1 \sigma_2} \Phi_k^*(\mathbf{r}_1, \sigma_1) \Phi_{\bar{k}}^*(\mathbf{r}_2, \sigma_2) \\ & \times V^\tau(\mathbf{r}_1, \sigma_1; \mathbf{r}_2, \sigma_2) \\ & \times [\Phi_l(\mathbf{r}_1, \sigma_1) \Phi_{\bar{l}}(\mathbf{r}_2, \sigma_2) - \Phi_{\bar{l}}(\mathbf{r}_1, \sigma_1) \Phi_l(\mathbf{r}_2, \sigma_2)]. \end{aligned} \quad (4)$$

Here $\Phi_k(\mathbf{r}, \sigma)$ is the single-particle eigenfunction of \hat{h} in the space (\mathbf{r}) and spin (σ) representation and $\Phi_{\bar{k}}(\mathbf{r}, \sigma)$

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is its time reversal counterpart. $V^\tau(\mathbf{r}_1, \boldsymbol{\sigma}_1; \mathbf{r}_2, \boldsymbol{\sigma}_2)$ is the δ -pairing force [6]

$$V^\tau(\mathbf{r}_1, \boldsymbol{\sigma}_1; \mathbf{r}_2, \boldsymbol{\sigma}_2) = V_0^\tau \frac{1 - \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2}{4} \delta(\mathbf{r}_1 - \mathbf{r}_2). \quad (5)$$

In the following we consider the proton-proton (p-p) and neutron-neutron (n-n) part of the interaction only. Taking this into account, one obtains

$$G_{kl} = V_{k\bar{k}l\bar{l}} = V_0 \int d^3r \rho_k(\mathbf{r}) \rho_l(\mathbf{r}), \quad (6)$$

where

$$\rho_k(\mathbf{r}) = |\Phi_k(\mathbf{r})|^2 \quad (7)$$

and V_0 is the pairing interaction strength as adjusted in ref. [10]. The pairing gap equations become

$$\Delta_k = \frac{1}{2} \sum_{l>0} G_{kl} \frac{\Delta_l}{\sqrt{(e_l - \lambda)^2 + \Delta_l^2}}, \quad (8)$$

where e_l is the single-particle energy and the Fermi level λ is determined from the particle number equation

$$N = \sum_{k>0} \left(1 - \frac{e_k - \lambda}{\sqrt{(e_k - \lambda)^2 + \Delta_k^2}} \right). \quad (9)$$

The coupled set of eqs. (8) and (9) is solved numerically by the appropriate iteration procedure.

3 Collective pairing Hamiltonian

Following ref. [11] we construct the monopole pairing operator (see appendix A) which characterizes the amplitude of excitations connected with vibrations of the pair density:

$$\hat{A} = \frac{1}{2} \sum_{k>0} \left(e^{-2i\phi} c_k^\dagger c_k^\dagger + e^{2i\phi} c_{\bar{k}} c_{\bar{k}} \right). \quad (10)$$

The pair condensate can be described by the mean value of the operator (10) in the BCS-like state

$$|\alpha\phi\rangle = e^{iN\phi} \prod_{k>0} \left(u_k + v_k e^{-2i\phi} c_k^\dagger c_k^\dagger \right) |0\rangle, \quad (11)$$

where N is the number of particles, ϕ is the gauge angle and the average pairing gap is given by the expectation value of the operator (10):

$$\alpha = \langle \alpha\phi | \hat{A} | \alpha\phi \rangle = \sum_{k>0} u_k v_k. \quad (12)$$

Using (11) as a generator function and α, ϕ as generator coordinates and following the steps of ref. [2] the collective Hamiltonian

$$\begin{aligned} \hat{\mathcal{H}}_{\text{coll}} = & -\frac{\hbar^2}{2\sqrt{\det\gamma_{\alpha\alpha}}} \frac{\partial}{\partial\alpha} \sqrt{\det\gamma_{\alpha\alpha}} \mathcal{M}_{\alpha\alpha}^{-1} \frac{\partial}{\partial\alpha} \\ & -\frac{1}{2} \hbar^2 \mathcal{M}_{\phi\phi}^{-1} \frac{\partial^2}{\partial\phi^2} \\ & -i\hbar \frac{\text{Im} \left\langle \alpha\phi \left| \frac{\partial}{\partial\phi} \hat{H} \right| \alpha\phi \right\rangle}{\gamma_{\phi\phi}} \frac{\partial}{\partial\phi} + V(\alpha), \end{aligned} \quad (13)$$

