SIMPLIFIED H—F—B PAIRING CALCULATION AND THE VCP METHOD

By Z. Bochnacki*, E. B. Balbutsev

Joint Institute for Nuclear Research, Dubna

and M. Płoszajczak

Institute of Nuclear Physics, Cracow**

(Received March 12, 1976)

A simple version of the H–F–B pairing calculation, in which the H–F–B average single particle field is approximated by the phenomenological potential with parameters depending on the energy gap, is discussed. It is shown that the corrections to the standard pairing calculation those obtained are approximately included in the VCP method, proposed by the authors earlier. These corrections are important when the energy gain due to the pairing correlations is calculated. It is also concluded that VCP approximately takes into account the particle number projection effects.

1. Introduction

The pairing correlation effect on nuclear properties is usually obtained from an approximate diagonalization of the constant matrix element pairing force and the single particle (s.p.) Hamiltonian, containing a phenomenological potential and kinetic energy operator. Most of the effort to improve the description of the pairing correlation effect has been directed to improving the method of approximate diagonalization of such a Hamiltonian. A somewhat different approach to the problem of finding a simple description of the pairing correlation was developed by the authors of the present paper in [1–5]. Within the framework of this approach, which from now on will be referred to as VCP (volume conserving pairing), an attempt was made to improve the properties of the Hamiltonian itself by imposing some conditions, in particular the volume conservation condition. The VCP calculations have shown that pairing can be quite well accounted for without introducing any new phenomenological parameters apart from those of the s. p. potential.

* On leave from the Institute of Nuclear Physics, Cracow.
** Address: Instytut Fizyki Jądrowej, Radzikowskiego 152, 31-342 Kraków, Poland.

However, the arguments on the basis of which the additional VCP conditions were introduced met with some criticism. A more general foundation of the method is, therefore, needed in order to see what kind of improvement is introduced by VCP in comparison to the standard pairing calculation.

It is the purpose of this paper to show that VCP is an approximation of the full H−F−B method. It approximates the H−F−B calculation under the assumption, that the phenomenological potential reproduces well the shape of the H−F−B average s. p. field and that the state-independent energy gap Δ can be used. In comparison with the usual pairing calculation, VCP includes corrections arising from the fact that the phenomenological potential with constant parameters cannot approximate the H−F−B average s. p. field for finite changes of Δ.

The way in which the conditions connecting the parameters of the phenomenological Hamiltonian can be obtained within the H−F−B method is discussed in the second Section. The third one deals with the problem of practical use of the conditions thus obtained. In the last Section some questions concerning the particle number projection are discussed.

2. Relation between the s. p. and pairing parameters

1. In practical pairing calculations the Hartree-Fock part of the more general H−F−B problem is assumed to be solved. The H−F−B average s. p. field can be written as

$$U_{\nu\nu'} = \sum_{\mu} \langle \nu, \mu | V | \nu', \mu \rangle \tilde{n}_{\mu}, \tag{1}$$

where V is the antisymmetrized two-body force, and $\tilde{n}_{\mu}$ are the generalized occupation numbers, equal to the squares of the pairing amplitudes: $\tilde{n}_{\mu} = v_{\mu}^2$. The change of U caused the variation of $\tilde{n}$ is

$$\delta U_{\nu\nu'} = \sum_{\mu} \langle \nu, \mu | V | \nu', \mu \rangle \delta \tilde{n}_{\mu}. \tag{2}$$

