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Влияние принципа Паули на свойства двухфононных состояний

Показано, что в рамках квазичастично-фононной модели ядра можно корректно учесть перестановочные соотношения между квазичастицами, образующими фононы. Исследован случай четно-четных деформированных ядер. Получены точные и приближенные секулярные уравнения. Показано, что поправки, связанные с учетом принципа Паули велики для двухфононных компонент волновых функций, составленных из одинаковых фононов.

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Djolos R.V., Molina J.L., Soloviev V.G. **E4 - 12250**

Influence of the Pauli Principle on the Two-Phonon States

It is shown that the commutation relations between quasiparticles forming phonons can correctly be taken into account within the quasiparticle-phonon nuclear model. The case of the even-even deformed nuclei is studied. Exact and approximate secular equations are obtained. The corrections arising due to the Pauli principle are shown to be large for the two-phonon components of the wave functions, when the phonons are identical.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

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1. Introduction

The generalization of the Hartree-Fock Variational Principle suggested by N.N.Bogolubov[1] (then called the Hartree-Fock-Bogolubov Variational Principle[2-4])and his method of time-dependent selfconsistent field[5] made the basis for the modern microscopic nuclear theory[6-9].

These methods resulting in the recent quasiparticle-phonon nuclear model[10] allow one to correctly describe the properties of the one-quasiparticle and one-phonon excited states, the distribution of one-quasiparticle[11] and one-phonon[12] components over more complex states at intermediate excitation energies and to calculate the photoabsorption[13] and one-nucleon transfer reaction strength functions. The proporties of the highly excited states have been well described without free parameters since the interaction constants were fixed while analyzing the properties of the low-lying states.

The consideration of the two-phonon states, the wave functions of which contain the components with four quasiparticles, should include the effects of antisymmetrization of the wave functions with respect to permutation of quasiparticles of different phonons. Many papers were devoted to the influence of the Pauli principle on the many-phonon states. Usually the boson representations for the fermion operators were used[14,15] and mainly the purely collective states were considered.

This paper considers the influence of the Pauli principle on the two-phonon states. Besides purely collective states we shall discuss all two-phonon states. In the framework of the quasiparticle-phonon nuclear model we obtain the equations for the excited state wave functions containing one- and two-phonon components, the commutation relations being strictly taken into account.

2. The Model Hamiltonian and Commutation Relations

Let us consider doubly even deformed nuclei. In this case the model Hamiltonian expressed through the phonon operators Q_g^+, Q_g, is

$$H_M = H_v + H_{vq} \tag{1}$$

$$\begin{aligned} H_v = \sum_q \varepsilon(q) B(qq) - \frac{1}{2} \sum_{\substack{gg' \\ g=\lambda\mu i \\ g'=\lambda\mu i'}} x^{(\lambda)} \sum_{q q' q_2 q_2'} f^{\lambda\mu}(qq') u_{qq'} (\psi^g_{qq'} + \varphi^g_{qq'}) \cdot \\ \cdot f^{\lambda\mu}(q_2 q_2') u_{q_2 q_2'} (\psi^{g'}_{q_2 q_2'} + \varphi^{g'}_{q_2 q_2'}) Q_g^+ Q_{g'} , \end{aligned} \tag{2}$$

$$\begin{aligned} H_{vq} = -\frac{1}{2\sqrt{2}} \sum_{\substack{g q q' \\ q_2 q_2'}} u_{q_2 q_2'} v_{qq'} f^{\lambda\mu}(q_2 q_2') (\psi^g_{q_2 q_2'} + \varphi^g_{q_2 q_2'}) f^{\lambda\mu}(qq') \cdot \\ \cdot \left\{ (Q_g^+ + Q_g) B(qq') + B(qq')(Q_g^+ + Q_g) \right\} , \end{aligned} \tag{3}$$

where

$$Q_g^+ = \frac{1}{2} \sum_{qq'} \left\{ \psi^g_{qq'} A^+(qq') - \varphi^g_{qq'} A(qq') \right\} ,$$

$$A^+(qq') = \frac{1}{\sqrt{2}} \sum_\sigma \sigma \alpha^+_{q-\sigma} \alpha^+_{q\sigma} , \quad \text{or} \quad \frac{1}{\sqrt{2}} \sum_\sigma \alpha^+_{q\sigma} \alpha^+_{q'\sigma} ,$$

$$B(qq') = \sum_{\sigma} \alpha^{+}_{q\sigma}\alpha_{q'\sigma} \quad , \qquad \text{or} \qquad \sum_{\sigma} \sigma \alpha^{+}_{q-\sigma}\alpha_{q'\sigma} \ .$$

