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Fixed Particle Number and Angular Momentum Double-Projected BCS Wave Functions

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In this paper, a method for projecting the usual BCS states simultaneously onto the eigenstates of particle number and angular momentum is suggested. Fomenko's method of projection in the occupation number space, which leads to rapidly converging series, seems to be very suitable to a subsequent projection onto the eigenstates of angular momentum. For simplicity, the deformation is restricted to be axially symmetric, and general double-projection formulas are established in this case. Simple numerical model calculations, using the adiabatic assumption, show that it is important to project the BCS states onto the particle-number eigenstates before computing the rotational spectrum and the moment of inertia.

1. INTRODUCTION: NUMBER-CONSERVING PAIRING

A straightforward diagonalization of the residual forces in many nuclear calculations becomes unmanageable whenever the nucleus is away from a closed shell, because of the numerous nearly degenerate configurations that are possible for a few nucleons moving in an unfilled major shell.

The BCS theory[1-7] allows for avoiding this difficulty, but the trial function used in the variational process is not an eigenfunction of the number of particles. The dispersion in the number (which is of the same order as the square root of the number of particles) is practically negligible in the theory of superconductivity. In nuclear physics, the errors connected with nonconservation of the number of particles are considerable because of the smaller relative density of the levels of the average nuclear field. Thus, the BCS approximation yields relatively poor results both for the ground-state and for the first-excited-state energies; this is undoubtedly due to the spurious components contained in the BCS wave functions. Furthermore, the presence of these unphysical components seems to be the reason for the existence of an unphysical critical value G_c of the pairing force strength, below which there is no solution to the BCS equations, except for the trivial one that gives no configuration mixing at all.[8-12]

Several methods have been proposed, dealing with the problem of number conservation in pairing correlations:

(i) Bayman's steepest descent method[13-15] which taken in its simplest formulation is the usual BCS approximation,[13] and the improvements to this approach by Iwamoto and Onishi, with the large-fluctuations approximation.[16]

(ii) Lipkin's method of the curvature of the separation energy as function of particle number.[17-20]

(iii) Methods of projection: the Kerman, Lawson, and Macfarlane[21] exact diagonalization method [projected BCS (PBCS)] and [fixed BCS (FBCS)][15] method where the variation is done after the projection of fixed particle components rather than before. The PBCS and FBCS methods differ by the order in which projection and variation are performed. The methods of Refs. 9, 13, 22, and 23 can also be considered as projection methods. Fomenko's approximation[22] consists in the substitution of integrals by summations, which in the practical use, are rapidly converging.

(iv) The equations-of-motion methods have been extensively discussed by Salusti,[24] Jean,[25] and Klein and his co-workers.[26,29] Mauger and Evans, developing an idea by Covello and Salusti,[27] also take into account the Pauli principle.[28]

(v) Algebraic methods, approximately conserving the number of particles have been shown to be powerful approaches to the study of pairing interactions.[28-30]

(vi) The spurious effects of the dispersion in the number of particles can be approximately eliminated within the random-phase approximation (RPA).[11,31,32] We can quote also the broken-pair approximation using the Tamm-Dancoff method.[33]

(vii) Boson expansions have been used by Sorensen and Kleber.[34]

(viii) The second-order perturbation theory yields good numerical results for low values of the pairing-force parameter.[11]

(ix) Variational methods[11,29,35,36] and

(x) generator-coordinate methods[37,38] have been used in the pairing correlation problem.

(xi) Let us mention too the method of the eigen wave functions strictly conserving the number of particles.[39] Finally, we note that the Lipkin-Nogami method[17,19,40] recently reviewed[41] in its different applications with or without projection or orthogonalization seems to be applicable for any value of the coupling strength, although it is less accurate than perturbation theory[11] for $G \leq G_c$.

The projected wave functions, like the BCS func-

tions, are not eigenfunctions of the angular momentum. A few calculations[37,42] use generator-coordinate methods to obtain the rotational spectra of the ground state from the BCS wave functions.

In this work, we propose a double projection of the BCS wave functions: First, we select, by projection, the components corresponding to an exact number of particles; then, we select by projection on the angular momentum, the rotational spectra of even-even nuclei. To our knowledge, this program does not appear to have been performed, so it seems to us necessary to investigate the importance of the dispersion of the number of particles in a wave function intended to be split up into components with a fixed angular momentum.

In the following section, we present the method of double projection of the usual BCS state. In Sec. III, the practical calculation, with the approximations used, is outlined. The results obtained by model calculations are discussed in Sec. IV.

II. GENERAL METHOD OF DOUBLE PROJECTION

The BCS wave function is projected with respect to the particle number by the method of Fomenko.[22] A general method of angular momentum projection of the obtained wave function is then outlined.