The H−F self-consistency of U means, in particular, that the change of the s. p. states ν introduced by δU will give no linear contribution to the energy change at the H−F−B energy minimum. At the H−F−B minimum U can, therefore, be approximated by an $\tilde{n}$ independent phenomenological potential U^0. With the potential U^0 the BCS equations can be written and solved for Δ and the chemical potential λ in the usual way. The change of the s. p. energy is given in such a calculation by the familiar formula

$$\delta E_{\text{s.p.}} = \delta \{ \sum_{\nu} \varepsilon_{\nu}^0 \tilde{n}_{\nu} \},$$

where ε_{ν}^0 are the s. p. energies calculated with the potential U^0. It is easy to see that the contribution of δU to the energy change is automatically included here. From (1) and (2) we have

$$\sum_{\nu} \delta U_{\nu\nu} \tilde{n}_{\nu} = \sum_{\nu} U_{\nu\nu} \delta \tilde{n}_{\nu} \tag{3}$$

and the s. p. contribution to the energy change takes the form

$$\delta E_{\text{s.p.}} = \sum_{\nu} T_{\nu\nu}\delta\tilde{n}_{\nu} + \delta(\tfrac{1}{2}\sum_{\nu} U_{\nu\nu}\tilde{n}_{\nu}) \simeq \sum_{\nu}(T_{\nu\nu}+U_{\nu\nu})\delta\tilde{n}_{\nu} \simeq \delta(\sum_{\nu}\varepsilon^{0}_{\nu}\tilde{n}_{\nu}), \tag{4}$$

where T is the kinetic energy operator. Thus, by choosing a right shape of the potential U^0 and connecting its parameters a_i to the experimental quantities one can hope to approach the self-consistent solution for Δ, λ and associated quantities at the H−F−B minimum.

The situation is different when the energy change for finite differences of $\tilde{n}$ (or Δ) is to be calculated. This is, in particular, the case when the energy gain due to the pairing correlation $B_{\Delta} = E(\Delta = 0) - E(\Delta)$ is the required quantity. It follows from (1) that $E(\Delta = 0)$ and $E(\Delta)$ should be calculated with different s. p. potentials. The error introduced by calculating them with the same phenomenological potential U^0 cannot be eliminated by a better choice of its shape or parameters.

Another source of an even more serious error is due to the fact that the phenomenological potentials used in practical calculation can hardly pretend to reproduce the H−F self-consistency at the H−F−B minimum. When the energy change calculated by means of them is extrapolated to $\Delta = 0$, the use of (3) or (4) means that the entire potential change δU is included, also that part of it, which would be compensated for by a kinetic energy change in the self-consistent calculation.

2. An obvious generalization of the standard BCS procedure, which would be free from the inaccuracies mentioned above, consists in approximating U with the phenomenological potential $\tilde{U}^0$, the parameters $\tilde{a}_i$ of which change with $\tilde{n}$. The dependence of $\tilde{a}_i$ on $\tilde{n}$ should be consistent with the expressions (1) and (2). In order to solve the H−F−B problem simplified in this way, the energy minimum with respect to the pairing amplitude variations and the variations of the s. p. states ν, caused by the change of $\tilde{U}^0$ with Δ, should be found.

The relations between the parameters of $\tilde{U}^0$, implied by expression (1), can be obtained from (3) by writing δU as

$$\delta U_{\nu\nu} = \sum_{i}\left(\frac{\partial\tilde{U}^{0}_{\nu\nu}}{\partial\tilde{a}_i}\right)\delta\tilde{a}_i.$$

Equation (3) then takes the form

$$\sum_{\nu}\sum_{i}\left(\frac{\partial\tilde{U}^{0}_{\nu\nu}}{\partial\tilde{a}_i}\right)\delta\tilde{a}_i\tilde{n}_{\nu} = \sum_{\nu}\tilde{U}^{0}_{\nu\nu}\delta\tilde{n}_{\nu}. \tag{5}$$

It follows from (1) and (2) that if $\tilde{U}^0$ splits into parts which come from different components of the two-body force, relation (5) can be written separately for each part and its parameters.

