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COLLECTIVE HAMILTONIAN DERIVED FROM THE PAIRING-PLUS-QUADRUPOLE MODEL

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The microscopic collective hamiltonian for the axial quadrupole vibrations was derived from the QQ+PP model. The generator coordinate method and the generalized gaussian overlap approximation was used. The results were compared with the cranking estimates. The zero-point correction to the potential energy was found important. The mass parameters for the full two-body hamiltonian are nearly the same as for the mean-field approximation to that hamiltonian.

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1. *Introduction*

The microscopic collective hamiltonian is usually derived from the pairing-plus-quadrupole model (QQ+PP) [1] under the cranking approximation (e.g. Ref. [2]). Apart from a great success this approach has some disadvantages.

First, one begins there with the time-dependent Schrödinger equation while the nuclear vibration is a typical stationary process. Second, within the cranking model, one obtains a classical Hamilton function only. A quantal collective hamiltonian is then obtained after a somewhat arbitrary quantization procedure (see e.g. discussion in Ref. [3]).

The method proposed by Brink and Weiguny [4] is free of these disadvantages. Using the generator coordinate method (GCM) [5] and the gaussian overlap approximation (GOA) they obtained directly the quantal collective hamiltonian. This approach was since that time widely applied and discussed (Ref. [6]). A generalized version of the GCM+GOA theory in which one assumes only that the overlap of generating functions can be transformed to a Gauss function [7] is used in the present work.

There are two essential differences in the form of the collective hamiltonians in the

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cranking and in the GCM+GOA approaches. First, the metric tensor is assumed to be equal to the mass tensor in the cranking model, while in GCM the tensor of the widths of the overlap play the role of a metric. Second, the potential energy in GCM is determined accurately and not just up to an arbitrary scalar function as in the cranking model. It is equal to the Hartree-Fock energy, corrected by the so-called zero-point energy [8].

In Ref. [9] the mass parameters for the mean-field potential (MF) evaluated in both the cranking and GCM approaches were compared. The GCM inertia reaches only about 2/3 of the magnitude of the cranking masses. Also it was shown there that in the case of the hamiltonian with MF the GCM zero-point correction to the potential energy is identically zero. It was proven in the paper [10] that the particle number and angular momentum projection does not influence, in GOA, the magnitude of the mass parameters. The projection affects the potential energy only.

The aim of the present work is to investigate how the mass parameters and the zero-point energies are changed, when we take hamiltonian with two-body interaction instead of the mean field hamiltonian. For the pure pairing hamiltonian the effect was appreciable [11]. Now we take the pairing-plus-quadrupole hamiltonian [1]. Using the eigenfunctions of the axially deformed mean-field hamiltonian as the generator functions we construct the collective hamiltonian for the axial quadrupole vibrations.

The mass parameters for QQ+PP hamiltonian are rather close to those evaluated with the mean-field hamiltonian. They are almost equal, apart from small higher order and exchange terms, in all selfconsistency points. On the other hand, the zero-point correction does not vanish, as it did for MF. It has a magnitude of the order of 1 MeV and oscillates with deformation.

Results of our investigations can be easily generalized to the hamiltonians containing a two-body long range interaction in the local approximation [12], and the formalism presented here can be then applied to any multipolarity vibration, or spontaneous fission process [13].

The paper is organized as follows. Sect. 2 contains the description of our model and all useful formulae. The results and discussion are in Sect. 3 and at the end of the paper some conclusions are drawn.

2. *The model*

a) The pairing-plus-quadrupole hamiltonian

Following paper [1] we have assumed the hamiltonian in the form:

$$\hat{H} = \hat{H}_{sp} + \hat{H}_{QQ} + \hat{H}_{pair}, \tag{1}$$

where $\hat{H}_{sp}$ is the spherical single-particle hamiltonian of the Nilsson type [14] and $\hat{H}_{QQ}$ is the quadrupole-quadrupole long range interaction and $\hat{H}_{pair}$ stands for the pairing hamiltonian.