is derived. In eq. (13) $\gamma_{\alpha\alpha}, \gamma_{\phi\phi}$ are related to the widths of the Gaussian overlap and $\mathcal{M}_{\alpha\alpha}^{-1}, \mathcal{M}_{\phi\phi}^{-1}$ are the components of the inverse mass tensor. The quantities appearing in eq. (13) are analogous to the general expressions obtained for the Δ and ϕ coordinates in the monopole pairing case [2]. $V(\alpha)$ is the collective pairing potential equal to

$$V(\alpha) = \langle \alpha\phi | \hat{H} | \alpha\phi \rangle - \mathcal{E}_0, \quad (14)$$

where \mathcal{E}_0 is the so-called zero-point energy. The collective pairing Hamiltonian (13) is Hermitian with the Jacobian

$$d\tau = \sqrt{\gamma_{\alpha\alpha} \gamma_{\phi\phi}} \alpha d\alpha d\phi. \quad (15)$$

It means that the eigenfunctions of (13) should be orthogonal with the above measure.

The mean value of the Hamiltonian (1) is evaluated using the constraints $N = \text{const}$ and $\alpha = \text{const}$, which leads to minimization of the average value of the operator

$$\hat{H}' = \hat{H} - \lambda(\hat{N} - \langle \alpha\phi | \hat{N} | \alpha\phi \rangle) - \xi(\hat{A} - \langle \alpha\phi | \hat{A} | \alpha\phi \rangle), \quad (16)$$

calculated in the BCS state (11). Here λ and ξ are Lagrange multipliers.

The expectation value of the BCS Hamiltonian in eq. (14) is given by

$$\begin{aligned} E_{\text{BCS}} = \langle \alpha\phi | \hat{H} | \alpha\phi \rangle = \\ 2 \sum_{k>0} e_k v_k^2 - \frac{1}{2} \sum_{k>0} \frac{\Delta_k^2}{E_k} - \sum_{k>0} G_{kk} v_k^4, \end{aligned} \quad (17)$$

where $E_k = \sqrt{(e_k - \lambda)^2 + \Delta_k^2}$ is the quasiparticle energy.

The final expressions for the nonvanishing components of the metric and mass tensors are

$$\gamma_{\alpha\alpha} = \sigma^2 \sum_k \frac{(e_k - \lambda)^2}{16E_k^4}, \quad (18)$$

$$\gamma_{\phi\phi} = \sum_k \frac{\Delta_k^2}{E_k^2}, \quad (19)$$

$$\mathcal{M}_{\alpha\alpha}^{-1} = \sum_k E_k \sigma^2 / \gamma_{\alpha\alpha}^2, \quad (20)$$

$$\mathcal{M}_{\phi\phi}^{-1} = \sum_k \frac{\Delta_k^2}{E_k} / \gamma_{\phi\phi}^2, \quad (21)$$

where σ is equal to

$$\sigma = \left(\sum_k \frac{(e_k - \lambda)^2}{4E_k^3} \right)^{-1}. \quad (22)$$

The zero-point energy appearing in eq. (14) reads

$$\begin{aligned} \mathcal{E}_0 = \mathcal{E}_0^\alpha + \mathcal{E}_0^\phi = \\ \frac{1}{2} \left(\sum_k \frac{(e_k - \lambda)^2}{16E_k^3} \sigma^2 / \gamma_{\alpha\alpha} + \sum_k \frac{\Delta_k^2}{E_k} / \gamma_{\phi\phi} \right). \end{aligned} \quad (23)$$

The first term in eq. (23) represents the collective correlations in the ground-state energy, whereas the second corresponds to the approximate particle number projection [4].

An alternative method of treating collective vibrations is the cranking model [12, 13]. The mass parameters in this case read

$$\mathcal{M}_{\alpha\alpha}^{\text{cr}} = 2\sigma^2 \sum_k \left(\frac{e_k - \lambda}{16E_k^3} \right)^2, \quad (24)$$

$$\mathcal{M}_{\phi\phi}^{\text{cr}} = \sum_k \frac{\Delta_k^2}{E_k^3} \quad (25)$$

and the collective potential is usually assumed to be equal to E_{BCS} (17).