A. Projection in the Occupation-Number Space

The method of Ref. 22, which may be applied to the description of all the excited states with nonzero seniority, has the advantage of replacing the Fowler-Darwin type integrals by discrete sums. It seems very suitable in practical calculations. A system of P pairs of particles (neutrons or protons), interacting through the pairing effect, is generally described by the Hamiltonian

$$H=\sum_{\nu}(E_{\nu}-\lambda_f)(a_{\nu}^{\dagger}a_{\nu}+a_{\bar{\nu}}^{\dagger}a_{\bar{\nu}})-G\sum_{\nu,\nu'}a_{\nu'}^{\dagger}a_{\bar{\nu}'}^{\dagger}a_{\bar{\nu}}a_{\nu}\,, \tag{1}$$

where $a_{\nu}^{\dagger}$ and a_{ν} are the creation or annihilation operators for a particle with an individual energy E_{ν} in the state $|\nu\rangle$; λ_f and G correspond to the chemical potential and the pairing constants, respectively; the $|\bar{\nu}\rangle$ state is obtained from $|\nu\rangle$ by time reversal.

In the BCS theory, the trial wave function used in the variational calculation is represented by

$$|\psi_0\rangle=\prod_{\nu}(u_{\nu}+v_{\nu}a_{\nu}^{\dagger}a_{\bar{\nu}}^{\dagger})|0\rangle\,. \tag{2}$$

$|0\rangle$ is the true particle vacuum and v_{ν}, u_{ν} are the occupation and inoccupation amplitudes in the state $|\nu\rangle$, respectively. They satisfy the normalization condition ($u_{\nu}^2+v_{\nu}^2=1$) and are determined from the conditions of minimization of the energy and average conservation of the number of particles in the $|\psi_0\rangle$ state, the chemical potential being regarded as a Lagrange multiplier. The $|\psi_0\rangle$ ket describes a mixing of states with number of pairs of particles: $P\pm1$, $P\pm2$, ... The trial ket

$$|\psi_1\rangle=(-1)^P\prod_{\nu}(u_{\nu}-v_{\nu}a_{\nu}^{\dagger}a_{\bar{\nu}}^{\dagger})|0\rangle \tag{3}$$

has the same physical properties as $|\psi_0\rangle$, the components corresponding to a given number of pairs of particles being the same in both cases.

It is clear that the two (unnormalized) kets $|\psi_{\pm}\rangle$ defined by

$$|\psi_{\pm}\rangle=|\psi_0\rangle\pm|\psi_1\rangle \tag{4}$$

describe states with a number of pairs differing from P by an even or odd integer, respectively.

More generally, we consider the kets

$$|\psi_n\rangle=C\left\{\sum_{k=0}^{n+1}\epsilon_k\eta_k^{-P}\prod_{\nu}(u_{\nu}+\eta_k v_{\nu}a_{\nu}^{\dagger}a_{\bar{\nu}}^{\dagger})+\text{c.c.}\right\}|0\rangle \tag{5}$$

with

$$\eta_k=e^{i(k\pi)/n+1}$$

and

$$\epsilon_k=\begin{cases}1 & \text{if } k=0 \text{ or } n+1\\ \frac{1}{2} & \text{if } 0<k<n+1\,,\end{cases}$$

and where n is a nonnegative integer and C, a normalization constant. In Eq. (5), only the components, corresponding to numbers of pairs $P\pm2l\times(n+1)$, differ from zero (l is an integer $l\geq0$). If $2(n+1)>\max(P,\Omega-P)$ (Ω represents the total pairs degeneracy of the system[43]) the $|\psi_n\rangle$ state coincides with the component having P pairs of particles. In fact, the components, with a number of pairs very different from P, have very small amplitudes; it is possible to observe a convergence for the $|\psi_n\rangle$ set with $n\sim3,4$.

B. Projection Description of the Rotational Bands

While the Hamiltonian of the system, given in Eq. (1), has the axial symmetry, the projected wave function of Eq. (5), like the trial wave function of Eq. (2), does not correspond to a given angular momentum. Therefore, it is necessary to take out the components with well determined values of the angular momentum J and of its projection K on the symmetry axis $0z$. First of all, in agreement with Ref. 37, we remark that the projected state can be written, without any approx-

imation:

$$|\psi_n\rangle = C\left\{\sum_{k=0}^{n+1}\epsilon_k\eta_k^{-P}\left(\prod_{\nu>0}u_\nu\right)\times\exp\left(\tfrac{1}{2}\eta_k\sum_{\alpha\beta}f_{\alpha\beta}a_\alpha^\dagger a_\beta^\dagger\right)+\text{c.c.}\right\}|0\rangle, \tag{6}$$

where $f_{\alpha\beta}$ is the general form of the correlation function

$$f_{\alpha\beta}=\frac{v_\alpha}{u_\alpha}\delta_{\alpha\tilde{\beta}}.$$

The projected wave function, describing a system of P pairs of particles with an angular momentum J and its $0z$ component K, is given by the integral[44]

