VOLUME CONSERVING PAIRING IN RARE EARTH NUCLEI

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Equilibrium pairing in the deformed rare earth nuclei is calculated by varying energy expression along the trajectory of the constant mean square radius. The Nilsson potential is used in the calculations and its parameters are the only input data for the problem. The resulting equilibrium values of the proton and neutron energy gaps are compared with the values obtained by the standard procedure of fitting the pairing strength to the experimental odd-even mass differences.

1. Introduction

Pairing is well known to be one of the most important phenomena in the structure of nuclear states at low excitation energy. A great deal of consideration has been given to the problem of finding the best methods for its treatment. However, for heavy nuclei most of the work has been concentrated on the search for good methods of diagonalization of the pairing Hamiltonian with the phenomenological constant taken as the pairing force strength. It is far from obvious that even the exact diagonalization of the constant matrix element pairing force takes one close to the physical situation. Even assuming that the relevant matrix element of the real two-body force in the nucleus, namely: $\langle \nu, \tilde{\nu}|V|\nu', \tilde{\nu}'\rangle = G_{\nu\nu'}$, where $|\tilde{\nu}\rangle$ is the time reversed $|\nu\rangle$ state, varies slowly in the Fermi surface region, the average pairing strength:

$$G = \frac{\sum\limits_{\nu,\nu'} G_{\nu\nu'} u_\nu v_\nu u_{\nu'} v_{\nu'}}{\left(\sum\limits_{\nu} u_\nu v_\nu\right)^2} \tag{1}$$

is still a function of many nuclear parameters. In particular, it should depend rather strongly on the energy gap Δ, which determines the pairing amplitudes u, v. This is due to

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the fact that, even if one starts with all $G_{\nu\nu'} = G^0$ and performs the calculation in a limited, symmetric with respect to the Fermi surface λ, single particle state region, the renormalization of G, connected with the use of the limited single particle space, will increase it near the edges of the region, far from the Fermi surface, more than at the Fermi surface. The averaging (1) of the renormalized $G_{\nu\nu'} = G^0 + \delta G_{\nu\nu'}$ will give G small for small Δ (for which the weight function $u_\nu v_\nu$ is picked at the Fermi surface), and larger G value for larger values of Δ (for which the weight function becomes more and more flat).

The dependence of G on Δ may turn out to be important when the pairing potential $E(\Delta)$ is used, *e. g.* in calculating the Coriolis-antipairing effect in the rotational spectra. Of course, all the effects connected with variation of the pairing matrix element could be accounted for in the framework of the theory which uses the real nuclear two-body force as a starting point. This, however, is obviously a very complicated problem, and it seems useful to look for some simpler, approximate solutions.

The one proposed in [1–4] consists in constructing a variational procedure in which the equilibrium values of the energy gaps Δ_{eq} and the corresponding average matrix element $G(\Delta_{eq})$ are determined for a given nuclear state. Apart from postulated rules for varying the energy with respect to the energy gap Δ, which allow for the changes of G with Δ, the only input parameters of the procedure are those of the single particle potential. Thus the comparison of the equilibrium energy gaps obtained in this way with the experimental odd-even mass differences (or with the energy gaps obtained for the phenomenological value of the pairing strength) can be used as a straightforward test of the theory. Such a test was performed for the case of some spherical nuclei and gave satisfactory results [2, 3]. In the present paper the results obtained for the deformed rare earth nuclei with the Nilsson single particle potential as the input data are presented and compared with the values of the pairing parameters obtained by fitting the experimental odd-even mass differences.

2. *Variational procedure and its connection with the H–F energy changes*

In order to allow for the effective pairing strength $\tilde{G}$ changes with Δ, and use these changes in the variational procedure, consider the limit in which $\tilde{G}$ changes in such a way that every values of Δ is the self-consistent one in the BCS approximation

$$\Delta = \tilde{G}(\Delta) \sum_\nu u_\nu v_\nu \quad \text{or} \quad \tilde{G}(\Delta) = (\tfrac{1}{2} \sum_\nu 1/E_\nu)^{-1}, \tag{2}$$

where E_ν is the quasiparticle energy of the state ν. The pairing contribution to the energy is then:

$$E_p = -\Delta \sum_\nu u_\nu v_\nu. \tag{3}$$

For a small single particle space (3) can differ strongly from the constant G expression

$$E_p(G = \text{const.}) = -G (\sum_\nu u_\nu v_\nu)^2 \tag{4}$$

in all but two points: the curves intercept at $\Delta = 0$ and at the point $\tilde{G}(\Delta) = G$. In the limit of very large single particle space $\tilde{G}$ becomes very small for any finite value of Δ, thus it becomes very flat as a function of Δ. If the variational procedure assures stability of the equilibrium value of Δ in this limit we turn back to the constant G approximation. Thus, in enlarging the single particle space we get closer to the real variation of the effective $\tilde{G}$ with Δ, which should lie somewhere between the constant and the "self-consistent" case.