4 Diagonalisation of the collective pairing Hamiltonian

Having found the collective potential, the mass and the metric tensors, we can evaluate the collective Hamiltonian numerically. Only the vibrational spectra will be constructed here as the quasirotational states correspond to the bands built from the ground-states function of the neighbouring even-even isotopes (or isotones). In the first step we perform a transformation from the α -coordinate to a new variable x in which the mass parameter \mathcal{M}_{xx} is nearly constant:

$$\mathcal{M}_{xx} \approx \mathcal{M}_{\alpha\alpha} \left(\frac{\partial\alpha}{\partial x} \right)^2 = \text{const}. \quad (26)$$

The mass parameter $\mathcal{M}_{\alpha\alpha}$ is a rapidly decreasing function of α and can be approximated by the function

$$\mathcal{M}_{\alpha\alpha} = \frac{b}{(\alpha + \alpha_0)^2}, \quad (27)$$

where α_0 and b parameters are chosen to approximate the mass parameter in the best way. Variables x and α are connected through the equation

$$x = \sqrt{b/\mu} \ln \left(1 + \frac{\alpha}{\alpha_0} \right), \quad (28)$$

where μ is an arbitrary constant. The basis states used to diagonalise the Hamiltonian (13) are generated by the harmonic-oscillator Hamiltonian

$$\hat{H}_B = -\frac{\hbar^2}{2\mathcal{M}_{xx}} \frac{d^2}{dx^2} + \frac{1}{2} \mathcal{M}_{xx} \omega^2 x^2, \quad (29)$$

with the frequency ω determined from the plateau condition of the energy $\partial E/\partial\omega \approx 0$, where E is the ground-state energy of the collective Hamiltonian (13). In our case only the even eigenstates are picked (see [2]):

$$\hat{H}_B \psi_i = \left(i + \frac{1}{2} \right) \psi_i, \quad i = 0, 2, 4, \dots \quad (30)$$

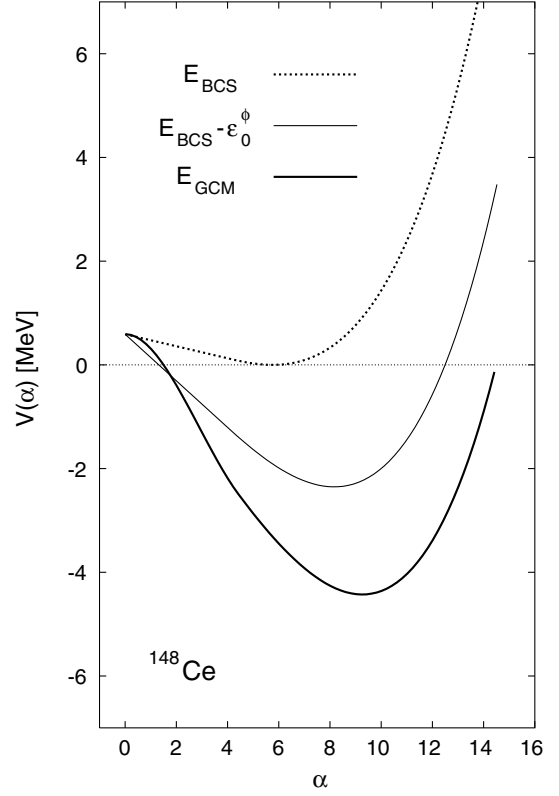


Fig. 1. Pairing potentials: the BCS energy (dotted line), the GCM collective potential (solid line) and the particle number corrected BCS energy $E_{\text{BCS}} - \mathcal{E}_0^\phi$ (thin solid line) as functions of the collective coordinate α for protons in ^{148}Ce . The zero value on the abscissa corresponds to the minimum of the BCS energy.

These eigenstates which satisfy the usual normalization conditions

$$\int_0^\infty \psi_i \psi_j dx = \delta_{ij} \quad (31)$$

are employed to calculate the matrix elements of the collective Hamiltonian (eq. 13). The diagonalization was performed in a basis of $N_{\text{max}} = 19$ oscillator shells.

5 Results

We have considered a few nuclei in the rare-earth region. The $A = 165$ parameter set of the single-particle Nilsson potential is used [14]. The δ -pairing strengths as obtained in ref. [10] are

$$\begin{aligned} V_0^{\text{neutrons}} &= 230 \text{ MeV fm}^3, \\ V_0^{\text{protons}} &= 240 \text{ MeV fm}^3. \end{aligned} \quad (32)$$

The fit of the V_0 parameters was done for the pairing window with $2\sqrt{15}n$ levels closest to the Fermi energy where $n = N$ for neutrons and $n = Z$ for protons [14].