$$\psi_J^K(n)=\int_0^\pi \sin\theta\, d\theta\int_0^{2\pi}d\phi\int_0^\pi d\gamma D_{K0}^J(\phi\theta\gamma)\Psi_n(\phi\theta\gamma), \tag{7}$$

where $\Psi_n(\phi\theta\gamma)$ is the ψ_n function rotated through Euler angles ϕ, θ, γ:

$$|\Psi_n(\phi\theta\gamma)\rangle = C\left\{\sum_{k=0}^{n+1}\epsilon_k\eta_k^{-P}\prod_\nu u_\nu\right)\times\exp\left(\tfrac{1}{2}\eta_k\sum_{\alpha\beta}F(\phi\theta\gamma)a_\alpha^\dagger a_\beta^\dagger\right)+\text{c.c.}\right\}|0\rangle. \tag{8}$$

In the notation of Ref. 37, we have

$$F_{\alpha\beta}(\phi\theta\gamma)=\sum_{\alpha'\beta'}d_{\alpha\alpha'}(\phi\theta\gamma)d_{\beta\beta'}(\phi\theta\gamma)f_{\alpha'\beta'}$$

and

$$d_{\alpha\beta}=\langle\alpha|e^{-i\phi J_z}e^{-i\theta J_y}e^{-i\gamma J_z}|\beta\rangle.$$

Because of the axial symmetry of the system with P pairs of particles, we have $K=0$ and the energies of the states with angular momentum J are

$$E_J^P(n)=\frac{\langle\psi_J(n)|H|\psi_J(n)\rangle}{\langle\psi_J(n)|\psi_J(n)\rangle}=\frac{\int_0^\pi\sin\theta\,d\theta\langle\psi_n|HR(\theta)|\psi_n\rangle P_J(\cos\theta)}{\int_0^\pi\sin\theta\,d\theta\langle\psi_n|R(\theta)|\psi_n\rangle P_J(\cos\theta)}, \tag{9}$$

where we note $\psi_J^{K=0}$ by $\psi_J(n)$, and the rotation operator through a θ angle around the $0y$ axis, by $R(\theta)=e^{-i\theta J_y}$. The operators H and $R(\theta)$ conserve the number of particles and connect only the terms of the number-projected wave function [Eq. (5)] having the same number of particles; consequently the overlap integrals become

$$\mathcal{N}(n,\theta)=\langle\psi_n|R(\theta)|\psi_n\rangle=2(n+1)C\langle\psi_n|R(\theta)|\psi_0\rangle,$$
$$\mathcal{H}(n,\theta)=\langle\psi_n|HR(\theta)|\psi_n\rangle=2(n+1)C\langle\psi_n|HR(\theta)|\psi_0\rangle. \tag{10}$$

Using the commutation relations

$$\left[a_\alpha,\exp\left(\frac{1}{2}\sum_{\beta\beta'}F_{\beta\beta'}a_\beta^\dagger a_{\beta'}^\dagger\right)\right]=\sum_\delta F_{\alpha\delta}a_\delta^\dagger\exp\left(\frac{1}{2}\sum_{\beta\beta'}F_{\beta\beta'}a_\beta^\dagger a_{\beta'}^\dagger\right)$$

and the identity

$$R(\theta)|\psi_0\rangle=\left(\prod_{\nu>0}u_\nu\right)\exp\left(\frac{1}{2}\sum_{\alpha\beta}F_{\alpha\beta}a_\alpha^\dagger a_\beta^\dagger\right)|0\rangle, \tag{11}$$

we finally obtain

$$\mathcal{N}(n,\theta)=2(n+1)C^2\sum_{k=0}^{n+1}\epsilon_k\eta_k^{-P}\left(\prod_{\nu>0}u_\nu\right)^2N(k,\theta)+\text{c.c.}, \tag{12a}$$

$$\mathcal{H}(n,\theta)=2(n+1)C^2\sum_{k=0}^{n+1}\epsilon_k\eta_k^{-P}\left(\prod_{\nu>0}u_\nu\right)^2H(k,\theta)\times N(k,\theta)+\text{c.c.} \tag{12b}$$

with

$$N(k,\theta)=\exp\{\tfrac{1}{2}\mathrm{tr}[\ln(1+\eta_kM)]\} \tag{13a}$$

and

$$H(k,\theta)=\sum_\alpha(E_\alpha-\lambda_f)\rho_{\alpha\alpha}-G\sum_{\alpha\beta}(2\rho_{\alpha\beta}\rho_{\tilde{\alpha}\tilde{\beta}}+\bar{K}_{\alpha\tilde{\alpha}}K_{\tilde{\beta}\beta}). \tag{13b}$$

In Eqs. (13), ρ and K are matrices defined by

$$\rho=\frac{\eta_kM}{1+\eta_kM};$$

$$K_{\alpha\beta}=\sum_\delta\left(\frac{1}{1+\eta_kM}\right)_{\alpha\delta}F_{\delta\beta}$$

and

$$\bar{K}_{\alpha\beta}=\sum_\delta\left(\frac{\eta_k}{1+\eta_kM}\right)_{\delta\alpha}f^*_{\delta\alpha} \tag{13c}$$

and M is a θ-dependent square matrix given by

$$M_{\alpha\beta}(\theta)=\sum_\delta F_{\alpha\delta}(\theta)f_{\beta\delta}. \tag{13d}$$