In practical calculation the expression (3) for the pairing contribution to the energy can be used for the single particle space large enough to ensure stability of the resulting equilibrium values of Δ with respect to the variations of the cut-off energy. Indeed, the constant value of Δ for a finite single particle energy interval may be considered as a step function approximation to a more realistic dependence of Δ on ν, which should also be varied in a more complete variational approach.

The next problem is to construct such an expression for the single particle contribution to the energy change with Δ which would take into account the rearrangement change of the single particle potential parameters, corresponding to the configuration change introduced by pairing correlations. In [1] the volume conservation was proposed as the simplest candidate for the condition determining the rearrangement changes. The motivation of such a choice is as follows. Pairing correlations in a system described by a single particle potential with Δ-independent parameters change the volume of the system. This means, in particular, that the average particle density $\varrho = A/V$ is changed. For the saturated system the energy change should not contain contributions proportional to $\delta\varrho$ while for the Δ independent parameters of the single-particle potential it does. The difficulty can be overcomed by calculating the energy change for a given nuclear state at $\varrho =$ constant or $V =$ constant. This in turn can be achieved by an appropriate change of the single particle potential parameters with Δ. The changes quadratic in $\delta\varrho$ are also eliminated in this way, but they can be estimated to be very small.

The meaning of the rearrangement changes of the single particle potential parameters imposed by the constant volume condition is clearly seen in the case of the harmonic oscillator potential. Here the oscillator frequency ω is the only parameter and the volume of the system can be connected with the mean square radius. Thus the condition of constant volume may be written as

$$\langle r^2\rangle_{\mathrm{BCS}} = \sum_{\nu} r_{\nu\nu}^2 2v_\nu^2 = (E_0 + \delta E_\Delta)\frac{\hbar}{m\omega(\Delta)} = \text{const.}, \tag{5}$$

where E_0 and $E_0 + \delta E_\Delta$ are the sums of the single particle energies, measured in $\hbar\omega$ units, at $\Delta = 0$ and at a finite Δ value, respectively. The rearrangement change of ω is thus given by

$$\frac{\omega(\Delta)}{\omega_0} = \frac{E_0 + \delta E_\Delta}{E_0}; \quad \omega_0 = \omega(\Delta = 0). \tag{6}$$

If the whole rearrangement is given by (6), only half of the potential energy should be summed in the energy expression, and we get:

$$E_{\text{s.p.}}(\Delta) = \hbar\omega(\Delta)\,(E_0+\delta E_\Delta)\,\tfrac{3}{4} = \hbar\omega_0[\text{const.} + \tfrac{3}{2}\,\delta E_\Delta + O(\delta E_\Delta)^2], \tag{7}$$

where we used (6) to write the energy in the Δ-independent units. It is easy to see the origin of the factor 3/2 appearing in (7) from the point of view of the Hartree-Fock approximation. The 2/2 part is simply the H–F rearrangement in the potential term, giving back factor 1 in the energy changes. The remaining 1/2 comes from the kinetic energy change corresponding to the H–F change of the h. osc. potential, its value being determined by the equality of the potential and kinetic energy contributions for the harmonic oscillator. So large a rearrangement change of the kinetic energy is thus specific for the harmonic oscillator. In the case of the Saxon-Woods potential the corresponding change of the kinetic energy contribution would be connected with the change in the diffuseness of the edge of the potential, caused by the pairing configuration change.

Summing the contributions (3) and (7) we get the expression

$$E(\Delta) = \frac{\omega(\Delta)}{\omega_0}\left[\frac{3}{4}\,(E_0+\delta E_\Delta) - \Delta \sum_\nu u_\nu v_\nu\right] \tag{8}$$

which can now be varied to obtain the equilibrium value of Δ.