The term $\hat{H}_{QQ}$ contains the interactions among neutrons (nn), protons (pp) and between neutrons and protons (np):

$$\hat{H}_{QQ} = -\tfrac{1}{2}\{\chi_{nn}\hat{Q}_n^+\hat{Q}_n + \chi_{np}(\hat{Q}_n^+\hat{Q}_p + \hat{Q}_p^+\hat{Q}_n) + \chi_{pp}\hat{Q}_p^+\hat{Q}_p\}. \tag{2}$$

For simplicity we took only the axially symmetric component of $\hat{Q}$ operators

$$\hat{Q} = \sum_{i} r_i^2 Y_{20}(i), \tag{3}$$

where the sum runs over all protons (p) or neutrons (n). This approximation is not severe when one discusses axially symmetric vibrations because the missing components of $\hat{Q}$ appear in exchange terms only.

The pairing term $\hat{H}_{pair}$ is taken in the usual form:

$$\hat{H}_{pair} = -G_n \hat{P}_n^+ \hat{P}_n - G_p \hat{P}_p^+ \hat{P}_p \tag{4}$$

with

$$\hat{P} = \sum_{\nu > 0} a_{\bar{\nu}} a_\nu .$$

The form of hamiltonian $\hat{H}_0$ and its parameters are standard [15]. Two major shells $N = 4, 5$ for protons and $N = 5, 6$ for neutrons, were included in the calculations.

The strength of the quadrupole-quadrupole forces was taken

$$\chi_{nn} = \chi_{np} = \chi_{pp} = 250/A^{5/3} \text{ MeV} \tag{5}$$

and that of the pairing interaction was equal to:

$$G_n = 22/A \text{ MeV} \quad \text{and} \quad G_p = 27/A \text{ MeV}. \tag{6}$$

It is the standard choice of parameters for rare-earth region calculations [1].

Using the Hartree-Fock-Bogolubov approximation the hamiltonian $\hat{H}$ (1) can be written in a linearized form:

$$\hat{H}_{MF} = \hat{H}_{sp} - (\chi_{nn}\langle \hat{Q}_n \rangle + \chi_{np}\langle \hat{Q}_p \rangle)\hat{Q}_n - G_n(\langle \hat{P}_n^+ \rangle \hat{P}_n + \langle \hat{P}_n \rangle \hat{P}_n^+)$$
$$-(\chi_{np}\langle \hat{Q}_n \rangle + \chi_{pp}\langle \hat{Q}_p \rangle)\hat{Q}_p - G_p(\langle \hat{P}_p^+ \rangle \hat{P}_p + \langle \hat{P}_p \rangle \hat{P}_p^+). \tag{7}$$

It is the so-called mean-field hamiltonian. The averaging $\langle\ \rangle$ in (7) is taken over the BCS wave function:

$$|\text{BCS}\rangle = \prod_{\nu > 0} (u_\nu + v_\nu a_\nu^+ a_{\bar{\nu}}^+)\,|\text{vac.}\rangle \tag{8}$$

which is composed of eigenstates of a deformed single-particle hamiltonian:

$$\hat{H}_0(\beta) = -\frac{\hbar^2}{2m}\Delta + \tfrac{1}{2} m\omega_0^2 r^2[1 - 2\beta Y_{20}(\vartheta, \varphi)]$$
$$-\kappa[2\vec{l}\cdot\vec{s} + \mu(\vec{l}^2 - \langle \vec{l}^2 \rangle_N)]. \tag{9}$$

The hamiltonian $\hat{H}_0'(\beta)$ is identical to $\hat{H}_{sp}$ in (1) when the quadrupole deformation is $\beta = 0$.