We use the following notation: $f^{\lambda\mu}(qq')$ are the matrix elements of the operator of the multipole moment λ with projection μ, $\alpha^{+}_{q\sigma}$ is the quasiparticle creation operator, $\mathcal{E}(q)=\sqrt{C^2+(E(q)-\lambda)^2}$, $E(q)$ is the single-particle energy, C is the correlation function, λ is the chemical potential; $u_{qq'} = u_q v_{q'} + u_{q'} v_q$, $v_{qq'} = u_q u_{q'} - v_q v_{q'}$ where u_q and v_q are the Bogolubov transformation coefficients, and $(q\sigma)$ are the quantum numbers of the single-particle state, $\sigma = \pm 1$.

Using the secular equation defining the energies ω_g of the one-phonon states in the RPA

$$1 = 2\varkappa^{(\lambda)} \sum_{qq'} \frac{\left(f^{\lambda\mu}(qq')\, u_{qq'} \right)^2 \varepsilon(qq')}{\varepsilon^2(qq') - \omega_g^2} \tag{4}$$

and the relation

$$\frac{1}{2}\sum_{qq'} \varepsilon(qq')\, \ell^{gg'}(qqq') - \frac{1}{4\varkappa^{(\lambda)}\sqrt{Y_g Y_{g'}}} = \omega_g \delta_{gg'} \tag{5}$$

where

$$\ell^{gg'}(qq'q_2) = \psi^{g}_{q_2 q'} \psi^{g'}_{q_2 q} + \varphi^{g}_{q_2 q} \varphi^{g'}_{q_2 q'} \ , \tag{5'}$$

$$\varepsilon(qq') = \varepsilon(q) + \varepsilon(q')$$

$$Y_g = \sum_{qq'} \frac{\left(f^{\lambda\mu}(qq')\, u_{qq'} \right)^2 \varepsilon(qq')\, \omega_g}{\left(\varepsilon^2(qq') - \omega_g^2 \right)^2} \ ,$$

then H_v and H_{vq} can be rewritten as follows:

$$H_v = \sum_q \varepsilon(q) B(qq) - \frac{1}{4} \sum_{\substack{g=\lambda\mu i \\ g'=\lambda\mu i'}} \frac{1}{\varkappa^{(\lambda)} \sqrt{Y_g Y_{g'}}} Q_g^+ Q_{g'} \,, \tag{6}$$

$$H_{vq} = -\frac{1}{4} \sum_g \frac{1}{\sqrt{Y_g}} \sum_{qq'} v_{qq'} f^g(qq') \{ (Q_g^+ + Q_g) B(qq') + B(qq')(Q_g^+ + Q_g) \} . \tag{7}$$

Note that these results are obtained under the assumption of a small number of quasiparticles in the ground nuclear state

$$\langle \Psi_0 | B(qq') | \Psi_0 \rangle = 0 .$$

If the isovector part of the multipole-multipole interaction will be taken into account, formula (4) and others will be of a more complex form (see ref.[10]).

The phonon operators satisfy the following commutation relations[16]

$$[Q_g, Q_{g'}^+] = \delta_{gg'} - \frac{1}{2} \sum_{q_1 q_2 q} (\psi^g_{qq_2} \psi^{g'}_{qq_1} - \varphi^g_{qq_1} \varphi^{g'}_{qq_2}) B(q_1 q_2) .$$

Now we calculate the double commutator

$$[[Q_{g_1}, Q_{g_2}^+], Q_{g_3}^+] = \sum_g (\mathcal{K}(g g_1 g_2 g_3) Q_g^+ + \tilde{\mathcal{K}}(g g_1 g_2 g_3) Q_g) \,, \tag{9}$$

where

$$\mathcal{K}(g g_1 g_2 g_3) = -\frac{1}{2} \sum_{\substack{q_1 q_2 \\ q_3 q_4}} (\psi^{g_1}_{q_1 q_2} \psi^{g_2}_{q_1 q_3} - \varphi^{g_1}_{q_1 q_3} \varphi^{g_2}_{q_1 q_2})(\psi^{g_3}_{q_4 q_2} \psi^{g}_{q_4 q_3} + \varphi^{g_3}_{q_4 q_3} \varphi^{g}_{q_4 q_2}) \,, \tag{10}$$

$$\tilde{\mathcal{K}}(g g_1 g_2 g_3) = -\frac{1}{2} \sum_{\substack{q_1 q_2 \\ q_3 q_4}} (\psi^{g_1}_{q_1 q_2} \psi^{g_2}_{q_1 q_3} - \varphi^{g_1}_{q_1 q_3} \varphi^{g_2}_{q_1 q_2})(\psi^{g_3}_{q_4 q_2} \varphi^{g}_{q_4 q_3} + \varphi^{g_3}_{q_4 q_3} \psi^{g}_{q_4 q_2}) . \tag{10'}$$