It is interesting to examine the case of the harmonic oscillator potential, in which relation (5) determines the $\tilde{n}$-dependence of the single parameter, i. e. the oscillator strength ω. (The dependence should be the same for the widely used Nilsson potential, since the

spin orbit force can be connected with different component of the two-body interaction.) We have $\tilde{U}^0_{\nu\nu} = \frac{1}{2}\hbar\omega\bar{r}^2_{\nu\nu}$, where $\bar{r}^2_{\nu\nu} = N_\nu + \frac{3}{2}$, N_ν being the oscillator quantum number of the s. p. state ν, and (5) can be written as

$$\sum_\nu \tfrac{1}{2}\hbar\bar{r}^2_{\nu\nu}\delta\omega\tilde{n}_\nu = \sum_\nu \tfrac{1}{2}\hbar\omega\bar{r}^2_{\nu\nu}\delta\tilde{n}_\nu$$

or

$$\frac{\delta\omega}{\omega} = \frac{\delta\langle\bar{r}^2\rangle_{\mathrm{BCS}}}{\langle\bar{r}^2\rangle_{\mathrm{BCS}}},$$

where $\langle\bar{r}^2\rangle_{\mathrm{BCS}} = \sum_\nu \bar{r}^2_{\nu\nu}\tilde{n}_\nu$. Integrating this equation we get

$$\langle\bar{r}^2\rangle_{\mathrm{BCS}}/\omega = \text{const.}$$

or

$$\langle r^2\rangle_{\mathrm{BCS}} = \frac{\hbar}{m\omega}\langle\bar{r}^2\rangle_{\mathrm{BCS}} = \text{const.} \tag{6}$$

which tells us that the mean square radius of the nucleus should not be influenced by the pairing correlation. Condition (6) is just the condition which has been used in the VCP method.

3. It is easy to see the effect that relation (6) may have on the pairing energy gain B_Δ. With the $\tilde{n}$-independent h. o. potential we would have the s. p. contribution

$$\delta E_{\mathrm{s.p.}} = \omega_0\{\sum_\nu \bar{r}^2_{\nu\nu}n_\nu - \sum_{\nu>0}\bar{r}^2_{\nu\nu}2v^2_\nu\} = -\omega_0\delta\langle\bar{r}^2\rangle,$$

where $\delta\langle\bar{r}^2\rangle$ is the difference of the mean square of the dimensionless radius for $\Delta \neq 0$ and $\Delta = 0$ states. With the $\tilde{n}$-dependent h. o. potential $\tilde{U}^0$ the s. p. energy expression must be written with the factor 3/4, ensuring that the potential energy is counted once:

$$\tilde{E}_{\mathrm{s.p.}} = \omega_\Delta\,\tfrac{3}{4}\sum_{\nu>0}\bar{r}^2_{\nu\nu}2v^2_\nu = \omega_\Delta\,\tfrac{3}{4}\{\langle\bar{r}^2\rangle_{\Delta=0} + \delta\langle\bar{r}^2\rangle\}. \tag{7}$$

From (6) we have

$$\frac{\omega_\Delta}{\omega_0} = \frac{\langle\bar{r}^2\rangle_\Delta}{\langle\bar{r}^2\rangle_{\Delta=0}} = 1 + \frac{\delta\langle\bar{r}^2\rangle}{\langle\bar{r}^2\rangle_{\Delta=0}} \tag{8}$$

and thus

$$\tilde{E}_{\mathrm{s.p.}} = \omega_0\,\tfrac{3}{4}\left\{\left(1 + \frac{\delta\langle\bar{r}^2\rangle}{\langle\bar{r}^2\rangle_{\Delta=0}}\right)(\langle\bar{r}^2\rangle_{\Delta=0} + \delta\langle\bar{r}^2\rangle)\right\} \simeq \tilde{E}_{\Delta=0} + \tfrac{3}{2}\,\omega_0\delta\langle\bar{r}^2\rangle. \tag{9}$$

The kinetic energy correction included by using the $\tilde{n}$-dependent potential $\tilde{U}^0$ can, therefore, be as large as 1/2 of the s. p. contribution to the pairing energy gain, and it can significantly reduce B_Δ. This can be important in the equilibrium deformation calculation, and can be of primary importance in the Coriolis-antipairing calculation, where B_Δ essentially determines the value of the spin, at which the transition to the $\Delta = 0$ phase takes place.

