On a Variable of the Quasi-particle Transformation of the Hamiltonian of an Odd-Nucleus

Doğan Demirhan * and Fevzi Büyükkiliç

Ege University, Faculty of Science, Department of Physics, Bornova-Izmir, Turkey

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The canonical transformation of the general BCS Hamiltonian has been performed. The energy spectrum of $_{73}Ta^{181}$ is determined and the calculated energy values are plotted as a function of the auxiliary variable z of the transformation for three different values of the deformation parameter.

1. Introduction

In the investigation of the structure of nuclei, BCS (Bardeen-Cooper-Schrieffer) [1–3], TDA (Tamm-Dancoff Approximation) and PBCS (Projected BCS) approximations [4–6] are often used methods. In the present paper, the quasi-particle creation and annihilation operators that are introduced in the BCS formalism, are taken as a function of an additional parameter σ which is also a function of an other variable z in terms of the states being occupied or unoccupied.

The canonical transformation of the general Hamiltonian of the nucleus has been performed in terms of this new variable using the transformations proposed by Dias and Krmpotic [7].

The main objective of the present paper is to investigate the role of the variable z and to calculate the energy spectrum of an odd-mass nucleus, namely $_{73}Ta^{181}$, in order to rationalize the dependence of the results on z.

2. Theory

The general Hamiltonian in BCS formalism is

$$H = \sum_{i>0} (\varepsilon_i - \lambda)(a_i^+ a_i + a_{-i}^+ a_{-i}) - G \sum_{i,j>0} a_j^+ a_{-j}^+ a_{-i} a_i, \quad (1)$$

where ε_i is the single-particle energy, λ the chemical potential, G the pairing constant, and a_i^+ and a_i are creation and annihilation operators. The canonical transformations between a_i^+ and a_i and the quasi-particle creation and annihilation operators α_i^+ and α_i are the following [8, 9]:

$$\begin{aligned} a_i^+ &= \sqrt{\sigma_i}\,(u_i \alpha_i^+ + z v_i^* \alpha_{-i}), \\ a_i &= \sqrt{\sigma_i}\,(u_i^* \alpha_i + z v_i \alpha_{-i}^+), \\ a_{-i}^+ &= \sqrt{\sigma_i}\,(u_i^* \alpha_{-i}^+ - z v_i \alpha_i), \quad \sigma_i = (u_i^2 + z^2 v_i^2)^{-1}, \\ a_{-i} &= \sqrt{\sigma_i}\,(u_i \alpha_{-i} - z v_i^* \alpha_i^+), \quad u_i^2 + v_i^2 = 1, \end{aligned} \quad (2)$$

where u_i^2 and v_i^2 are the probabilities of the ith state to be unoccupied or not. z is an auxiliary variable in the formalism to obtain states with exact particle number.

The quasi-particle operators satisfy the equation

$$\alpha_i |\mathrm{BCS}\rangle = \langle \mathrm{BCS}| \alpha_i^+ = 0, \quad (3)$$

where

$$|\mathrm{BCS}\rangle = |0\,z\rangle = \prod_{i>0} (u_i + z v_i a_i^+ a_{-i}^+)|0\rangle \quad (4)$$

is the vacuum state of the quasi-particle state.

By substituting (2) into (1) one obtains the following Hamiltonian:

$$H = H_{00} + H_{11} + H_{20} + H_{22} + H_{31} + H_{40}, \quad (5)$$

where

$$\begin{aligned} H_{00} &= \sum_{i>0} z^2 \sigma_i [(\varepsilon_i - \lambda)\, 2 v_i^2 - \Delta u_i v_i - G z^2 v_i^4 \sigma_i], \\ H_{11} &= \sum_{i>0} A(i)(\alpha_i^+ \alpha_i + \alpha_{-i}^+ \alpha_{-i}), \\ A(i) &= \sigma_i [(\tilde{\varepsilon}_i - \lambda)(u_i^2 - z^2 v_i^2) + 2 \Delta z^2 u_i v_i], \\ \tilde{\varepsilon}_i &= \varepsilon_i - G v_i^2 z^2 \sigma_i, \qquad \Delta = G \sum_{i>0} u_i v_i \sigma_i, \\ H_{20} &= \sum_{i>0} B(i)(\alpha_i^+ \alpha_{-i}^+ + \alpha_{-i} \alpha_i), \\ B(i) &= z \sigma_i [(\tilde{\varepsilon}_i - \lambda)\, 2 u_i v_i - \Delta (u_i^2 - z^2 v_i^2)], \\ H_{22} &= \sum_{i,j} [R(i,j) D(i,j) \alpha_j^+ \alpha_{-j}^+ \alpha_{-i} \alpha_i \\ &\quad + R(i,j) F(i,j) \alpha_j^+ \alpha_{-i}^+ \alpha_j \alpha_{-i}], \end{aligned}$$

Reprint requests to Dr. D. Demirhan, Department of Physics, Faculty of Science, Ege University, Bornova-İzmir/Türkei.

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$$R(i,j) = -\tfrac{1}{4} G \sigma_i \sigma_j, \qquad F(i,j) = 4 u_i v_i u_j v_j,$$
$$D(i,j) = u_i^2 u_j^2 + z^4 v_i^2 v_j^2,$$
$$H_{31} = \sum_{i,j} C(i,j)(\alpha_j^+ \alpha_{-j}^+ \alpha_{-i}^+ \alpha_{-i} + \alpha_{-i}^+ \alpha_{-i} \alpha_{-j} \alpha_j),$$
$$C(i,j) = +\tfrac{1}{2} G z u_i v_i \sigma_i \sigma_j (u_j^2 - z^2 v_j^2),$$
$$H_{40} = \sum_{i,j} Q(i,j)(\alpha_j^+ \alpha_{-j}^+ \alpha_{-i}^+ \alpha_i^+ + \alpha_i \alpha_{-i} \alpha_{-j} \alpha_j),$$
$$Q(i,j) = -\tfrac{1}{4} G z^2 u_j^2 v_i^2 \sigma_i \sigma_j. \qquad (6)$$

In order to investigate the role of the variable z and exhibit the dependence of the results on z, in the following section we present an application of the formalism by calculating the energy spectrum of the nucleus $_{73}TA^{181}$.

3. An Application: Energy Spectrum of $_{73}Ta^{181}$

The odd-nucleus $_{73}Ta^{181}$, having an odd number of protons and even number of neutrons, is considered as a quasi-particle outside an even-even core, and the core is represented by a BCS wave function.

The matrix elements of the Hamiltonian (5) are calculated. The parameters in this matrix operator are single-particle energies, the quantities λ, u_i, v_i, G, and the auxiliary variable z.

The single-particle energies are determined by diagonalizing the Lamm Hamiltonian [10, 11] whose matrix elements have been calculated using asymptotic base wave functions. In these calculations, for the protons 64 states, corresponding to the quantum numbers $N = 4,5$ whose energies are between $5.5\,\hbar\omega_0(\varepsilon)$ and $8.5\,\hbar\omega_0(\varepsilon)$, have been considered. For the protons, $\varkappa = 0.0577$ and $\mu = 0.65$ are taken. Three different values, namely 0.20, 0.25 and 0.30, of the deformation parameter ε are used.

The chemical potential λ, the pairing constant G and the occupation probabilities u_i^2 and v_i^2 are calculated in a self consistent way in BCS formalism for given single particle energies ε_i and the gap parameter Δ. For the proton $\Delta = 12/\sqrt{A}$, where A is the mass number of $_{73}Ta^{181}$.

In the calculation of the matrix elements eight different values starting from 0.25 with 0.25 step intervals are given for the variable z. We shall discuss the role of z in analytical calculations in the last section of the paper. It will be seen that by giving various values to this variable, the relative weight of components with different particle numbers in BCS is changed. This in turn brings about a correction of the chemical potential λ, and we expect that at the end of the computations, results consistent with usual BCS treatment will be obtained.