3. The case of the deformed nucleus

Owing to the Coriolis-antipairing effect, pairing correlations change drastically within the rotational band of the deformed nucleus. To get the equilibrium pairing for a given rotational state, the ground state of the nucleus in particular, the wave functions projected on the right value of the angular momentum should be used in fact for calculation of the energy and the mean square radius. The first order projection correction to the energy expression will be discussed in the next section. The mean value of the scalar squared radius operator may be calculated for the deformed state because the projection on the $I = 0$ ground state amounts to giving of equal weights to every orientation of the deformed object with respect to the laboratory coordinate system. The main effect of working with the projected state is hidden here in the volume definition — for projected state we are forced to define it in the laboratory reference frame and connect it with the mean square radius in contrast *e. g.*, to the equilibrium deformation calculation, in which the intrinsic volume of the ellipsoidal density distribution should rather be conserved, while the mean square radius varies with deformation. This also means that different expressions for the energy changes should be used in the two cases. To be as close as possible to the standard equilibrium deformation calculation by the Bès-Szymański method [5] we use here their expression for the energy change with deformation, with our equilibrium values of the pairing energy gaps, determined by varying (8) at a fixed deformation. Such a procedure corresponds approximately to fitting the nuclear radius to the $A^{1/3}$ dependence at equilibrium values of the pairing energy gaps.

4. Corrections terms

The obvious corrections to the harmonic oscillator single particle potential are the Nilsson $\hat{l} \cdot \hat{s}$ and $l(l+1)$ terms. We take them with the r-independent Nilsson parameters:

$$U^{ls} = -\kappa[2\hat{l} \cdot \hat{s} + \mu(l(l+1) - \langle \hat{l}^2 \rangle_N)], \tag{9}$$

where $\langle \hat{l}^2 \rangle_N$ is the average of the single particle angular momentum square for the N-th oscillator shell, and (9) is measured in the $\hbar\omega$ units. It is difficult to conclude anything about the rearrangement change with Δ of the purely phenomenological parameters κ and μ. As their values are determined with respect to the change of the sum of the harmonic oscillator single-particle energies, we include (9) to the energy-change expression (8) with the same 3/2 factor as that multiplying the change of the single particle energies sum δE_Δ. (Note that a factor 1.25 was used in [2, 3, 4]. The difference in the resulting Δ_{eg} values is small. The factor 3/2 leads to a somewhat better relation between proton and neutron energy gaps.) The value of κ and μ for the rare earth region were taken from [6]. Working with a large single particle space one must, however, ensure a reasonable behaviour of the single particle energies for very large value of N, far above the Fermi surface. For these states the product $\kappa \cdot \mu$ should go to zero. Otherwise the states with very large N would emerge everywhere, even far below the Fermi surface. We keep κ constant for all the states and let μ decrease in such a way that the product $\kappa \cdot \mu$ decreases according to the extrapolations of [6] for A-values large enough to shift the Fermi surface up to the shell considered. The decrease in μ starts at $N = 6$ for protons and $N = 7$ for neutrons (about $2\hbar\omega$ above the Fermi surface). The rate of the decrease has practically no effect on the equilibrium values of Δ, provided it is kept in reasonable limits.

The next correction term comes from the approximate projection on the chosen value of the total angular momentum I. It is taken in the form given in the [7]:

$$\delta E^I_{\text{rot}} = -\frac{\hbar^2 \langle \hat{I}^2 \rangle}{2\mathcal{J}} + \frac{\hbar^2}{2\mathcal{J}} I(I+1), \tag{10}$$

where $\mathcal{J}$ is the moment of inertia, and the average is taken over the deformed BCS state. The expression (10) has the following simple physical meaning. If the energy (8) with the correction (9) is assumed to be the average value of the real nuclear Hamiltonian over the deformed state and the real Hamiltonian dependence on the angular momentum has the form of the rotational energy operator $\hbar^2 \hat{I}^2 / 2\mathcal{J}$, the average value of this operator should be replaced by its value for a fixed angular momentum I. The correction (10) increases the values of the equilibrium energy gaps for $I = 0$ ground state and approximately accounts for the Coriolis-antipairing effect for larger I. In the calculation the cranking model formula is used for the moment of inertia $\mathcal{J}$.

Another correction term used in the calculation is the RPA-correction to the ground state energy. It is essentially the RPA–BCS difference in the energy of the zero-point vibration in this state [8]. Its form is given in [2]. This correction increases the equilib-

rium energy gaps by a few per-cent. It has been checked by calculation that it can be replaced here by the familiar term:

$$-\tilde{G}\sum_{\nu} v_{\nu}^4. \tag{11}$$

This is connected with the fact that for the cases of very small equilibrium values of Δ, where BCS+RPA approximation of [8] should improve the results, a very flat or two minima curve is obtained for the energy as a function of Δ and dynamical pairing calculations similar to those of [9] should be performed. On the other hand, for larger values of Δ the BCS approximation, with the term (11) included, works quite well.