Then

$$\langle \Psi_0 | Q_{g_2'} Q_{g_1'} Q_{g_1}^+ Q_{g_2}^+ | \Psi_0 \rangle = \delta_{g_1 g_1'} \delta_{g_2 g_2'} + \delta_{g_1 g_2'} \delta_{g_2 g_1'} + \mathcal{K}(g_2' g_1' g_1 g_2) \tag{11}$$

The values of the coefficients $\mathcal{K}(g_2' g_1' g_1 g_2)$ specify the degree of influence of the Pauli principle on the two-phonon states.

3. Exact Equations of the Model

Now we write the excited state wave function of a doubly even deformed nucleus as a superposition of the one- and two-phonon components

$$\Psi_n = \Big\{ \sum_i R_i^n(\lambda\mu) Q_g^+ + \frac{1}{\sqrt{2}} \sum_{g_1 g_2} P_{g_1 g_2}^n(\lambda\mu) Q_{g_1}^+ Q_{g_2}^+ \Big\} \Psi_0 . \tag{12}$$

Its normalisation condition has the form

$$\langle \Psi_n^* | \Psi_n \rangle = \sum_i (R_i^n(\lambda\mu))^2 + \sum_{g_1 g_2} (P_{g_1 g_2}^n(\lambda\mu))^2 + \\ + \frac{1}{2} \sum_{\substack{g_1 g_2 \\ g_1' g_2'}} P_{g_1 g_2}^n(\lambda\mu) P_{g_1' g_2'}^n(\lambda\mu) \mathcal{K}(g_1' g_2' g_1 g_2) = 1 . \tag{13}$$

Calculate the average value of $H_v + H_{vq}$ over the state (12)

$$\langle \Psi_n^* | H_M | \Psi_n \rangle = \sum_i \omega_i (R_i^n(\lambda\mu))^2 + \sum_{g_1 g_2} (\omega_{g_1} + \omega_{g_2})(P_{g_1 g_2}^n(\lambda\mu))^2 + \\ + \frac{1}{2} \sum_{\substack{g_1 g_2 \\ g_1' g_2'}} (\omega_{g_1} + \omega_{g_2}) \mathcal{K}(g_1' g_2' g_1 g_2) P_{g_1 g_2}^n(\lambda\mu) P_{g_1' g_2'}^n(\lambda\mu) - \tag{14}$$

$$-\frac{1}{8}\sum \frac{1}{x^{(\lambda)}\sqrt{Y_g}}\left(\frac{K(g_2' g g_1 g_2)}{\sqrt{Y_{g_1'}}}+\frac{K(g_1' g g_1 g_2)}{\sqrt{Y_{g_2'}}}\right)P^{n}_{g_1 g_2}(\lambda\mu)P^{n}_{g_1' g_2'}(\lambda\mu)-$$

$$-2\sum_{i g_1 g_2} U_{g_1 g_2}(\lambda\mu i)R^{n}_{i}(\lambda\mu)P^{n}_{g_1 g_2}(\lambda\mu)- \tag{14}$$

$$-\sum_{i g_1 g_2}\sum_{g g_3}\sum_{q q' g_3}\Gamma^{g}_{qq'}\{\ell^{\lambda\mu i g_3}_{(qq'g_3)}K(g g_3 g_1 g_2)+\ell^{g_1 g_3}_{(qq'g_3)}K(\lambda\mu i g g_2 g_3)+$$

$$+\ell^{g_2 g_3}_{(qq'g_3)}K(\lambda\mu i g g_1 g_3)\}R^{n}_{i}(\lambda\mu)P^{n}_{g_1 g_2}(\lambda\mu) \quad ,$$

where

$$\Gamma^{g}_{qq'}=\frac{v_{qq'}}{2\sqrt{Y_g}}f^{\lambda\mu}(qq')$$

and $U_{qq'}(\lambda\mu i)$ is given by (9.75) in ref. /7/.