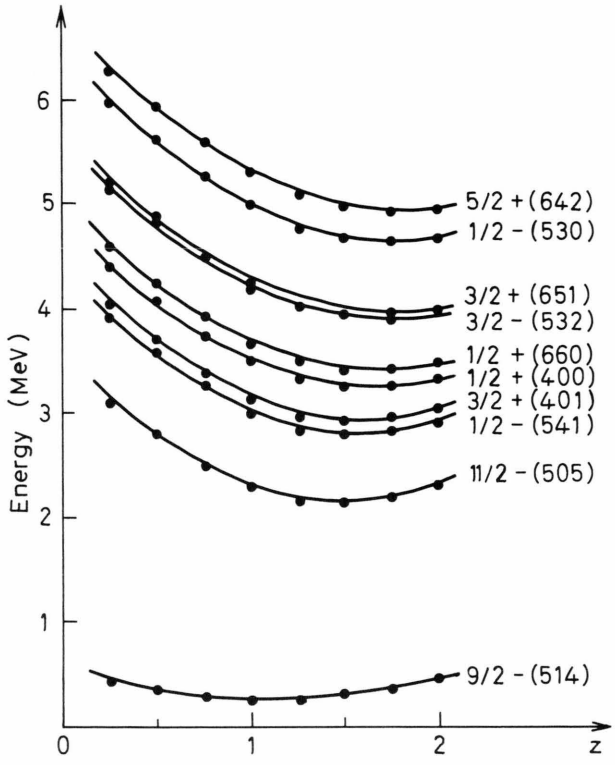

Fig. 1. Variation of the Excitation Energy with respect to z for $\varepsilon = 0.20$.

Table 1. Quantities Calculated for the Nucleus $_{73}Ta^{181}$.

ε	Fermi surface		Chemical potential	Pairing constant	Fluctuation
	State	Energy ($\hbar\omega_0(\varepsilon)$)	($\hbar\omega_0(\varepsilon)$)	G(MeV)	
0.20	5/2+(402)	5.9150	5.9249	0.1214	2.5704
0.25	5/2+(402)	5.9774	5.9478	0.1192	2.6180
0.30	7/2+(404)	5.9658	5.9478	0.1154	2.7542

The Fermi surfaces, chemical potentials and pairing constants determined for $_{73}Ta^{181}$ by the above mentioned choice of the quantities are presented in Table 1.

In Figs. 1–3 the calculated eigenvalue energies are plotted with respect to the variable z for three different deformation parameters.

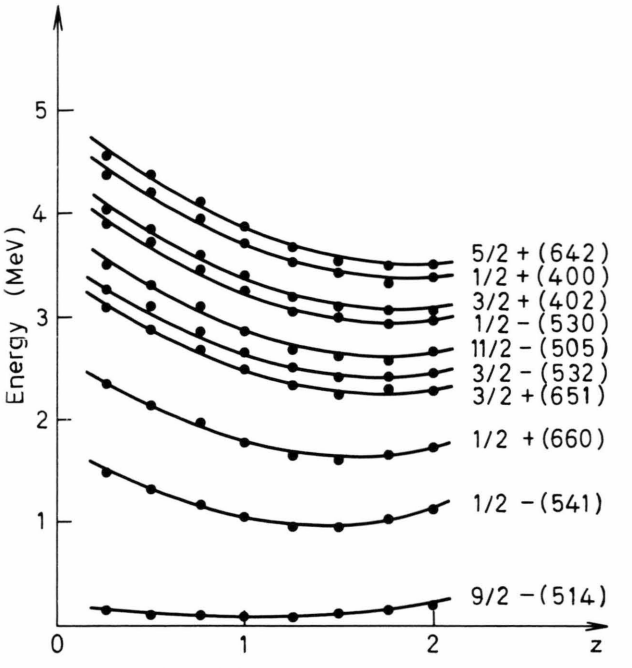

Fig. 2. Variation of the Excitation Energy with respect to z for $\varepsilon = 0.25$.