Finally, the Coulomb energy change is also included:

$$E_{\mathrm{C}} = E_{\mathrm{C}}^{0}\left[\frac{\langle r_p^2\rangle_{\Delta=0}}{\langle r_p^2\rangle_{\Delta}}\right]^{1/2}, \tag{12}$$

where E_{C}^{0} is the sharp-edge, deformed charge distribution Coulomb energy (see *e. g.* [6]) and the square root factor accounts for the change of the proton distribution radius with Δ. The proton mean square radius may change with Δ because only the mean square radius of the total (protons + neutrons) density distribution is conserved in the variational procedure.

The effect of the Coulomb energy correction on the equilibrium values of the energy gaps is small. It slightly increases the proton energy gaps and leaves the neutron energy gaps unchanged.

5. Details of the calculation and results

As mentioned above, the Nilsson potential was used as the single particle component of the Hamiltonian. Quadrupole and hexadecapole deformations were included. The parameters were taken from [6] where also the details of the form of the potential can be found. The potential was diagonalized within one oscillator shell in the stretched coordinate system ξ, η, ζ (to account for the quadrupole $N, N+2$ oscillator shell coupling). Then the BCS equation:

$$\sum_{\nu} 2v_{\nu}^2 = \text{number of particles} \tag{13}$$

was solved to obtain the Fermi energy λ for a set of Δ-values, for protons and neutrons. The main advantage of the simple Nilsson potential from the point of view of our calculations consists in the fact that the rearrangement change of the oscillator frequency ω changes only the energy scale for the single-particle energies here, and the equation (13) can be solved only once for each value of Δ in our variational procedure.

With the single particle states, single-particle energies and pairing amplitudes obtained

in this way the expression giving the energy change with Δ was constructed by summing the contributions (8), (9), (10), (11) and (12) for protons and neutrons:

$$\frac{\omega(\Delta)}{\omega_0}\left[\frac{3}{4}\sum_{\nu}\varepsilon_{\nu}^{\text{Nilsson}}2v_{\nu}^2+\frac{3}{4}\sum_{\nu}U_{\nu\nu}^{ls}2v_{\nu}^2-\right.$$

$$\left.-\Delta\sum_{\nu}u_{\nu}v_{\nu}-\tilde{G}\sum_{\nu}v_{\nu}^4+\delta E_{\text{rot}}\right]+E_{\text{C}} \tag{14}$$

and the ratio

$$\frac{\omega(\Delta)}{\omega_0}=\sum_{\nu}r_{\nu\nu}^2 2v_{\nu}^2\Big/\sum_{\nu}r_{\nu\nu}^2 n_{\nu}, \tag{15}$$

where $r_{\nu\nu}^2$ is the matrix element of r^2 for the Nilsson wave functions, measured in units of $\hbar/m\omega$, and n_{ν} are the occupation numbers for $\Delta = 0$, was calculated. All the summations in (14), (15) run over proton and neutron states.

Equilibrium values of Δ_{p} and Δ_{n} were determined by finding the minimum of (14) with respect to both variables. Stability of the solutions with respect to the cut-off energy variations was not investigated. The cut-off energy was kept constant and equal to 12 $\hbar\omega$

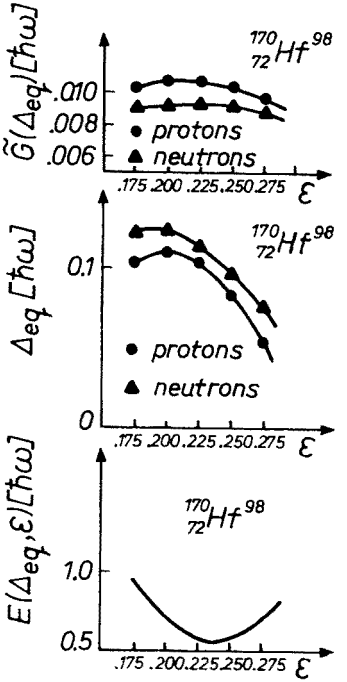

Fig. 1. The deformation dependence of the calculated equilibrium pairing energy gaps and the corresponding $\tilde{G}(\Delta_{\text{eq.}})$ values for ^{170}Hf. The energy function of Ref. [6] calculated with $\Delta = \Delta_{\text{eq.}}$ shows the position of the equilibrium deformation

both for the proton and neutron single particle spectrum. Such a large single particle space ensures that for the highest values of $\Delta_{eq.}$ (about 0.17 $\hbar\omega$) which we get, the changes of $\Delta_{eq.}$ are less than 0.01, when the cut-off is shifted up by 1 $\hbar\omega$. They are still smaller at $\Delta_{eq.} \approx 0.9$–0.11, which is a typical $\Delta_{eq.}$-value at equilibrium deformations.