Figure 1 shows the pairing potentials for BCS and GCM models. The dotted line represents the pure BCS energy (17) as a function of the collective coordinate α ,

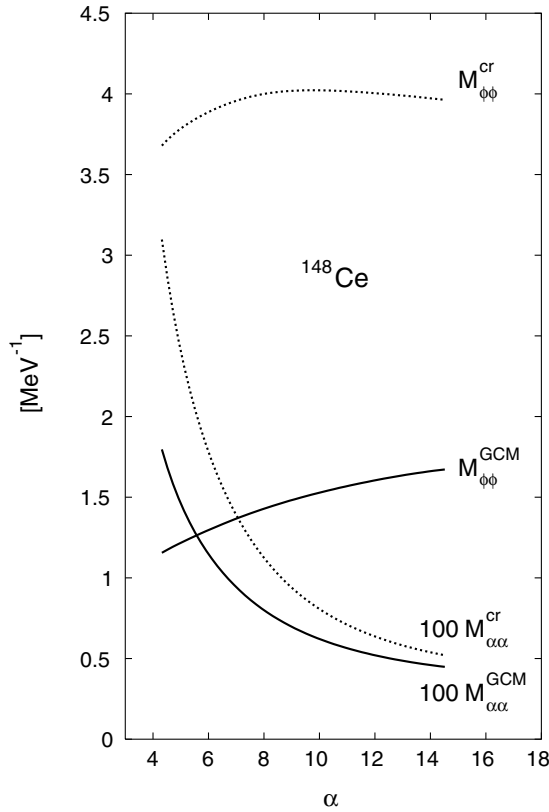


Fig. 2. Components of GCM and the cranking mass parameters for protons in ^{148}Ce . The $M_{\alpha\alpha}$ components are multiplied by a factor 100. The components $M_{\phi\phi}$ are in natural units.

whereas the solid line corresponds to the GCM collective potential (14). The particle number corrected BCS energy, *i.e.*, the one with extracted \mathcal{E}_0^ϕ energy is also shown (thin solid line). The zero value on the abscissa corresponds to the minimum of the BCS energy. The particle number projected energy is about 2 MeV deeper than the BCS energy minimum and its position is shifted in the direction of larger α . Analogously, the GCM ground-state energy which additionally contains the zero-point energy corresponding to the pure α vibrations has a minimum shifted by a similar amount towards larger α .

The $M_{\alpha\alpha}$ and $M_{\phi\phi}$ components of the mass tensor for both GCM and the cranking model are shown in fig. 2. The ratio of the α -component of the cranking mass (dotted line) to the GCM mass (solid line) is close to 2/3 in the vicinity of the minimum of the GCM potential. The decrease of the collective mass with α (or Δ) has a significant influence on the spontaneous fission half-lives of heavy nuclei, as shown for the Δ collective coordinate, as well as on the height of the fission barriers (see, *e.g.*, [15]). Similarly, in case of the collective Bohr model calculations [16,17] the inclusion of the coupling of quadrupole vibrations improves significantly the agreement with the experimental data.

In fig. 3 we show the collective potential $V(\alpha)$ (solid line), the GCM mass parameter $M_{\alpha\alpha}(\alpha)$ (dotted line) and the probability density $P = |\Phi_0(\alpha)|^2 \sqrt{\gamma_{\alpha\alpha}\gamma_{\phi\phi}}$ of the

