

correct if the crossed cuts in the N 's were given functions. It is interesting to note that, depending on the coupling constants c and d , the inelastic contribution to M_{22} can have a very large effect on the position of a resonance, even if it has an energy considerably below the inelastic threshold. Another amusing point is the possibility of a bound state in the $(M'-M')$ system of mass M_0 which should yield a two-particle cut in M_{22} starting at $(M_0+\mu)^2$. Continuing analytically in the coupling constant a , one sees that this cut arises from the $I_4(s)$ terms in $M_{22}(s)$. The procedure for performing this continuation has been described elsewhere.²⁵ The essential point is that since D_{11} develops

²⁵ R. Blankenbecler, M. Goldberger, S. MacDowell, and S. Treiman (to be published). For a preliminary account see R. Blankenbecler, *Proceedings of the 1960 Annual International*

a zero at the bound-state mass, the s' integral in I_4 must be deformed to avoid the resulting singularity of the integrand. This procedure then yields an "anomalous threshold" beginning at the point $(M_0+\mu)^2$. By picking out the residue at M_0 in the variable w , one can calculate the processes $(M_0+\mu \rightarrow M_0+\mu)$ and $(M+M \rightarrow \mu+M_0)$ from M_{33} and M_{23} , respectively.

One final observation concerns the possibility of a three-particle bound state. This occurs when the denominator in M_{22} develops a zero below the point $4M^2$. The bound-state pole is also seen to be present in M_{23} and M_{33} due to the general structure of the solutions.

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Self-Consistent Field Theory of Nuclear Shapes*

MICHEL BARANGER

Carnegie Institute of Technology, Pittsburgh, Pennsylvania

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The Hartree-Fock equations are generalized to include pairing effects on the same footing with field-producing effects. In addition to the Hartree potential, there enters a pairing potential. When applied to a spherically symmetric shell-model Hamiltonian, these equations may possess deformed solutions. Application is made to pairing plus quadrupole forces, with results identical to those of Belyaev and Kisslinger and Sorensen. The spherical shape becomes unstable when some collective vibration of the spherical nucleus reaches zero frequency.

1. INTRODUCTION

THE question to be considered here is the calculation of nuclear shapes starting from a spherically symmetric Hamiltonian. In a Hartree-Fock type of theory, all nuclei are deformed except at closed shells. It is well known that residual interactions tend to keep nuclei spherical for a while as one goes away from closed shells. Since a prominent effect of residual interactions is to produce pairing correlations, one might think that the inclusion of pairing¹ effects together with the Hartree-Fock field would be able to give realistic estimates of shapes.

This problem has been treated by Belyaev,² who gave it an approximate solution for the case where the single-particle levels are degenerate and the two-body force is a combination of pairing force and quadrupole force. In this paper, we would like to consider the more practical case of nondegenerate single-particle levels and also to develop a formalism which can be used with

any two-body interaction. The inclusion of a general two-body interaction was also considered by Belyaev at the beginning of his paper, but his solution involves three successive canonical transformations, which makes it of limited practical value. In the present work, a single transformation is made, the generalized Bogolyubov transformation.³ It differs from the more familiar Bogolyubov-Valatin transformation⁴ in the following way. In the latter, a specific assumption is made about the bound state (the Cooper pair) into which pairs of particles are allowed to condense; for instance, in the application to spherical nuclei,^{5,6} the two particles are assumed to have opposite angular momenta. On the other hand, in the generalized transformation, the bound-state wave function is left completely arbitrary and is determined by minimizing the

³ N. N. Bogolyubov, *Uspekhi Fiz. Nauk* **67**, 549 (1959) [translation: *Soviet Phys.—Uspekhi* **67**(2), 236 (1959)]. See also Y. Nambu, *Phys. Rev.* **117**, 648 (1960).

⁴ N. N. Bogolyubov, *Nuovo cimento* **7**, 794 (1958); J. G. Valatin, *Nuovo cimento* **7**, 843 (1958).

⁵ L. S. Kisslinger and R. A. Sorensen, *Kgl. Danske Videnskab. Selskab, Mat.-fys. Medd.* **32**, No. 9 (1960).