It is worthwhile noting here that the selfconsistency condition for the mean-field hamiltonian (7) reads:

$$\chi_{nn}\langle\hat{Q}_n\rangle+\chi_{np}\langle\hat{Q}_p\rangle = \beta m\omega^2_{0(n)}$$
$$\chi_{np}\langle\hat{Q}_n\rangle+\chi_{pp}\langle\hat{Q}_p\rangle = \beta m\omega^2_{0(p)}. \quad (10)$$

We assume in the paper the same frequency ω_0 for protons (p) and neutrons (n):

$$\hbar\omega_0 = 41/A^{1/3}\ \text{MeV}. \quad (11)$$

Further on we have assumed β to be thegener ator coordinate. The BCS wave function (or better to say the product of the BCS wave function for protons and neutrons) composed of the single-particle states of $\hat{H}_0(\beta)$ is taken as the generator function $|\beta\rangle$. The pairing energy gap Δ and the Fermi level λ are obtained from the set of BCS equations and they depend here on β. It means that these parameters of the mean-field pairing hamiltonian are not taken as the independent generator coordinates (refer also to paper [11]).

b) The form of the collective hamiltonian

The generator coordinate method allows one to derive the collective hamiltonian $\hat{H}_{coll}$ when one assumes that the overlap of the generator functions can be transformed into gaussian form [4, 6–8]. We quote here the equation for $\hat{H}_{coll}$ when only one generator coordinate (β) is present:

$$\hat{H}_{coll} = \frac{-1}{2\sqrt{\gamma(\beta)}}\frac{d}{d\beta}\sqrt{\gamma(\beta)}/\mathrm{m}(\beta)\frac{d}{d\beta}+V(\beta), \quad (12)$$

a more general multidimensional form is given e.g. in Ref. [9]. The GCM mass parameter is equal to:

$$\mathrm{m}^{-1}(\beta) = \frac{1}{2\gamma^2}\left[\langle\beta|\frac{\overleftarrow{d}}{d\beta}\hat{H}\frac{\overrightarrow{d}}{d\beta}|\beta\rangle_L-\langle\beta|\hat{H}\frac{\overrightarrow{d}^2}{d\beta^2}|\beta\rangle_L+\frac{d\ln\gamma}{d\beta}\langle\beta|\hat{H}\frac{\overrightarrow{d}}{d\beta}|\beta\rangle\right], \quad (13)$$

where index L denotes the linked matrix element [8]. The width of the overlap (γ) plays the role of a metric in (12) and is given by:

$$\gamma(\beta) = \langle\beta|\frac{\overleftarrow{d}}{d\beta}\frac{\overrightarrow{d}}{d\beta}|\beta\rangle. \quad (14)$$

The collective potential:

$$V(\beta) = \langle\beta|\hat{H}|\beta\rangle-\varepsilon_0(\beta) \quad (15)$$

is corrected by the so-called zero-point energy [8]:

$$\varepsilon_0(\beta) = \frac{1}{2\gamma}\left[\frac{d}{d\beta}\langle\beta|\hat{H}\frac{\overrightarrow{d}}{d\beta}|\beta\rangle-\langle\beta|\hat{H}\frac{\overrightarrow{d}^2}{d\beta^2}|\beta\rangle_L\right]. \quad (16)$$

c) The microscopic expressions for the matrix elements

The matrix elements appearing in Eqs. (13, 14, 16) have to be evaluated microscopically. The derivative $\frac{d}{d\beta}$ is, in the BCS picture, the two-quasiparticle operator:

$$\frac{d}{d\beta}|\beta\rangle = \sum_{\nu,\mu>0} A_{\nu\mu}\alpha_\nu^+ \alpha_{-\mu}^+|\beta\rangle, \tag{17}$$

where the sum runs over all neutron and proton orbitals and

$$A_{\nu\mu} = -\frac{\langle\nu|\frac{d\hat{H}_0}{d\beta}|\mu\rangle}{E_\nu+E_\mu}(u_\nu v_\mu+u_\mu v_\nu)-\tfrac{1}{2}\,\delta_{\nu\mu}\left(\frac{\Delta}{E_\nu^2}\,\frac{d\lambda}{d\beta}+\frac{e_\nu-\lambda}{E_\nu^2}\,\frac{d\Delta}{d\beta}\right). \tag{18}$$