The typical results for $\Delta_{eq.}$ at different deformations and the $\Delta_{eq.}$ values at the equilibrium deformations for nuclei in the rare earth region are shown in Figs 1 and 2. The values of Δ of [6], corresponding to the constant G fitted to the experimental odd-even mass differences in the rare earth region, are also shown for comparison.

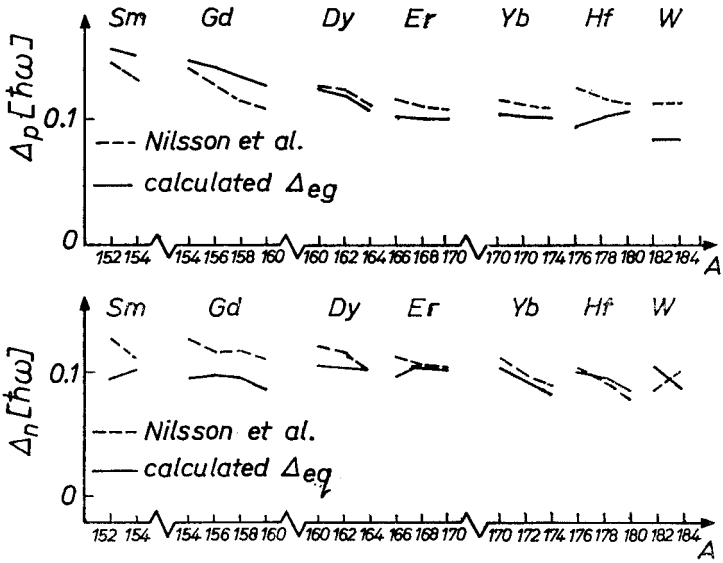

Fig. 2. The calculated ground state equilibrium pairing energy gaps for protons and neutrons (Δ_p and Δ_n respectively) in the rare earth region. The phenomenological constant G energy gaps of Ref. [6] are shown for comparison

It is seen from Fig. 1 that, owing to the strong equilibrium pairing dependence on the deformation, the calculation of the equilibrium deformation must be performed with the calculated $\Delta_{eq.}$ values in order to determine what is the ground state pairing in a real nucleus. As the hexadecapole deformation ε_4 was not determined in the calculations, the quadrupole deformation ε was varied along the line $\varepsilon_4 = \alpha\varepsilon$ with α chosen for each nucleus to give the result of [6] for ε_4 at the equilibrium value of ε. The equilibrium values of ε obtained with $\Delta_{eq.}$ are smaller on the average by 10% than the values obtained in [6].

6. *Conclusion*

The results for the ground state pairing energy gaps appear quite satisfactory. This is seen from the Fig. 2 if one remembers that the typical error of Δ determination from the odd-even mass differences is of the order of 0.01 and that it is probably much larger at

the edges of the deformed region, where the changes in the deformation energies lead to additional uncertainties. However, the systematic character of the discrepancies, together with the too small values of the ground state deformation obtained, suggest that they may be physically significant. On the other hand, they seem to be within the reach of the small change of the single-particle potential parameters κ and μ, which should probably be chosen much more carefully for our calculations, because they are the only input parameters here and there is no room for correcting the results by the choice of some other phenomenological quantities. The opposite sign of the discrepancies for protons and neutrons suggests that the difference between the proton and the neutron potentials is too large and should be decreased.

Satisfactory results for the ground state deformations tempt one to draw some conclusions concerning pairing beyond the equilibrium deformation. Fig. 1 shows that it varies faster with ε than the constant G pairing. The average pairing matrix element $\tilde{G}(\Delta_{\text{eq.}})$ comes close to the critical value at some deformations and is not a monotonic function of ε as assumed in some calculations. It is probable, however, that the inclusion of the quadrupole pairing term, suggested in [10], both in phenomenological and our pairing calculations would bring the two pictures much closer to each other, because such a term would obviously influence the dependence of energy gaps on deformation.

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