The energies of the excited states η_n and the functions $R^{n}_{i}(\lambda\mu)$ and $P^{n}_{g_1 g_2}(\lambda\mu)$ can be determined using the variational principle

$$\delta\{\langle\Psi_n^{*}|H_M|\Psi_n\rangle-\eta_n\langle\Psi_n^{*}|\Psi_n\rangle\}=0 .$$

As a result of calculations we get the following system of equations:

$$(\omega_i-\eta_n)R^{n}_{i}(\lambda\mu)-\sum_{g_1 g_2}U_{g_1 g_2}(\lambda\mu i)P^{n}_{g_1 g_2}(\lambda\mu)-\frac{1}{2}\sum\Gamma^{g}_{qq'}P^{n}_{g_1 g_2}(\lambda\mu)\cdot \tag{15}$$

$$\cdot\{\ell^{\lambda\mu i g_3}_{(qq'g_3)}K(g g_3 g_1 g_2)+\ell^{g_1 g_3}_{(qq'g_3)}K(\lambda\mu i g g_2 g_3)+\ell^{g_2 g_3}_{(qq'g_3)}K(\lambda\mu i g g_1 g_3)\}=0$$

$$(\omega_{g_1}+\omega_{g_2}-\eta_n)P^{n}_{g_1 g_2}(\lambda\mu)+\frac{1}{4}\sum_{g_1' g_2'}(\omega_{g_1}+\omega_{g_2}+\omega_{g_1'}+\omega_{g_2'}-2\eta_n)K(g_1 g_2 g_1' g_2')P^{n}_{g_1' g_2'}(\lambda\mu)-$$

$$-\frac{1}{16}\sum_{gg_1'g_2'}\frac{1}{x^{(\lambda)}\sqrt{Y_g}}\left(\frac{\mathcal{K}(g_1'gg,g_2)}{\sqrt{Y_{g_1'}}}+\frac{\mathcal{K}(g_1'gg,g_2)}{\sqrt{Y_{g_2'}}}\right)P^{n}_{g_1'g_2'}(\lambda\mu)-$$

$$-\frac{1}{16}\sum_{gg_1'g_2'}\frac{1}{x^{(\lambda)}\sqrt{Y_g}}\left(\frac{\mathcal{K}(g_1gg_1'g_2')}{\sqrt{Y_{g_1}}}+\frac{\mathcal{K}(g_1gg_1'g_2')}{\sqrt{Y_{g_2}}}\right)P^{n}_{g_1'g_2'}(\lambda\mu)-\tag{16}$$

$$-\sum_i U_{g_1g_2}(\lambda\mu i)R_i^n(\lambda\mu)-\frac{1}{2}\sum_i R_i^n(\lambda\mu)\sum_{gg_3}\sum_{gg'g_3}\Gamma^{g}_{gg'}\cdot$$

$$\cdot\left\{\ell^{\lambda\mu ig_3}(gg'g_3)\mathcal{K}(gg_3g_1g_2)+\ell^{g_1g_3}(gg'g_3)\mathcal{K}(\lambda\mu igg_2g_3)+\ell^{g_2g_3}(gg'g_3)\mathcal{K}(\lambda\mu igg_1g_3)\right\}=0.$$

Assuming $\mathcal{K}(g_1g_2g_3g_4)$ and $\ell^{gg'}(g_1g_2g_3)$ to be equal to zero, we arrive at the system of equations obtained in ref./7/ within the quasiboson approximation. Obtaining $R_i^n(\lambda\mu)$ from (15) and substituting it into (16), we get a homogeneous system of equations with respect to $P^n_{g_1g_2}(\lambda\mu)$. To determine the energies η_n, one should diagonalise the matrix in the space of the two-phonon states g_1g_2. For the deformed nuclei the matrix is obtained of a very high order, thus necessitating the transition to the approximate equations.

4. Approximate Equations

Among the matrix elements of the Hamiltonian connecting the two-phonon states we shall preserve only those which do not change the quantum numbers of the two-phonon states. Then equation (16) will be

$$\Big\{(\omega_{g_1}+\omega_{g_2}-\eta_n)(1+\mathcal{K}(g_2g_1g_1g_2)-\frac{1}{4}\sum_i\Big(\frac{\mathcal{K}(g_1g_2g_2\lambda_1\mu_1 i)}{x^{(\lambda_1)}\sqrt{Y_{\lambda_1\mu_1 i}Y_{g_1}}}+$$