The calculation of the preceding expressions is simplified by the use of the identity[37]

$$\mathrm{Tr}[\ln(1+\eta_kM)]=\ln[\det(1+\eta_kM)] \tag{14}$$

which reduces the calculation of Eq. (12) to that of the determinant of $(1+\eta_kM)$. It is easy to demonstrate that if L is the order of the M matrix,

then the following relation holds:

$$\det(1+\eta_k M)=\sum_{\nu=0}^{L}\eta_k^{\nu}\sum_{i_1<i_2<i_3\cdots<i_\nu}\det\begin{bmatrix}M_{i_1i_1} & M_{i_1i_2} & \cdots & M_{i_1i_\nu}\\ M_{i_2i_1} & M_{i_2i_2} & \cdots & M_{i_2i_\nu}\\ \vdots & \vdots & \cdots & \vdots\\ M_{i_\nu i_1} & M_{i_\nu i_2} & \cdots & M_{i_\nu i_\nu}\end{bmatrix}=\sum_{\nu=0}^{L}\eta_k^{\nu}M_\nu, \tag{15}$$

where η_k^{ν} represents the νst power of η_k and M_ν is a summation over C_L^{ν} determinants of order ν ($M_0=1$; $M_1=\sum_{i=1}^{L}M_{ii};\ldots$).[45] Equation (15) allows us to transform Eq. (12a) after eliminating the imaginary part:

$$\mathcal{N}(n,\theta)=4(n+1)C^2\sum_{k=0}^{n+1}\epsilon_k\Big(\prod_{\nu>0}u_\nu\Big)^2 r_k\cos\xi_k=\Big(\sum_{k=0}^{n+1}\epsilon_k R_k\cos\psi_k\Big)^{-1}\sum_{k=0}^{n+1}\epsilon_k\Big(\prod_{\nu}u_\nu\Big)^2 r_k\cos\xi_k, \tag{16a}$$

where we set:

$$\gamma_\nu=2u_\nu v_\nu,\quad \delta_\nu=u_\nu^2-v_\nu^2,\quad x_k=\frac{k\pi}{2(n+1)},\quad R_k=\prod_\nu(1-\gamma_\nu^2\sin^2x_k)^{1/2},\quad \psi_k=\sum_\nu\phi_{\nu k}+(\Omega-2P)x_k, \tag{16b}$$

$$\tan\phi_{\nu k}=-\delta_\nu\tan x_k,\quad |\phi_{\nu k}|\le\tfrac{1}{2}\pi,\quad r_k^2=\sum_\nu M_\nu^2+2\sum_{\nu\neq\mu}M_\nu M_\mu\cos[2(\nu-\mu)x_k],\quad \tan\xi_k=\frac{\sum_\nu M_\nu\sin[2(\nu-P)x_k]}{\sum_\nu M_\nu\cos[2(\nu-P)x_k]}.$$

These equations constitute the solution of the problem of the double projection of the BCS wave function. Some simplifying hypotheses may be made to yield more manageable expressions.

III. PROJECTION WITHIN THE ADIABATIC ASSUMPTION

When many nucleons are moving in a highly deformed well, it is well known that the adiabatic assumption and the Peierls-Yoccoz projection method approximately lead to the same results. The overlap integrals $\mathcal{N}(n,\theta)$ and $\mathcal{H}(n,\theta)$ are then very small except in the neighborhood of $\theta=0$ and $\theta=\pi$. Furthermore, the symmetry of the wave function $|\psi_n\rangle$ through a π rotation around $0z$ and the hermiticity of the Hamiltonian and of the angular momentum involve the symmetry properties

$$\begin{aligned}&\mathcal{N}(n,\pi-\theta)=\mathcal{N}(n,\theta),\quad &&\mathcal{H}(n,\pi-\theta)=\mathcal{H}(n,\theta),\\ &\mathcal{N}(n,-\theta)=\mathcal{N}(n,\theta),\quad &&\mathcal{H}(n,-\theta)=\mathcal{H}(n,\theta)\end{aligned} \tag{17}$$

which permit the integration from 0 to $\frac{1}{2}\pi$ in Eq. (9) (for even J) and the expansion of $\mathcal{N}$ and $\mathcal{H}$ in powers of $\sin^2\theta$ [$N(n,0)=1$].