It has been shown recently [6, 7] that in the usual BCS calculation the particle number projection, which enlarges B_Δ, wipes out or pushes to high spins the point of the phase transition. It follows from (9) that in the standard BCS one actually works with too large values of B_Δ. Thus, the conclusion of [6, 7] that the Coriolis-antipairing effect cannot be the basic mechanism responsible for the anomalies in the rotational spectra are not really demonstrated in this situation.

3. Pairing calculation with the Δ-dependent h. o. potential

At the value of ω corresponding to the H−F−B minimum, $\omega = \omega_{eq}$, the pairing contribution to the energy expression can be calculated in the same way as for the Δ-independent potential and has, therefore, the familiar form:

$$E_{\text{pair.}} = -\omega_{eq}\Delta \sum_{\nu>0} u_\nu v_\nu, \tag{10}$$

where Δ is connected with the ratio of the pairing force strength G to ω by the BCS equation

$$\Delta = \frac{G}{\omega_{eq}} \sum_{\nu>0} u_\nu v_\nu. \tag{11}$$

In order to get the value of ω_{eq} we have to find the point, at which the energy of the system, equal to the sum of the s. p. contribution (7) and the pairing contribution (10),

$$\tilde{E} = \omega\{\tfrac{3}{4} \sum_{\nu>0} \bar{r}^2_{\nu\nu} 2v^2_\nu - \Delta \sum_{\nu>0} u_\nu v_\nu\} \tag{12}$$

is stable against variations of ω:

$$\frac{d\tilde{E}}{d\omega} = \frac{d\tilde{E}}{d\Delta}\frac{d\Delta}{d\omega} = 0.$$

For $\dfrac{d\Delta}{d\omega} \neq 0$ (it is always different from zero for the pairing acting in a sufficiently large s. p., h. o. space) we get

$$\frac{d\tilde{E}}{d\Delta} = 0.$$

Thus, the value of Δ (in ω units) corresponding to the stability point can be obtained by finding the minimum of the energy $\tilde{E}$ with respect to Δ. The dependence of ω on Δ is given by (6) or (8). These relations also couple the equilibrium values ω_{eq} and Δ_{eq}

$$\omega_{eq} = \omega(\Delta_{eq}).$$

The procedure described above has been used in the VCP method. It should be pointed out that once the pairing contribution at the stability point is written as in form (10), no use is made of G and the BCS Eq. (11) for finding the Δ_{eq} value. Relation (6) couples

the s. p. and pairing parameters. They can be determined at the equilibrium point from the values of the same experimental quantities (the mean square radius of the nucleus in our case). Once ω_{eq} and Δ_{eq} are determined, Eq. (11) may be used to calculate G.

It should also be stressed that in order to use condition (6), the pairing calculation should be performed in a sufficiently large s. p. space. In one oscillator shell condition (6) is an identity and loses its physical meaning. This corresponds to the fact that with the h. o. degeneracies, the pairing force acting in one oscillator shell has no influence on the structure of the wave function. The pairing amplitudes are fixed in the degenerated case by the conservation of the average particle number and do not depend on G.

In the VCP calculation the term $-G\sum_{\nu} v_{\nu}^4$ has been added to the energy expression (12). This is consistent with the present derivation of the method since this r-independent term may be considered as an Δ-dependent correction to the constant term of the s. p. potential, which is not explicitly used in the calculation.

4. The particle number projection effect

The pairing calculation is often improved by projecting the right particle number component out of the BCS wave-function and only then performing the variation with respect to Δ (see, e. g., Refs [6, 7]). From the point of view of the BCS energy calculation the effect of the particle number projection amounts to a multiplication of G and the s. p. operator in the varied energy expression by the Δ-dependent factors. The factors are equal to the ratios of the projected and unprojected average values of the pairing force and the s. p. part of the Hamiltonian, respectively.