The matrix elements $\langle\beta|\hat{H}|\beta\rangle$, $\langle\beta|\hat{H}\frac{\vec{d}}{d\beta}|\beta\rangle$, $\langle\beta|\frac{\overleftarrow{d}}{d\beta}\hat{H}\frac{\vec{d}}{d\beta}|\beta\rangle$ and $\langle\beta|\hat{H}\frac{\vec{d}^2}{d\beta^2}|\beta\rangle$ were evaluated after transforming of the pairing-plus-quadrupole hamiltonian (1) into the quasiparticle (α_ν) picture.

The expectation value of the hamiltonian (1) is equal to:

$$\langle\beta|\hat{H}|\beta\rangle = \sum_\nu 2\langle\nu|\hat{H}_{sp}|\nu\rangle-\frac{\chi}{2}\left(\sum_\nu 2\langle\nu|\hat{Q}|\nu\rangle v_\nu^2\right)^2$$

$$-G\left(\sum_\nu u_\nu v_\nu\right)^2-G\sum_\nu v_\nu^4-\frac{\chi}{2}\sum_{\nu\mu}\langle\nu|\hat{Q}|\mu\rangle^2(u_\nu v_\mu+u_\mu v_\nu)^2. \tag{19}$$

χ and all operators here are expressed in intrinsic units [1, 14]. The last term contains the exchange part of the $\hat{H}_{QQ}$ interaction.

The expression for the other matrix elements of $\hat{H}$ (1) are rather long and we will not quote them here for lack of space. It is worthwhile to write them down at the selfconsistent points, where the equations simplify significantly:

$$\langle\beta|\frac{\overleftarrow{d}}{d\beta}\hat{H}\frac{\vec{d}}{d\beta}|\beta\rangle_L = \Sigma_1-\chi\Sigma_1^2+\ldots \tag{20}$$

$$\langle\beta|H\frac{\vec{d}^2}{d\beta^2}|\beta\rangle_L = -\chi\Sigma_1^2+\ldots \tag{21}$$

where

$$\Sigma_i = \sum_{\nu\mu}\frac{(\langle\nu|\hat{Q}|\mu\rangle)^2}{(E_\nu+E_\mu)^i}(u_\nu v_\mu-u_\mu v_\nu)^2. \tag{22}$$

We have omitted in (20–21) all higher order and exchange terms and that containing the derivatives $\frac{d\Delta}{d\beta}$ and $\frac{d\lambda}{d\beta}$.

Using the notation (22) one can write down the equation (14) for γ in a very short form:

$$\gamma(\beta) = \Sigma_2. \tag{23}$$

The selfconsistency condition (10) can be written in a different foım [12]

$$d\beta = \chi d\langle\beta|\hat{Q}|\beta\rangle \tag{24}$$

which leads to an estimate of the quadrupole-quadrupole strength

$$\chi^{-1} = \frac{d}{d\beta}\langle\beta|\hat{Q}|\beta\rangle \simeq 2\Sigma_1. \tag{25}$$

Using the last estimate of χ and the formulae (20–23) we ca get a simple estimate of the collective mass parameter $\mathfrak{m}$ (13):

$$\mathfrak{m}(\beta) = \frac{2(\Sigma_2)^2}{\Sigma_1} \tag{26}$$

and the zero-point correction (16) to the potential energy

$$\xi_0(\beta) = \frac{\gamma}{2\mathfrak{m}} = \frac{\Sigma_1}{4(\Sigma_2)^2}. \tag{27}$$

The formulae (26) and (27) are valid at the selfconsistent points only.