A. Overlap Integrals and Rotational Spectrum

$\mathcal{N}(n,\theta)$ and $\mathcal{H}(n,\theta)$ expand as:

$$\mathcal{N}(n,\theta)=1-d_1\sin^2\theta+d_2\sin^4\theta+\cdots, \tag{18a}$$

$$\mathcal{H}(n,\theta)=h_0+D_1\sin^2\theta+D_2\sin^4\theta+\cdots. \tag{18b}$$

When keeping out only the first-order term (in θ^2), we obtain

$$\begin{aligned}&P_J(\cos\theta)\simeq 1-\frac{J(J+1)}{4}\theta^2,\\ &\mathcal{N}(n,\theta)\simeq 1-d_1\theta^2,\\ &\mathcal{H}(n,\theta)\simeq(h_0+h_1\theta^2)(1-d_1\theta^2),\\ &h_1=D_1+h_0d_1,\end{aligned} \tag{19}$$

and the rotational energy spectrum takes the same form as for the pure BCS wave function[46]:

$$E_J^P(n)=h_0+h_1\frac{N_2(J,d_1)}{N_0(J,d_1)}, \tag{20a}$$

$$N_l(J,d_1)=\frac{(l/2)!}{2d_1^{l/2+1}}\left(1-\frac{J(J+1)}{4d_1}\left(\frac{l}{2}+1\right)\right). \tag{20b}$$

The expansion of Eq. (20a) to the first order in $[J(J+1)]/4a_1$ leads to the spectrum

$$E_J^P(n)=h_0+\frac{h_1}{d_1}+\frac{\hbar^2J(J+1)}{2\mathcal{J}}, \tag{21}$$

where $\mathcal{J}=-2\hbar^2(d_1^2/h_1)$ stands for the moment of inertia. The quantities h_0, h_1, and d_1 are obtained from a comparison between Eqs. (10) and (18):

$$\begin{aligned}&h_0=\langle H\rangle_n;\quad d_1=\tfrac{1}{2}\langle J_y^2\rangle_n,\\ &h_1=\tfrac{1}{2}(\langle H\rangle_n\langle J_y^2\rangle_n-\langle HJ_y^2\rangle_n),\end{aligned} \tag{22}$$

where the notation $\langle\ \rangle_n$ means the average value over $|\psi_n\rangle$.

B. Matrix Elements for Even-Even Systems

The matrix elements of Eqs. (22) are evaluated in the quasiparticles representation obtained by the canonical transformation of Bogoliubov-Valatin[2,3] (the vacuum is the BCS state $|\psi_0\rangle$). In this representation, the operators H and J_y^2 can be written

$$H=\sum_{i,j=0}^{4}H_{ij},\quad |i-j|=0,2,$$

and

$$J_y^2 = \sum_{i,j=0}^{4} (J_y^2)_{ij}\,, \quad |i-j| = 0, 2\,, \tag{23}$$

where H_{ij} and $(J_y^2)_{ij}$ stand for the sums of the components of H and J_y^2, respectively, with i creation operators and j destruction operators of quasiparticles.

The operators H, J_y^2, and HJ_y^2 conserve the number of particles and connect the only components having the same number of particles in Eq. (5), so that we have:

$$\langle H\rangle_n = 2(n+1)C\langle\psi_n|H|\psi_0\rangle\,, \tag{24a}$$

$$\langle J_y^2\rangle_n = 2(n+1)C\langle\psi_n|J_y^2|\psi_0\rangle\,, \tag{24b}$$

$$\langle HJ_y^2\rangle_n = 2(n+1)C\langle\psi_n|HJ_y^2|\psi_0\rangle\,. \tag{24c}$$

Because the kets $|\psi_n\rangle$ and $|\psi_0\rangle$ describe only pairs of quasiparticles, we introduce the following pair operators:

$$A_\nu = \alpha_{\tilde\nu}\alpha_\nu \quad \text{and} \quad A_{\tilde\nu}^\dagger = \alpha_\nu^\dagger \alpha_{\tilde\nu}^\dagger\,, \tag{25}$$

where $\alpha_\nu^\dagger$ and α_ν are the creation and destruction operators of quasiparticles. Each of the operators A_ν and $A_{\tilde\nu}^\dagger$ in Eq. (25) is its own time-reversal transform:

$$\begin{aligned} &\alpha_{\tilde\nu}^\dagger = T\alpha_\nu^\dagger T^{-1}\,, \quad A_\nu = TA_\nu T^{-1}\,,\\ &\alpha_{\tilde\nu} = T\alpha_\nu T^{-1}\,, \quad A_\nu^\dagger = TA_\nu^\dagger T^{-1}\,,\\ &\alpha_\nu = -T\alpha_{\tilde\nu}T^{-1}\,. \end{aligned} \tag{26}$$