The main projection effect comes in the standard calculation from the multiplication of G by the Δ-dependent factor. It can be accounted for by a redefinition of Δ in Eq. (11),

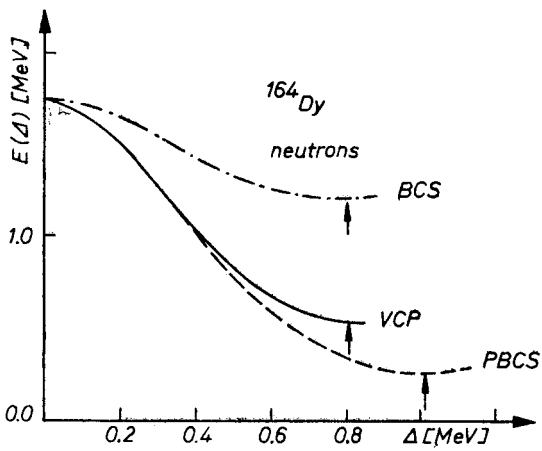

Fig. 1. The VCP $E(\Delta)$-curve for ^{164}Dy (full curve) is compared with the curves obtained in [7] by the BCS calculation with (PBCS) and without particle number projection (dashed and dash-dotted curves, respectively)

corresponding to calculating it with the Δ-dependent G [8]. The projection does not influence then the form of (10) of the pairing contribution used in our method.

The particle number projection effect could, therefore, influence the VCP results only through the Δ-dependent factor multiplying the s. p. part of the Hamiltonian. Here, however, it can be included in the ω dependence on Δ and condition (6) determines then the total Δ-dependence of ω, together with that part of it introduced by the projection. The VCP method "feels", therefore, the particle number projection only through the values of its parameters, and the projection is effectively accounted for when the parameters are determined from the experimental values of physical quantities.

In order to illustrate this conclusion, an example of the VCP $E(\Delta)$ curve is compared in Fig. 1 with the curves calculated by the usual BCS method and by the BCS with the particle number projection before the variation (PBCS). The Nilsson s. p. potential with $\omega_0 = 41/A^{1/3}$ MeV was used in all three cases. In VCP only the parameters of the Nilsson potential were required. The equilibrium deformation was determined by minimizing the energy expression with respect to quadrupole deformation. The details of the calculation may be found in Ref. [5]. The BCS and PBCS curves were calculated in [7] at the experimental equilibrium deformation and with G fitted to the experimental odd-even mass differences. It should be noted that the inclusion of the corrections discussed in this paper in the BCS and PBCS calculation would increase the minima in both cases.

The authors would like to thank Dr S. Frauendorf for supplying the BCS and PBCS curves for comparison with the result of VCP. They also thank Dr. I. N. Mikhailov for helpful discussions of the subject considered here.

REFERENCES

[1] Z. Bochnacki, *Phys. Lett.* **31B**, 187 (1970).
[2] E. B. Balbutsev, Z. Bochnacki, *Acta Phys. Pol.* **B3**, 287 (1972).
[3] E. B. Balbutsev, Z. Bochnacki, *Acta Phys. Pol.* **B3**, 283 (1972).
[4] E. B. Balbutsev, Z. Bochnacki, *Acta Phys. Pol.* **B5**, 397 (1974).
[5] Z. Bochnacki, M. Płoszajczak, E. B. Balbutsev, *Acta Phys. Pol.* **B6**, 769 (1975).
[6] F. Gruemmer, K. W. Schmid, Amand Faessler, *Nucl. Phys.* **A239**, 289 (1975).
[7] S. Frauendorf, *JINR report* E4-9101, Dubna 1975.
[8] I. N. Mikhailov, *Sov. Phys. JETP* **18**, 761 (1964).