⁶ M. Baranger, *Phys. Rev.* **120**, 957 (1960). We follow many of the notations of this paper. See also R. Arvieu and M. Vénéroni, *Compt. rend.* **250**, 992, 2155 (1960); T. Marumori, *Progr. Theoret. Phys. (Kyoto)* **24**, 331 (1960); G. E. Brown, J. A. Evans, and D. J. Thouless (to be published).

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¹ J. Bardeen, L. N. Cooper, and J. R. Schrieffer, *Phys. Rev.* **108**, 1175 (1957), referred to in the following as BCS; A. Bohr, B. R. Mottelson, and D. Pines, *Phys. Rev.* **110**, 936 (1958).

² S. T. Belyaev, *Kgl. Danske Videnskab. Selskab, Mat.-fys. Medd.* **31**, No. 11 (1959). Some of Belyaev's results were derived in a different way by A. Kerman, *Ann. Phys.* **12**, 300 (1961).

energy or by a self-consistency requirement. There results a set of equations (Sec. 2) which we call the Hartree-Bogolyubov equations and which generalize the Hartree-Fock equations. Although these equations arise naturally in the consideration of the general self-consistent field problem including pairing effects,⁷ they do not seem to have been written down previously in their full generality. They contain two potentials, the usual Hartree-Fock potential and another which describes pairing correlations and which we shall call the "pairing potential." Thus, these equations describe in a self-consistent manner what Bohr and Mottelson⁸ have called the two main effects of nuclear forces, the field-producing effect and the pairing effect. Other, less important effects are left in the residual interaction.

Although these equations always have a spherically symmetric solution, they also often possess in addition one or several deformed solutions. It is the solution with the lowest total energy which provides the stable shape of the nucleus. Hence, one is in possession of a framework which can allow one, "in principle," to answer such difficult questions as which nuclei are spherical, which are deformed, and whether the deformed ones are axially symmetric. The reader is referred to Belyaev's paper² for some very interesting qualitative discussions of these points. The answer that one expects is that nuclei are spherical at both ends of a shell, but strongly deformed in the middle.

In Sec. 3, we apply our formalism to nuclear forces consisting of a pairing force and a quadrupole force. The usefulness of this combination of interactions has been demonstrated in the recent work of Kisslinger and Sorensen.⁵ We find that our method, for this particular choice of forces, is identical to theirs and to Belyaev's. The deformations are quadrupolar, although not necessarily axially symmetric. We also investigate the stability of the spherically symmetric solution against small deformations. As a shell is being filled, the transition from spherical to deformed shape occurs exactly at the stage where the collective vibrations of the spherical nucleus, as calculated by the method of linearized equations of motion,⁶ reach zero frequency. Actually, this result is not dependent on the special forces assumed and we prove it in general. It is of interest in connection with the general theory of the stability of many-body systems. Unfortunately, nuclei are so small that nonlinear effects and zero-point motion are very important. Hence, it is expected that the vibrational frequencies computed on the spherical side and the deformations computed on the deformed side

will both be rather bad approximations near the transition.

2. HARTREE-BOGOLYUBOV EQUATIONS

Our point of departure is a spherically symmetric shell-model Hamiltonian with chemical potential

$$\mathcal{H} = H - \lambda \mathcal{N} \\ = \sum_{\alpha} (\epsilon_{\alpha} - \lambda) c_{\alpha}^* c_{\alpha} + \sum_{\alpha\beta\gamma\delta} \mathcal{V}_{\alpha\beta\gamma\delta} c_{\alpha}^* c_{\beta}^* c_{\delta} c_{\gamma}. \quad (1)$$

The c 's and c^* 's are a set of fermion creation and annihilation operators. We assume that the potential \mathcal{V} is sufficiently smooth to be treated by a Hartree-type approximation. In other words, we shall assume that problems associated with the repulsive core and the relationship of the effective two-body force to the observed nucleon-nucleon scattering have been solved. It is essential for the manipulations that follow to keep in mind the following symmetry properties of \mathcal{V} ,

$$\mathcal{V}_{\alpha\beta\gamma\delta} = -\mathcal{V}_{\beta\alpha\gamma\delta} = -\mathcal{V}_{\alpha\beta\delta\gamma} = \mathcal{V}_{\gamma\delta\alpha\beta}^*. \quad (2)$$