The expression (26) for collective inertia is essentially the same as that w hichone gets [10] taking the average mean field plus pairing hamiltonian

$$\hat{H}_G = \hat{H}_0(\beta)+\hat{H}_{pair}. \tag{28}$$

instead of the full pairing-plus-quadrupole hamiltonian (1).

The numerical calculations reported in the next section are based on the exact expression for all matrix elements entering the equations (13)–(16). The validity of the approximate formulae (20)–(22) and (25)–(28) is tested too.

For the sake of completeness we cite here the equation for the cranking inertia:

$$B(\beta) = 2\sum_{\nu\mu} A^*_{\nu\mu}A_{\mu\nu}(E_\nu+E_\mu)^{-1}, \tag{29}$$

where $A_{\nu\mu}$ is defined in (18). Neglecting in (18) the terms containing the derivatives $\frac{d\Delta}{d\beta}$ and $\frac{d\lambda}{d\beta}$ the expression (29) can be written in an even simpler form:

$$B(\beta) = 2\Sigma_3, \tag{30}$$

where Σ_3 is that of Eq. (22).

3. Results of the calculation

The numerical calculations were performed for a few nuclei in the rare-earth region. The results presented here are based on a typical representative of well deformed nuclei: ^{166}Er. All parameters of the calculation are standard [1, 2] and they are cited in Sec. 2 of the paper.

The expectation value of the pairing-plus-quadrupole hamiltonian (1) is plotted in Fig 1 as a function of deformation parameter β. It is equal to the selfconsistent energy V_{sc} [8] in the equilibrium configuration. Also in this point the selfconsistency condition $\beta = \chi\langle\beta|\hat{H}|\beta\rangle$ is satisfied and the linear term $\langle\beta|\hat{H}\frac{d}{d\beta}|\beta\rangle$ (see Eqs. (13) and (16)) vanishes. Please note that contrary to Ref. [8] the linear term vanishes in the selfconsistent points only.

The zero-point correction ξ_0 and the exchange term contributing to the collective potential V (Eqs. (15)–(16) and (19)) are drawn in Fig. 2. The zero-point energy is of the order of 1 MeV and fluctuates with growing deformation β. The amplitude of its oscillations is of the order 0.5 MeV. The fluctuation of the exchange term is much smaller.