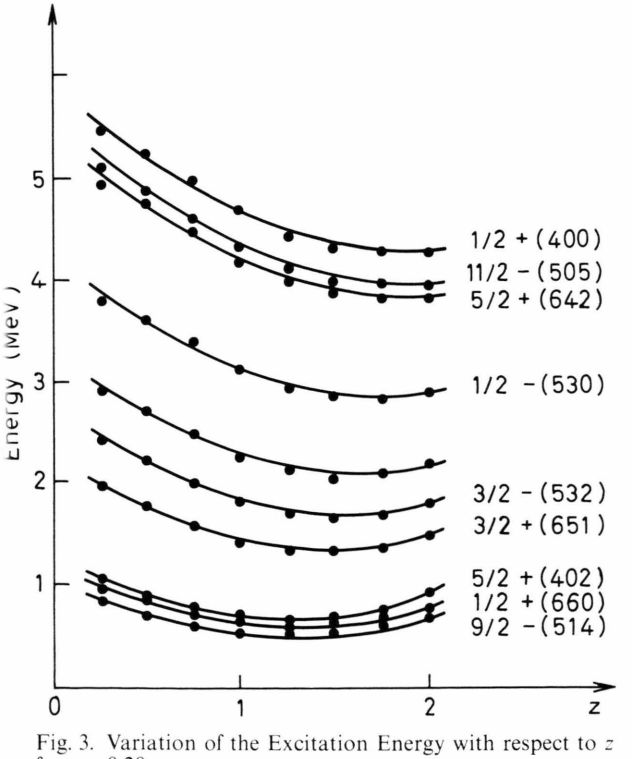

Fig. 3. Variation of the Excitation Energy with respect to z for $\varepsilon = 0.20$.

4. Conclusions

From the Table and the Figures we can conclude that the Fermi surface states and energies vary with respect to the deformation parameter of the nucleus. One can obtain different spectra by calculating single-particle energies for different values of the deformation parameter. This conclusion is consistent with the properties of the Nilsson model.

The chemical potential, pairing constant and fluctuation in the number of particles vary very little with respect to the deformation parameter but show greater variation in terms of the number of particles. This is an expected feature in the calculations, since Δ is kept constant for the effective pairing force.

The change in the energy values with respect to the variable z introduced in the Hamiltonian is given in Figures 1–3. All the curves show a minimum for values near $z = 1$. Energies which are close to the ground state are in agreement with the experimental data [12].

The energies plotted are only the energies above the Fermi energy. On the other hand, some states below the Fermi energy might have been included in the BCS calculations since such levels also contain a quasi-particle.

It is worth to discuss the variable z to some extent. z is a variable in the formalism introduced to obtain states with exact particle number. if the even-even core is represented by a BCS wave function, the ith state of the odd-nucleus which is the quasi-particle state reads

$$\alpha_i^+ |0\, z\rangle = (u_i^2 + z^2 v_i^2)^{1/2} \Big(\prod_{\substack{j>0 \\ j\neq i}} u_j \Big) a_i^+ \sum_k \frac{1}{k!} z^k \cdot \Big(\sum_{\substack{j>0 \\ j\neq i}} \frac{v_j}{u_j} a_j^+ a_{-j}^+ \Big)^k |0\rangle \tag{7}$$

Projection on a fixed particle number will then lead to results independent of z.

When the matrix elements of Hamiltonian (5) are calculated they will come out as a function of a residue integral of the form

$$I^k = (2\pi i)^{-1} \oint_C \mathrm{d}z\, z^{-k-1} \frac{\prod (u_i^2 + z^2 v_i^2)}{(u_p^2 + z^2 v_p^2) \ldots (u_t^2 + z^2 v_t^2)}, \tag{8}$$

where the origin is in the contour C and is the point of singularity of the transformation. The points $\pm i(u_p/v_p)$ etc. are not included in the contour. The problem is then the calculation of the residue integral by the known methods.

On the other hand, it may also be possible to represent the residue integral by finite sums through transformations similar to the Watson-Sommerfeld transform which we encounter in the transformation of the scattering amplitutes in the theory of scattering.

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