Using these properties, we obtain a quasiparticle representation where the vacuum is still $|\psi_0\rangle$ and where the projected state $|\psi_n\rangle$ becomes:

$$|\psi_n\rangle = C\left\{\sum_{k=0}^{n+1}\epsilon_k\eta_k^{-P}\prod_{\nu>0}(u_\nu^2+\eta_k v_\nu^2)\left(1+(\eta_k-1)\sum_\nu\frac{u_\nu v_\nu}{u_\nu^2+\eta_k v_\nu^2}A_\nu^\dagger + \frac{(\eta_k-1)^2}{2}\sum_{\nu\neq\mu>0}\frac{u_\nu v_\nu u_\mu v_\mu}{(u_\nu^2+\eta_k v_\nu^2)(u_\mu^2+\eta_k v_\mu^2)}A_\nu^\dagger A_\mu^\dagger + \cdots\right) + \text{c.c.}\right\}|\psi_0\rangle\,. \tag{27}$$

When H and J_y^2 directly act on $|\psi_0\rangle$ as in Eqs. (24), only the components without quasiparticle destruction operators give nonzero contributions. In Eqs. (24b) and (24c), the only nonzero contributions come from

$$\begin{aligned} &J_{00}^{(p)} = (J_y^2)_{00}\,, \quad J_{20}^{(p)} = \sum_k J_k^{20}A_k^\dagger\,, \quad J_{40}^{(p)} = \sum_{kl} J_{kl}^{40}A_k^\dagger A_l^\dagger\,,\\ &J_k^{20} = \sum_m |\langle k|J_y|m\rangle|^2(\gamma_k\delta_m - \gamma_m\delta_k)\,,\\ &J_k^{40} = (|\langle k|J_y|l\rangle|^2 + |\langle k|J_y|-l\rangle|^2)(u_k v_l - u_l v_k)^2\,, \end{aligned} \tag{28}$$

with the definitions of Eqs. (16b).

With the help of Eqs. (23), Eqs. (24a) and (24b) reduce to

$$\langle H\rangle_n = H_{00} + \langle H_{40}\rangle_n \tag{29a}$$

$$\langle J_y^2\rangle_n = J_{00}^{(p)} + \langle J_{20}^{(p)}\rangle_n + \langle J_{40}^{(p)}\rangle_n\,, \tag{29b}$$

$$\langle H_{20} + H_{02}\rangle_n = 0\,.$$

TABLE I. Specification of the quantum numbers corresponding to the energy levels $\nu = 1$–16 in the model with equidistant levels. The angular momenta j_ν and their projections m_ν are arbitrarily chosen.

ν	j_ν	m_ν	ν	j_ν	m_ν
1	$\frac{1}{2}$	$\frac{1}{2}$	9	$\frac{5}{2}$	$\frac{3}{2}$
2	$\frac{1}{2}$	$\frac{1}{2}$	10	$\frac{5}{2}$	$\frac{5}{2}$
3	$\frac{3}{2}$	$\frac{1}{2}$	11	$\frac{1}{2}$	$\frac{1}{2}$
4	$\frac{3}{2}$	$\frac{3}{2}$	12	$\frac{3}{2}$	$\frac{1}{2}$
5	$\frac{1}{2}$	$\frac{1}{2}$	13	$\frac{3}{2}$	$\frac{3}{2}$
6	$\frac{3}{2}$	$\frac{1}{2}$	14	$\frac{5}{2}$	$\frac{1}{2}$
7	$\frac{3}{2}$	$\frac{3}{2}$	15	$\frac{5}{2}$	$\frac{3}{2}$
8	$\frac{5}{2}$	$\frac{1}{2}$	16	$\frac{5}{2}$	$\frac{5}{2}$

TABLE II. Convergence versus n of several physical quantities (first column). The important discrepancies between $n=0$ and $n=2$ (especially for the energy and the moment of inertia) clearly show the imperative requirement of the projection in the occupation number space. For $n \geq 2$, the fluctuations of the particle number may be considered as negligible. In this case $P=4$, $G=0.8$ MeV, and $E_\nu = \nu$ MeV.

n	0	1	2	3	4
$\langle H\rangle_n - H_{00}$ (MeV)	−0.123	−1.383	−1.410	−1.410	−1.410
$\langle J_y^2\rangle_n$ ($\hbar^2$)	0.075	0.066	0.066	0.066	0.066
$\langle HJ_y^2\rangle_n$ (MeV $\hbar^2$)	−0.050	−0.065	−0.067	−0.067	−0.067
$\mathcal{J}$ (MeV^{-1})	19.86	15.30	14.92	14.92	14.92

Using Wick's theorem, and the expansion of $|\psi_n\rangle$ given in Eq. (27), Eqs. (29) give:

$$H_{00} = \sum_{\nu>0} [2(E_\nu - \lambda_f) - G v_\nu^2 - \tfrac{1}{2}\gamma_\nu \Delta],$$

$$\langle H_{40}\rangle_n = G \sum_{\nu\neq\mu>0} A_n^{\nu\mu} u_\mu^2 v_\nu^2; \quad J_{00}^{(p)} = \sum_{\nu\mu>0} J_{\nu\mu}^{40}, \tag{30}$$

$$\langle J_{20}^{(p)}\rangle_n = \frac{1}{2}\sum_{\nu>0} A_n^\nu J_\nu^{20}; \quad \langle J_{40}^{(p)}\rangle_n = 2\sum_{\nu\neq\mu>0} A_n^{\nu\mu} J_{\nu\mu}^{40}.$$

