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On the structure of the paired states

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Abstract. In this paper the quasi-particle structure of the ground state of the pairing Hamiltonian is analysed for the Ni isotopes and ^{206}Pb. The particle-number projected Bardeen–Cooper–Schrieffer states are used for describing the states under consideration. The quasi-particle amplitudes are evaluated in the saddle-point approximation. The amplitudes with the number of quasi-particles a multiple of four are shown to be comparable with the quasi-particle vacuum amplitude.

The value of the other quasi-particle amplitudes depends essentially on the system considered. In particular, the two-quasi-particle component can sometimes be comparable with the four-quasi-particle one (^{206}Pb).

On the basis of the data obtained it is concluded that the random phase approximation ground-state wave function with small admixture of the quasi-particle components, the components with the odd number of quasi-particle pairs being neglected completely, is rather poor.

1. Introduction

In this paper we consider the quasi-particle structure of the ground state of the pairing model (Belyaev 1959). Recently, a method for projecting the states of the Bardeen–Cooper–Schrieffer model (Bardeen *et al.* 1957—to be referred to as BCS) in the quasi-particle representation has been suggested (Fomenko 1970). Now it became possible to compare directly the ground-state wave functions of the pairing Hamiltonian with the wave functions of any other method which employs the quasi-particle representation. The random phase approximation (Baranger 1960—to be referred to as RPA) is of great interest in this connection, since this method in recent years is widely applied to the pairing Hamiltonian, in particular (Gupta 1964). Such comparison enables us to evaluate the possibilities of the RPA in describing the states of the pairing Hamiltonian because the projected BCS states give a very good approach to the exact solution for the ground states of nuclei. The overlap integrals with the exact solutions proved to be greater than 0·99, as was shown by Kerman *et al.* (1961).

2. The quasi-particle structure

It was shown (Fomenko 1970) that the projected BCS states describing P pairs of particles represent a superposition of states with an even number of quasi-particles. The wave function of the ground state with the seniority zero has the following form:

$$|\phi\rangle = \sum_{q=0}^{L} a_q |q\rangle\!\rangle \tag{1}$$

where

$$|q\rangle\!\rangle = \sum_{\nu_i} C_{\nu_i} A_{\nu_1}{}^{+} \dots A_{\nu_q}{}^{+} |0\rangle\!\rangle$$

$$\sum_{\nu_i} |C_{\nu_i}|^2 = 1.$$

Σ_{ν_i} denotes summation over all possible sets of indices $\nu_1, \dots, \nu_q$ (not equal to each other), $|0\rangle\!\rangle$ is the quasi-particle vacuum, $A_\nu = \alpha_{-\nu}\alpha_\nu$ where α_ν is the annihilation quasi-particle operator, the states ν and $-\nu$ being related to each other by time reversal. L is the total pair degeneracy of the system. Thus $|q\rangle\rangle$ represents a $2q$ quasi-particle state.

If q is an even number, we have for the amplitudes a_q and a_{q+1}:

$$a_q^2 = \left\{(n+1)\sum_{k=0}^{n+1} \epsilon_k R_k \cos\psi_k\right\}^{-1} \tag{2a}$$

$$\times \sum_{\nu_i}\left\{\sum_{k=0}^{n+1} \epsilon_k R_k \sin^q \chi_k \gamma_{\nu_1}\ldots\gamma_{\nu_q}\rho_{\nu_1}^{-1}\ldots\rho_{\nu_q}^{-1}\cos(\psi_k-\varphi_{\nu_1}-\ldots-\varphi_{\nu_q})\right\}^2$$

$$a_{q+1}^2 = \left\{(n+1)\sum_{k=0}^{n+1} \epsilon_k R_k \cos\psi_k\right\}^{-1} \tag{2b}$$

$$\times \sum_{\nu_i}\left\{\sum_{k=0}^{n+1} \epsilon_k R_k \sin^{q+1} \chi_k \gamma_{\nu_1}\ldots\gamma_{\nu_{q+1}}\rho_{\nu_1}^{-1}\ldots\rho_{\nu_{q+1}}^{-1}\sin(\psi_k-\varphi_{\nu_1}-\ldots-\varphi_{\nu_{q+1}})\right\}^2$$

with

$$\gamma_\nu = 2u_\nu v_\nu, \qquad \delta_\nu = u_\nu^2 - v_\nu^2, \qquad \rho_{\nu k} = (1-\sin^2\chi_k\gamma_\nu^2)^{1/2}$$

$$tg\varphi_{\nu k} = -\delta_\nu tg\chi_k, \qquad R_k = \prod_\nu \rho_{\nu k}, \qquad \psi_k = \sum_\nu \varphi_{\nu k} + (L-2P)\chi_k \tag{3}$$

$$\chi_k = \frac{\pi k}{2(n+1)}, \qquad \epsilon_k = \begin{cases} \frac{1}{2} \text{ for } k = 0,\ n+1 \\ 1 \text{ otherwise.} \end{cases}$$

The positive integer n determines the accuracy to which the projection is performed (for $2n \geqslant \max(P, L-P)$ the projection becomes exact).