$$+\frac{\mathcal{K}(g_1g_2g_1\lambda_2\mu_2 i)}{x^{(\lambda_2)}\sqrt{Y_{\lambda_2\mu_2 i}Y_{g_2}}}\Big\}P^n_{g_1g_2}(\lambda\mu)-\sum_i\big(U_{g_1g_2}(\lambda\mu i)+V_{g_1g_2}(\lambda\mu i)\big)R^n_i(\lambda\mu)=0, \tag{17}$$

where

$$V_{g_1g_2}(\lambda\mu i)=\frac{1}{2}\sum_{g_3g_3'}\sum_{qq'g_3}\Gamma^{g_3}_{qq'}\Big\{\ell^{\lambda\mu i g_3}(qq'g_3)\mathcal{K}(g_1g_2g_3'g_3)+$$

$$+\ell^{g_1g_3'}(qq'g_3)\mathcal{K}(g_3g_2\lambda\mu i g_3)+\ell^{g_2g_3'}(qq'g_3)\mathcal{K}(g_1g_3'\lambda\mu i g_3)\Big\}$$

Substituting $P^n_{g_1g_2}(\lambda\mu)$ from (17) into (15) we get

$$(\omega_i-\eta_n)R^n_i(\lambda\mu)-\sum_{i'}W_{ii'}R^n_{i'}(\lambda\mu)=0, \tag{18}$$

where

$$W_{ii'}=\sum_{g_1g_2}\frac{\big(U_{g_1g_2}(\lambda\mu i)+V_{g_1g_2}(\lambda\mu i)\big)\big(U_{g_1g_2}(\lambda\mu i')+V_{g_1g_2}(\lambda\mu i')\big)}{(\omega_{g_1}+\omega_{g_2}-\eta_n)(1+\mathcal{K}(g_1g_2g_2g_1))-\frac{1}{4}\sum_i\Big(\frac{\mathcal{K}(g_1g_2g_2\lambda_1\mu_1 i)}{x^{(\lambda_1)}\sqrt{Y_{\lambda_1\mu_1 i}Y_{g_1}}}+\frac{\mathcal{K}(g_1g_2g_1\lambda_2\mu_2 i)}{x^{(\lambda_2)}\sqrt{Y_{\lambda_2\mu_2 i}Y_{g_2}}}\Big)}. \tag{19}$$

Thus, the commutation relations being exactly taken into account result in the shift of the two-phonon poles in the secular equation

$$\theta(\eta_n)=det\,\|(\omega_i-\eta_n)\delta_{ii'}-W_{ii'}\|=0. \tag{20}$$

and in the interaction $V_{g_1g_2}(\lambda\mu i)$. As it follows from (19) the corrections to the two-phonon state energies, arising due to the Pauli principle, are specified by the values of the coefficients $\mathcal{K}(g_1g_2g_3g_4)$. It is seen from (13) that $\mathcal{K}(g_1g_2g_3g_4)$ enter into the normalization of the wave function. The diagonal coefficients $\mathcal{K}(g_1g_2g_1g_2)$ are negative and less than unity in the absolute value.

The values of $\mathcal{K}(g_1 g_2 g_3 g_4)$ for the low quadrupole with K = 2 and octupole with K=0 states of ^{166}Er are given in the Table. Similar results are obtained for ^{176}Hf and ^{228}Th . It is seen from the Table that the coefficients $\mathcal{K}(gggg)$ and $\mathcal{K}(gg'gg')$ are negative and less than unity in the absolute value, they exceed considerably all the rest coefficients. The fact that the coefficient $\mathcal{K}(223,223,223,223)$ is close to (-1) is caused by that the corresponding one-phonon state $Q^+_{223}|\Psi_0\rangle$ is similar to the two-quasiparticle one. Therefore the norm of the two-phonon state $Q^+_{223}Q^+_{223}|\Psi_0\rangle$ deviates strongly from the value obtained within the harmonic approximation, this being indicated by a large value of the coefficient $\mathcal{K}(223,223,223,223)$.

Thus, the commutation relations between quasiparticles forming phonons can correctly be taken into account within the quasiparticle-phonon nuclear model. The influence of the Pauli principle on the energies of the two-phonon states and radiative strength functions requires further investigation.

Table

Values of the coefficients for ^{166}Er

$\lambda_1\mu_1 i_1$	$\lambda_2\mu_2 i_2$	$\lambda_3\mu_3 i_3$	$\lambda_4\mu_4 i_4$	$\mathcal{K}(g_1 g_2 g_3 g_4)$
221	221	221	221	-0,617
222	222	222	222	-0,849
223	223	223	223	-0,996
301	301	301	301	-0,358
221	301	221	301	-0,151
221	221	221	222	0,094
221	221	221	223	0,001

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