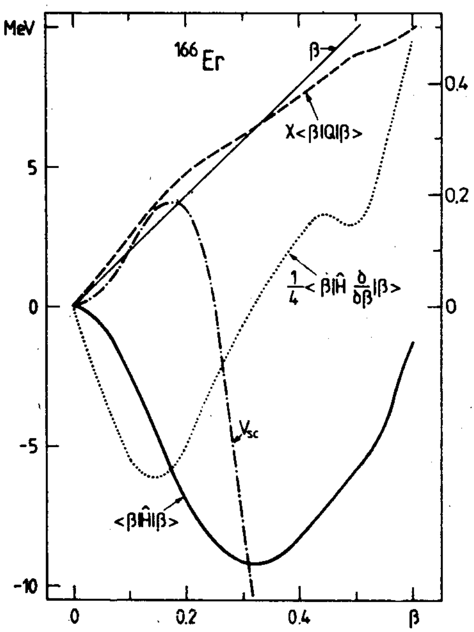

Fig. 1

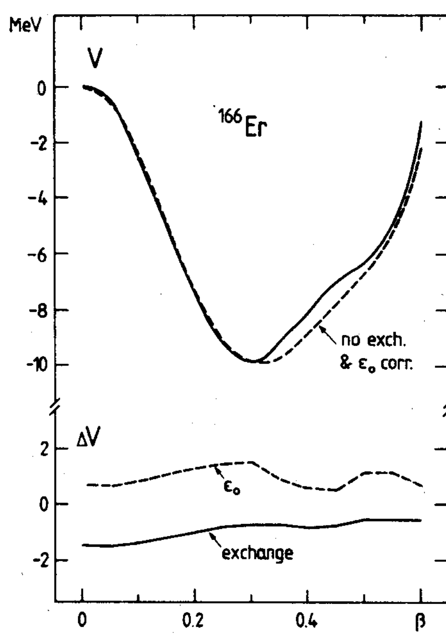

Fig. 2

Fig. 1. The expectation value of the pairing-plus-quadrupole hamiltonian, selfconsistent energy (V_{sc}), the linear term $\left\langle\beta\left|\hat{H}\frac{d}{d\beta}\right|\beta\right\rangle$ and the expectation value of the selfconsistent field $\chi\langle\beta|Q|\beta\rangle$ as functions of quadrupole deformation β

Fig. 2. The collective potential (V) with and without the zero-point correction (ε_0) and the exchange terms

The proton (p), neutron (n) parts and the whole (tot) width of the overlap of the generating functions is plotted in Fig. 3. It oscillates strongly as function of β suggesting that the curvature correction to $\mathfrak{m}$, Eq. (13) can be nonnegligible. The arrows indicate the equilibrium deformation.

The curvature correction, exchange terms and higher order pairing contributions to the collective mass parameter $\mathfrak{m}$ are presented in the bottom part of Fig. 4. They are

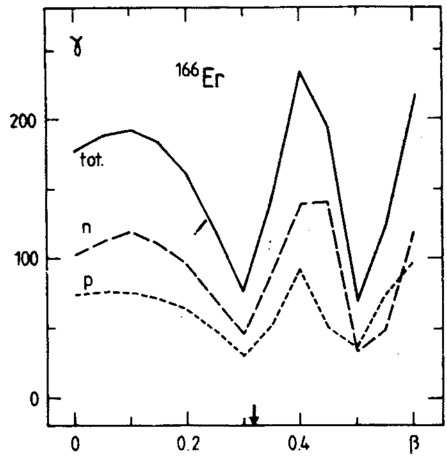

Fig. 3. The width of the overlap (γ) as well as its proton (p) and neutron (n) parts

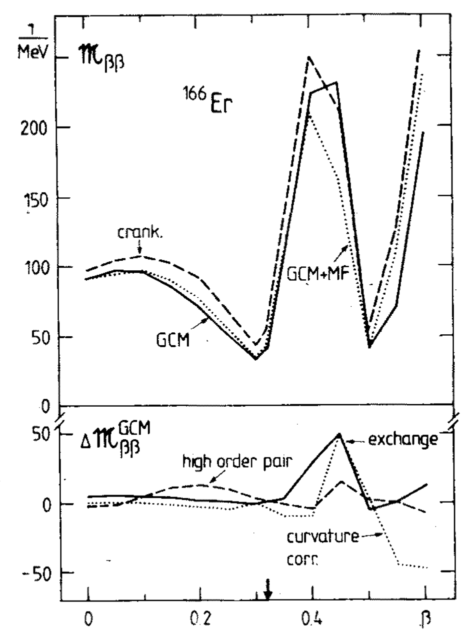

Fig. 4. The GCM masses for the full and the mean-field (MF) pairing-plus-quadrupole hamiltonians are compared with the cranking inertia. The contributions to the GCM mass due to exchange and higher order terms, as well as the curvature correction are plotted in the bottom part of the figure

especially predominant at deformation $\beta \simeq 0.45$. This effect is mainly connected with the small single-particle basis (see Sect. 2a) of the calculations.