The essential point to mention here is that R in (2) as a function of χ has a sharp maximum near $\chi = 0$ if the root-mean-square particle-number fluctuation is large, i.e. $\sigma^2 = \Sigma_\nu\gamma_\nu^2 \gg 1$. In this case $R(\chi)$ can be represented in the form

$$R(\chi) = \exp\left(-\frac{1}{2}\sigma^2\chi^2\right).$$

Further, let n be infinitely large. Then the sums over k will go over into integrals according to the following rule:

$$\sum_{k=0}^{n+1} f(\chi_k) \to \frac{2}{\pi} n \int_0^{\pi/2} f(\chi)\,d\chi.$$

All the integrands we get in (2) if $n \to \infty$ contain the sharply peaked function $R(\chi)$ and so they can be evaluated by the saddle-point method.†

The saddle-point approximation gives for the amplitudes:

$$a_q^2 = \left(\frac{2}{\pi}\right)^{1/2} \frac{\{(q-1)!!\}^2}{q!} \frac{1}{\sigma} \tag{4a}$$

$$a_{q+1}^2 = \left(\frac{2}{\pi}\right)^{1/2} \frac{\{(q+1)!!\}^2}{q!} \frac{\Sigma_\nu\gamma_\nu^2\delta_\nu^2}{\sigma^5}. \tag{4b}$$

† The saddle-point approximation is, as a rule, good enough for the ground states of even–even nuclei and sufficient for the purposes of the present paper as was shown by our exact calculations (based on the formulae (2)) for the most troublesome cases considered here.

From (4) one then obtains

$$\frac{a_2^2}{a_0^2} = \frac{1}{2} \tag{5a}$$

$$\frac{a_1^2}{a_2^2} = 2\frac{\Sigma_\nu \gamma_\nu^2 \delta_\nu^2}{\sigma^4}. \tag{5b}$$

However, according to the RPA one should have

$$\frac{a_2^2}{a_0^2} \ll 1 \tag{6a}$$

$$\frac{a_1^2}{a_2^2} \ll 1. \tag{6b}$$

One sees from (5*a*) that the quasi-particle admixture in the ground state cannot be regarded as small as is assumed in the RPA. We should emphasize that the relation (5*a*) for the vacuum and four-quasi-particle amplitudes is valid for an arbitrary system of particles if the root-mean-square particle-number fluctuation is large enough.

It follows from (4*a*) that the amplitudes of the states with the number of quasi-particles multiple to four decrease rather slowly as the number of quasi-particles increases:

$$a_0^2 \colon a_2^2 \colon a_4^2 \colon \ldots = 1 \colon \tfrac{1}{2} \colon \tfrac{3}{8} \colon \ldots . \tag{7a}$$

As for the two-quasi-particle states, a comparison of (5*b*) and (6*b*) can be performed only for a concrete system. We shall discuss this question below.

We shall note that, as follows from (4*b*), the weight of the states with the odd number of quasi-particle pairs increases with the number of quasi-particles:

$$a_1^2 \colon a_3^2 \colon a_5^2 \colon \ldots = 1 \colon \tfrac{9}{2} \colon \tfrac{75}{8} \colon \ldots . \tag{7b}$$

However, it should be emphasized that the saddle-point approximation becomes inapplicable when one considers a very large number of quasi-particles because of the quantities ρ_ν^{-1} in the formulae (2) which have a minimum at $\chi = 0$ and, if in large number, can dilute the sharp peak of the function $R(\chi)$. Thus the relations (4) are valid only for $q \ll L$, i.e., for the first quasi-particle components.

In the case of one degenerate level† the two-quasi-particle component remains in general. The projected wave function has the RPA structure in this case only when the level is half filled, i.e. when the number of particles and holes is equal (in this case $\delta = 0$).

In table 1 we represent the quantity a_1^2/a_2^2, i.e. the ratio of the two-quasi-particle component to the four-quasi-particle one. The chemical potential λ and the gap parameter Δ and the schemes of the single-particle levels for the nuclei given in table 1 are the same as those used by Kisslinger and Sorensen (1960). In table 1 the relative error $\delta E/E$ in the excitation energy of the seniority-zero states (the RPA compared with exact solutions) is given (we use here the data of Gupta 1964). It can be seen that the error in the excitation energy obtained according to the RPA is the larger the worse the relation (6*b*) is satisfied.

† It is worth noting that the projected BCS states become exact solutions for one degenerate level.

Table 1. Quasi-particle structure of the ground state

Nucleus	a_1^2/a_2^2	$\delta E/E$ (%)
^{58}Ni	0·25	10
^{60}Ni	0·10	9
^{62}Ni	0·07	5
^{64}Ni	0·09	7·5
^{66}Ni	0·23	9·5
^{206}Pb	0·59	42

3. Conclusions

Concluding the consideration, we can summarize that the basic assumptions of the RPA are rather poorly fulfilled when the ground states of the pairing model are treated (see (7*a*) and table 1), the accuracy of one of them (neglect of the components with the odd number of quasi-particle pairs) being different for different nuclei.

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