The generalized Bogolyubov transformation³ consists in re-expressing \mathcal{H} in terms of a new set of fermion operators, the quasi-particle operators, which are the most general linear combination of c 's and c^* 's,

$$a_i^* = \sum_{\alpha} (A_{\alpha}^i c_{\alpha}^* + B_{\alpha}^i c_{\alpha}). \quad (3)$$

Thus, every quasi-particle i possesses two wave functions: A_{α}^i , which is the wave function of its particle part; and B_{α}^i , which is the wave function of its hole part. The requirement that the a 's also form a set of fermion operators entails the orthogonality relations

$$\sum_{\alpha} (A_{\alpha}^i A_{\alpha}^j + B_{\alpha}^i B_{\alpha}^j) = \delta_{ij}, \quad (4a)$$

$$\sum_{\alpha} (A_{\alpha}^i B_{\alpha}^j + B_{\alpha}^i A_{\alpha}^j) = 0, \quad (4b)$$

$$\sum_i (A_{\alpha}^i A_{\beta}^{i*} + B_{\alpha}^i B_{\beta}^{i*}) = \delta_{\alpha\beta}, \quad (4c)$$

$$\sum_i (A_{\alpha}^i B_{\beta}^{i*} + B_{\alpha}^i A_{\beta}^{i*}) = 0, \quad (4d)$$

and the inverse relations

$$c_{\alpha} = \sum_i (A_{\alpha}^i a_i + B_{\alpha}^{i*} a_i^*). \quad (5)$$

When expressed in terms of quasi-particle operators, \mathcal{H} consists of four parts,

$$\mathcal{H} = \mathcal{H}_1 + \mathcal{H}_2 + \mathcal{H}_3 + \mathcal{H}_4. \quad (6)$$

The last term, \mathcal{H}_4 , contains products of four operators in normal order⁹; to avoid having to write 16 terms, we put it in the form

$$\mathcal{H}_4 = \sum_{\alpha\beta\gamma\delta} \mathcal{V}_{\alpha\beta\gamma\delta} \mathcal{N}(c_{\alpha}^* c_{\beta}^* c_{\delta} c_{\gamma}), \quad (7)$$

where it is understood that the normal ordering symbol

⁷ For instance, the solution of this problem by the method of reference 3 is actually equivalent to solving the Hartree-Bogolyubov equations, but the latter yield some additional information, namely, the single-particle excitations.

⁸ A Bohr, invited talk at the 1960 Spring meeting of the American Physical Society (unpublished); B. Mottelson, *Proceedings of the International Conference on Nuclear Structure, Kingston, Canada, 1960* (University of Toronto Press, Toronto, 1960), p. 525.

⁹ S. S. Schweber, H. A. Bethe, and F. de Hoffmann, *Mesons and Fields* (Row-Peterson and Company, Evanston, Illinois, 1955), Vol. I, p. 203.

N refers to the a 's, not the c 's. \mathcal{H}_3 contains products of two creation or two annihilation operators; we require that it vanish identically. \mathcal{H}_2 contains products of one creation and one annihilation operator; we require that it be of the form

$$\mathcal{H}_2 = \sum_i E_i a_i^* a_i, \quad (8)$$

with positive E_i . We use these two requirements, together with orthogonality relations (4), to determine the A 's and B 's. Finally, \mathcal{H}_1 is just a number. The significance of the various terms is clear. The vacuum of the quasi particles is taken as an approximation for the ground state of our system, a generalization of the BCS ground state, and its energy is \mathcal{H}_1 . The energies of the elementary excitations, or quasi particles, are given by E_i , while \mathcal{H}_4 is the residual interaction between quasi particles.

When the details are worked out, one finds that A and B must obey the equations

$$E_i A_\alpha^i = (\epsilon_\alpha - \lambda) A_\alpha^i + \sum_\gamma \Gamma_{\alpha\gamma} A_\gamma^i + \sum_\beta \Delta_{\alpha\beta} B_\beta^i, \quad (9a)$$

$$E_i B_\alpha^i = -(\epsilon_\alpha - \lambda) B_\alpha^i - \sum_\gamma \Gamma_{\alpha\gamma}^* B_\gamma^i - \sum_\beta \Delta_{\alpha\beta}^* A_\beta^i, \quad (9b)$$

which are easily seen to be compatible with the orthogonality relations. The quantities Γ and Δ are defined by