The A_n functions are defined as follows:

$$A_n^{\nu_1\nu_2\cdots\nu_s} = A^{-1} \sum_{k=0}^{n+1} \epsilon_k R_k \sin^s x_k \left(\prod_{i=1}^{s} \frac{\gamma_{\nu_i}}{\rho_{\nu_i k}^2}\right) \sum_{r=1}^{s+1} \cos[\psi_k + s\tfrac{1}{2}\pi + (s-2r)x_k]$$
$$\times \sum_{1=i_1<i_2<\cdots<i_r} \left(\prod_{t=1}^{r} v_{\nu_{i_t}}^2\right)\left(\prod_{l\neq i_1,\ldots,i_r} u_{\nu_l}^2\right), \tag{31}$$

$$A = \sum_{k=0}^{n+1} \epsilon_k R_k \cos\psi_k .$$

Similarly, using in Eq. (24c) the results of Eqs. (27) and (29b), we find:

$$\langle H J_y^2\rangle_n = K + \sum_\nu A_n^\nu B_1(\nu) + \sum_{\nu\neq\mu} A_n^{\nu\mu} B_2(\nu,\mu) + \sum_{\nu\neq\mu\neq\lambda} A_n^{\nu\mu\lambda} B_3(\nu,\mu,\lambda) + \sum_{\nu\neq\mu\neq\lambda\neq\rho} A_n^{\nu\mu\lambda\rho} B_4(\nu,\mu,\lambda,\rho), \tag{32}$$

where the first term

$$K = J_{00}^{(p)} H_{00} + 2G \sum_{\nu\neq\nu'} u_\nu^2 v_{\nu'}^2 J_{\nu\nu'}^{40}, \tag{33a}$$

comes from the component of $|\psi_n\rangle$ corresponding to zero pairs of quasiparticles, and so on until the last term which comes from the components of $|\psi_n\rangle$ corresponding to four pairs of quasiparticles:

$$B_1(\nu) = 2(\tilde{E}_\nu \delta_\nu - \gamma_\nu \Delta - \tfrac{1}{4} G \gamma_\nu^2) J_\nu^{20} - G \sum_{\nu'} (u_\nu^2 u_{\nu'}^2 + v_\nu^2 v_{\nu'}^2) J_{\nu'}^{20} + G\delta_\nu \sum_{\nu'\neq\nu} \gamma_{\nu'} J_{\nu\nu'}^{40},$$

$$B_2(\nu,\mu) = 2G\delta_\nu \gamma_\mu J_\mu^{20} + (4\tilde{E}_\nu \delta_\nu - 4\gamma_\nu \Delta - G\gamma_\nu^2 - 2G\gamma_\nu\gamma_\mu) J_{\nu\mu}^{40} - 2G \sum_{\rho\neq\nu} (u_\mu^2 u_\rho^2 + v_\mu^2 v_\rho^2) J_{\nu\rho}^{40}, \tag{33b}$$

$$B_3(\nu,\mu,\lambda) = 2G u_\nu^2 v_\mu^2 J_\lambda^{20} + 2G\delta_\nu \gamma_\mu J_{\lambda\mu}^{40},$$

$$B_4(\nu,\mu,\lambda,\rho) = G u_\nu^2 v_\lambda^2 J_{\mu\rho}^{40},$$

$$\tilde{E}_\nu = E_\nu - \lambda_f - G v_\nu^2, \tag{33c}$$

$$\Delta = G \sum_\nu u_\nu v_\nu . \tag{33d}$$

TABLE III. The fluctuations in the number of particles are less important in this case ($P=8$, $G=0.475$ MeV, $E_\nu = \nu$) than in the case presented in Table II, the number of pairs being multiplied by two. Again the convergence is physically satisfactory for $n=2$.

n	0	1	2	3	4
$\langle H\rangle_n - H_{00}$ (MeV)	−0.144	−1.340	−1.395	−1.395	−1.395
$\langle J_y^2\rangle_n$ ($\hbar^2$)	0.139	0.120	0.120	0.120	0.120
$\langle H J_y^2\rangle_n$ (MeV $\hbar^2$)	−0.099	−0.099	−0.100	−0.100	−0.100
$\mathcal{J}$ (MeV^{-1})	10.07	10.06	9.97	9.97	9.97

TABLE IV. Evolution of the rotational spectrum with the degree of extraction n of the unphysical components. The origin of the energies is set at $E_J = 0$, $P=8$, $G=0.475$ MeV (see Table III and the text).