In the upper part of Fig. 4 the mass parameters evaluated in the GCM approach for the full QQ+PP hamiltonian (GCM; Eq. (13)) and the average mean-field hamiltonian (GCM−MF; Eq. (26)) are compared with the cranking estimate of the inertia (Eq. (30)). The GCM+MF mass is always smaller than the cranking one, while this is not true for the GCM mass for the full hamiltonian. Also both the GCM estimates are nearly the same

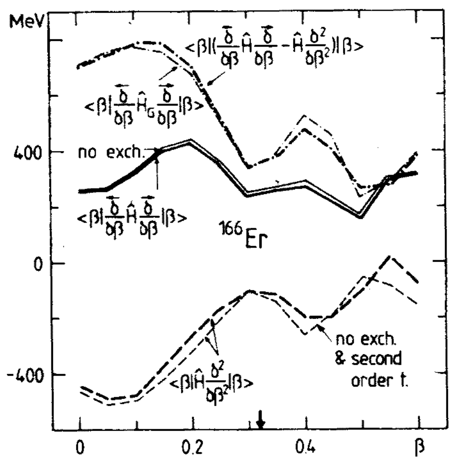

Fig. 5. The matrix elements entering the formulae for the GCM masses and zero-point energy

in the selfconsistent points. It means that the approximations (20)–(21) are really satisfied at these points.

The effect of the exchange and the higher order pairing terms on the magnitude of the matrix elements (20) and (21) entering the formula (23) for the mass parameter is presented in Fig. 5. This effect is usually smaller than 10% of the magnitude. The upper curves represent the accuracy of the approximations made in (20)–(21) and the estimate (25) of the coupling strength χ. If these approximations are accurate both curves should coincide. The deviations are smaller than 5% which is a measure of the quality of the approximations.

5. *Conclusions*

The following conclusions can be drawn from our investigations:

— the mass parameters evaluated in GCM+GOA model for the full pairing-plus-quadrupole hamiltonian and for the average mean-field potential are close to each other apart from the points in which the shell effects are large,

— the GCM masses are on the average by 20% smaller than the cranking inertias,

— the exchange and higher order pairing terms do not influence significantly the magnitude of the GCM mass parameters,

— the curvature correction term to the GCM inertia is equal to zero in all selfconsistent points and it is small for deformation $\beta < 0.4$,
— the zero-points correction to the potential energy is of the order of 1 MeV and oscillates with an amplitude of a 0.5 MeV as a function of deformation.

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REFERENCES

[1] M. Baranger, K. Kumar, *Nucl. Phys.* **62**, 113 (1965); **A110**, 490 (1968).
[2] K. Kumar, *Nucl. Phys.* **A231**, 189 (1974).
[3] H. Hofmann, *Z. Phys.* **250**, 14 (1977).
[4] D. M. Brink, A. Weiguny, *Nucl. Phys.* **A120**, 59 (1968).
[5] J. J. Griffin, J. A. Wheeler, *Phys. Rev.* **108**, 311 (1957); D. L. Hill, J. A. Wheeler, *Phys. Rev.* **89**, 1102 (1953).
[6] P. G. Reinhard, K. Goeke, preprint of Universität Erlangen-Nürnberg, FRG, 1985.
[7] A. Góźdź, *Phys. Lett.* **152B**, 281 (1985).
[8] P. Ring, P. Schuck, *The Nuclear Many-Body Problem*, Springer-Verlag 1980.
[9] A. Góźdź, K. Pomorski, M. Brack, E. Werner, *Nucl. Phys.* **A442**, 26 (1985).
[10] A. Góźdź, K. Pomorski, *Nucl. Phys.* **A451**, 1 (1986).
[11] A. Góźdź, K. Pomorski, M. Brack, E. Werner, *Nucl. Phys.* **A442**, 50 (1985).
[12] A. Bohr, B. R. Mottelson, *Nuclear Structure*, vol. 2, Benjamin 1975.
[13] K. Pomorski, Proc. of the Int. School-Seminar on Heavy Ion Physics, Dubna, USSR, 23–30, September 86.
[14] S. G. Nilsson, *Mat. Fys. Medd. Dan. Vidensk. Selsk.* **29**, No. 16 (1955).
[15] S. G. Nilsson, C. F. Tsang, A. Sobiczewski, Z. Szymański, S. Wycech, C. Gustafson, I. L. Lamm, P. Möller, B. Nilsson, *Nucl. Phys.* **A131**, 1 (1969).