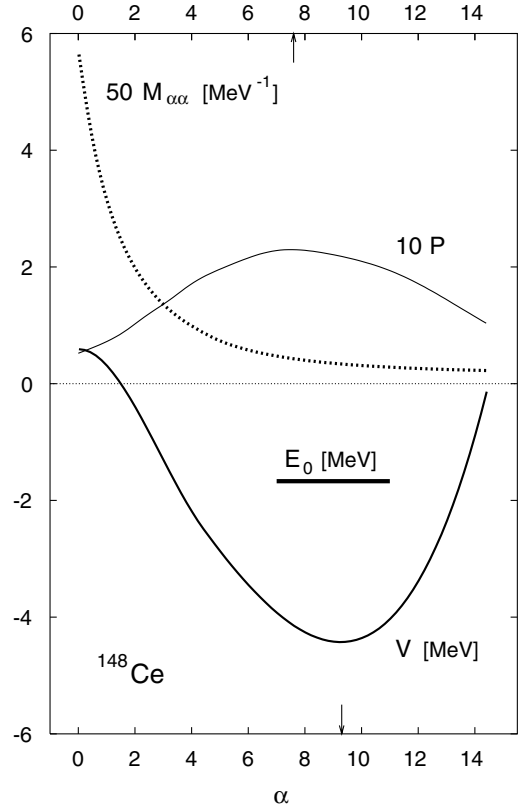


Fig. 3. The collective potential $V(\alpha)$ (solid line), the GCM mass parameter $M_{\alpha\alpha}(\alpha)$ (dotted line) and the probability density $P = |\Phi_0(\alpha)|^2 \sqrt{\gamma_{\alpha\alpha}\gamma_{\phi\phi}}$ (thin solid line) of the ground state for protons in ^{148}Ce . The ground-state energy E_0 is marked. The arrows indicate the positions of the minimum of the potential and the maximal value of the probability distribution on the α axis.

ground state (thin solid line). The short line segment in the middle of the figure marks the position of the ground-state energy. The arrows indicate the positions of the minimum of the potential (bottom scale) and the maximal value of the probability distribution (top scale). The α value of the equilibrium is 9.3 and the most probable value is 7.6. The latter is shifted towards smaller α values which implies the increase of the $M_{\alpha\alpha}$ by a 1.5 factor on average. This behaviour is common for the majority of nuclei in the considered region. As shown in ref. [16] in case of monopole pairing the use of the most probable value of the gap parameter (instead of the BCS gap) leads to a considerable improvement of the predictive power of the Bohr Hamiltonian.

6 Conclusions

The first-excited collective pairing vibrational states for even-even nuclei in the rare-earth region appear at energies close to 2.5 MeV for protons and 4.5 MeV for neutrons. Usually they have higher energies than two-quasiparticle excitations and consequently one has to include these correlations in the ground state, only.

Since the pairing vibrations are strongly coupled with shape degrees of freedom of the nucleus, it is hard to compare the results (which are similar to that obtained with the coordinate Δ) with experimental data.

Finally, it should be emphasized that the role of the collective coordinate α is analogous to the Δ -coordinate considered earlier.

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Appendix A. Multipole expansion of the $\delta(\mathbf{r})$ force

In the following we consider the short-range interaction operating between equivalent nucleons ($T = 1$, protons or neutrons)

$$\begin{aligned} V_{12}(\delta) &= V(\mathbf{r}_1, \boldsymbol{\sigma}_1; \mathbf{r}_2, \boldsymbol{\sigma}_2) \\ &= V_0 \frac{1 - \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2}{4} \delta^3(\mathbf{r}_1 - \mathbf{r}_2), \end{aligned} \quad (\text{A.1})$$

equal to $V_0 \delta^3(\mathbf{r})$ in case of the spin singlet ($S = 0$) and to 0 for the spin triplet ($S = 1$).

One can use the following representation of $\delta(\mathbf{r})$:

$$\delta^3(\mathbf{r}_1 - \mathbf{r}_2) = \frac{1}{r_1 r_2} \delta(r_1 - r_2) \delta(\cos \theta_1 - \cos \theta_2) \delta(\phi_1 - \phi_2). \quad (\text{A.2})$$

This form is very useful when separating the angular and radial parts. Using the relation

$$\begin{aligned} \delta(\cos \theta_1 - \cos \theta_2) \delta(\phi_1 - \phi_2) &= \\ \sum_K \frac{2K+1}{4\pi} \sum_M Y_{KM}^*(\theta_1, \phi_1) Y_{KM}(\theta_2, \phi_2), \end{aligned} \quad (\text{A.3})$$

and the angular-momentum algebra (see Talmi [18]), one gets the following energy shift of the identical ($T = 1$) particles state $|j_1 j_2 J\rangle$:

$$V_\delta(J) = V_0 F_R(n_1 l_1 n_2 l_2) I(j_1 j_2 J), \quad (\text{A.4})$$

where

$$F_R(n_1 l_1 n_2 l_2) = \frac{1}{4\pi} \int \frac{1}{r^2} R_{n_1 l_1}^2(r) R_{n_2 l_2}^2(r) dr \quad (\text{A.5})$$

and

$$\begin{aligned} I(j_1 j_2 J) &= \frac{(2j_1+1)(2j_2+1)}{1 + \delta_{n_1 n_2} \delta_{l_1 l_2}} \begin{pmatrix} j_1 & j_2 & J \\ 1/2 & -1/2 & 0 \end{pmatrix}^2, \\ & \quad (l_1 + l_2 + J \text{ even}). \end{aligned} \quad (\text{A.6})$$