J	n	0	1	2	3	4	5
2		0.297	0.298	0.301	0.301	0.301	0.301
4		0.991	0.992	1.004	1.004	1.004	1.004
6		2.082	2.083	2.108	2.108	2.108	2.108
8		3.570	3.571	3.614	3.614	3.614	3.614
10		5.454	5.456	5.522	5.522	5.522	5.522

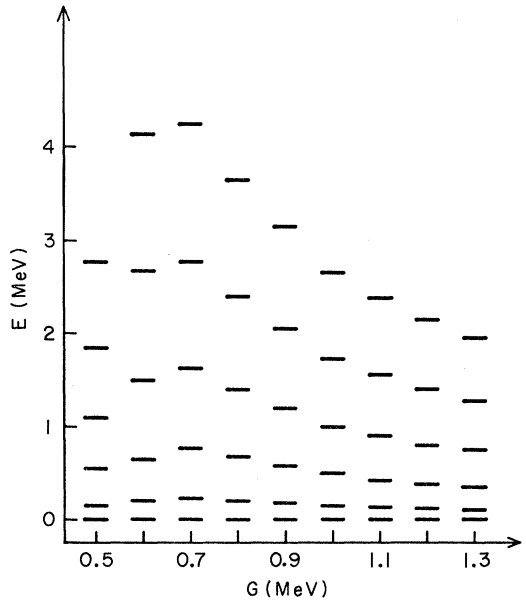

FIG. 1. Variation of the rotational spectrum versus the pairing force in the $P=4$ case; all the levels correspond to a complete projection in the occupation space ($n=6$).

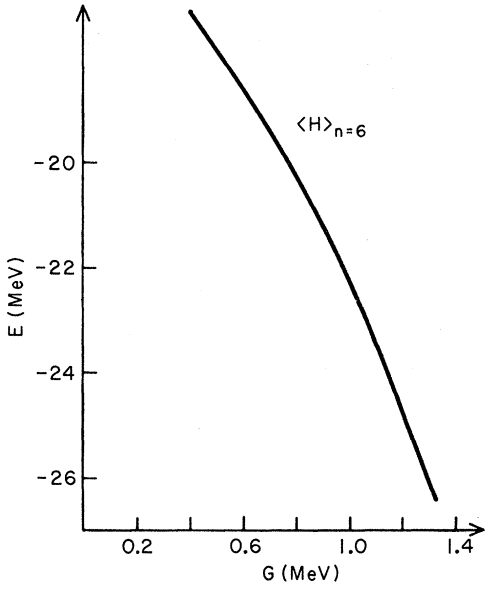

FIG. 2. Variations of the energy $\langle H\rangle_{n=6}$ versus the pairing force strength G (MeV), in the $P=4$ case and after convergence ($n=6$) of the particle-number projection procedure.

IV. APPLICATION TO MODEL CALCULATIONS: DISCUSSION

We performed two numerical calculations with Richardson's model with equidistant levels,[39] using the parameter values: $P=4$, $G=0.8$ and $P=8$, $G=0.475$.

This model assumes doubly degenerate levels which are equally separated by the unit energy. The number of particles equals the number of levels. Corresponding to each ν level of the model there are an angular momentum j_ν and its projection m_ν (see Table I). The average values over $|\psi_n\rangle$ for the operators H, J_y^2, HJ_y^2, and for the moment of inertia are given in Tables II and III. The results mainly show a very quick convergence with n for the calculated quantities. In fact, as soon as $n\geq 2$, the projected state $|\psi_n\rangle$ coincides with the exact wave function. The values of $\langle H\rangle_n - \langle H_{00}\rangle$ for $P=4$ and $G=0.8$ are the same as in Ref. 22.

The energy spectrum, calculated with Eq. (21) is tabulated versus n ($n=0,5$) in Table IV ($P=8$, $G=0.475$). Here too, we observe a very speedy convergence of the set $E_J^6(n)$.

In Fig. 1 we studied the evolution of the rotational spectrum versus G for $n\geq n_0$ [n_0 being the lowest integer such as $2(n_0+1)\geq \max(P, L-P)$], i.e., for an exact projection. The levels present a maxima for $0.6\leq G\leq 0.7$.

Figure 2 shows that $\langle H\rangle_{n=6}$ decreases rapidly versus the parameter of the pairing force.

In summary, we performed a double projection of the BCS wave function: Fomenko's method of projection in the occupation number space gives the number-projected wave function as a quickly converging series and thus seems very suitable to a further projection onto the eigenstates of the angular momentum. General formulas for this double projection have been established. We showed that numerical calculations may easily be performed if the adiabatic assumption is used. Only a calculation in the case of true nuclei can show if the strong dispersion (between $n=0$ and $n=2$) observed for the difference $\langle H\rangle_n - H_{00}$ and for the moment of inertia $\mathcal{I}$, is fortuitous or, on the contrary, a characteristic of the model. Nevertheless, the errors due to the fluctuations of the particle number can be important and it seems to us necessary to project out that part of the BCS wave function corresponding to the correct number of particles, before projecting onto the eigenstates of angular momentum. An application of this method to nuclei in the rare earth region is actually in progress.

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