Now we show that the δ interaction is separable in the *particle-particle* channel. To do this, we define the creation operators of a *pair* of particles coupled to the angular momentum JM :

$$P_{JM}^\dagger = \frac{1}{\sqrt{2}} \sum_{m_1 m_2} (j_1 m_1 j_2 m_2 | JM) c_{m_1}^\dagger c_{m_2}^\dagger \quad (\text{A.7})$$

and its Hermite conjugate

$$P_{JM} = \left(P_{JM}^\dagger \right)^\dagger. \quad (\text{A.8})$$

Here a_m^\dagger creates a nucleon in $(nljm)$ single-particle state. The δ interaction can be written in second quantized form

$$V_{12}(\delta) = \sum_{J, \text{even}} V_\delta(J) \sum_M P_{JM}^\dagger P_{JM}. \quad (\text{A.9})$$

Note that $V_\delta(J)$ does not depend on the third component M of the total angular momentum of a pair.

Since the pairing force is the interaction in the particle-particle channel with the third angular-momentum component $M = 0$, the operator P_{JM}^\dagger defined in eq. (A.7) simplifies to $P_J^\dagger \equiv P_{J, M=0}^\dagger$ and the summation in (A.7) runs over $m = m_1 = -m_2$ only.

The part of the interaction corresponding to $J = 0$ is the *classical pairing* (monopole pairing interaction). The next component $J = 2$ forms the *quadrupole* pairing force and so on. The monopole pairing term reads

$$V_\delta(0) \sum_{m, m'} c_m^\dagger c_m^\dagger c_{\bar{m}'} c_{m'}. \quad (\text{A.10})$$

The operator $c_{\bar{m}}^\dagger$ creates a particle in the time reversal state (\bar{m}) which is defined by

$$c_{\bar{m}}^\dagger = (-1)^{j-m} c_{-m}^\dagger. \quad (\text{A.11})$$

The quadrupole ($J = 2$) part of eq. (A.9) reads

$$V_\delta(2) \sum_{m, m'} (j_1 m j_2 - m | 20) (j_1 m' j_2 - m' | 20) c_m^\dagger c_m^\dagger c_{\bar{m}'} c_{m'}, \quad (\text{A.12})$$

etc. Each term in eq. (A.9) separates in a similar manner. The strength $V_\delta(J)$ of each multipole is different and depends on V_0 and the quantum numbers $(n_1 l_1 j_1)$, $(n_2 l_2 j_2)$ and J (see eq. (A.4)).

It is easy to show that for, *e.g.*, $j_1 = j_2 = 9/2$ the ratio $V_\delta(2)/V_\delta(0) \approx 0.24$, $V_\delta(4)/V_\delta(0) \approx 0.12$ etc. Therefore, the state $J = 0$ has the largest energy shift towards the lowest energies (assuming V_0 is a positive constant).

In analogy to eq. (10) one can define the following operators (only even J values are allowed; see eq. (A.9)):

$$\hat{A}_J = \frac{1}{2} (e^{-2i\phi} P_J^\dagger + e^{2i\phi} P_J), \quad J = 0, 2, 4, \dots \quad (\text{A.13})$$

The operators \hat{A}_J describe different multiplicities of the pairing field. Their average values are the multipole *deformations* of the pairing field. The mean-pairing-field Hamiltonian equivalent to the δ force expressed in terms of the field operators \hat{A}_J reads

$$\hat{V}_{12}(\delta) = \sum_{J, \text{even}} V_\delta(J) \alpha_J \hat{A}_J, \quad (\text{A.14})$$

where

$$\alpha_J = \langle \hat{A}_J \rangle \quad (\text{A.15})$$

is the *multipole deformation* of the pairing field. The term \hat{A}_0 corresponds to the operator \hat{A} used in the present paper (see eq. (10)) and describes the monopole-type deformation and the parameter α_0 corresponds to the collective deformation parameter α used in the text:

$$\alpha \sim \alpha_0. \quad (\text{A.16})$$

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