$$\Delta_{\alpha\beta} = -\Delta_{\beta\alpha} = 2 \sum_{\gamma\delta} \mathcal{U}_{\alpha\beta\gamma\delta} \kappa_{\gamma\delta}, \quad (10a)$$

$$\Gamma_{\alpha\gamma} = \Gamma_{\gamma\alpha}^* = 4 \sum_{\beta\delta} \mathcal{U}_{\alpha\beta\gamma\delta} \rho_{\beta\delta}, \quad (10b)$$

$$\kappa_{\gamma\delta} = -\kappa_{\delta\gamma} = \langle c_\delta c_\gamma \rangle = \sum_i A_\delta^i B_\gamma^{i*}, \quad (11a)$$

$$\rho_{\beta\delta} = \rho_{\delta\beta}^* = \langle c_\beta^* c_\delta \rangle = \sum_i B_\beta^i B_\delta^{i*}, \quad (11b)$$

where the symbol $\langle \dots \rangle$ denotes ground-state expectation value. The expression for \mathcal{H}_1 is

$$\mathcal{H}_1 = \sum_\alpha (\epsilon_\alpha - \lambda) \rho_{\alpha\alpha} + 2 \sum_{\alpha\beta\gamma\delta} \mathcal{U}_{\alpha\beta\gamma\delta} \rho_{\alpha\gamma} \rho_{\beta\delta} + \sum_{\alpha\beta\gamma\delta} \mathcal{U}_{\alpha\beta\gamma\delta} \kappa_{\alpha\beta}^* \kappa_{\gamma\delta}. \quad (12)$$

As usual, the chemical potential is determined by fixing the average number of particles

$$n = \langle \mathcal{N} \rangle = \sum_\alpha \rho_{\alpha\alpha}. \quad (13)$$

We have assumed that there was only one kind of particle, but one can easily generalize.

We see that $\Gamma_{\alpha\gamma}$ is the familiar Hartree-Fock self-consistent potential: $\rho_{\beta\delta}$ is the density of particles in the ground state, and $\Gamma_{\alpha\gamma}$ is the potential arising from this density. On the other hand, $\kappa_{\gamma\delta}$ is the wave function of the Cooper bound-pair state and gives rise to the other potential, $\Delta_{\alpha\beta}$, which couples together the particle and the hole parts of the quasi particle. It is a generalization of the quantity Δ (or ϵ_0 , half the energy gap) occurring in the BCS theory. Without it, Eqs. (9) would just be the Hartree-Fock equations. The additional potential $\Delta_{\alpha\beta}$ introduces pairing effects on an equal footing with the Hartree field. We call it the "pairing potential" and we call Eqs. (9) the "Hartree-Bogolyubov equations" (to be abbreviated in what

follows as HB equations). They are well suited to nuclear applications since the self-consistent field and the pairing seem to be responsible for a large fraction of systematic nuclear phenomena.⁸

There are many other ways to derive the HB equations. For instance, one can use a Green's function method.¹⁰ One can also show that \mathcal{H}_1 , as given in Eq. (12), is stationary against small changes in A and B about the solutions of the HB equations. It is clear that, to every solution with positive E_i , there corresponds another with energy $-E_i$, but the latter is of no physical interest. Like the Hartree-Fock equations, the HB equations are nonlinear, of course. To solve them, one procedure consists in picking two potentials Γ and Δ , calculating the corresponding A 's and B 's, using them to calculate new potentials, etc., . . . until the sequence of iterations converges, as in the usual Hartree procedure. Another method consists in picking a set of ρ 's and κ 's containing some parameters and obeying the supplementary conditions⁹

$$\sum_\gamma (\rho_{\alpha\gamma} \rho_{\gamma\beta} - \kappa_{\alpha\gamma}^* \kappa_{\gamma\beta}) = \rho_{\alpha\beta}, \quad (14a)$$

$$\sum_\gamma (\kappa_{\alpha\gamma} \rho_{\gamma\beta} + \kappa_{\beta\gamma} \rho_{\gamma\alpha}) = 0, \quad (14b)$$

and minimizing \mathcal{H}_1 to determine the best ρ and κ . Those can then be used to determine the best Γ and Δ by Eqs. (10). The supplementary conditions (14) follow easily from a consideration of ground-state expectation values of products of four c or c^* operators, or from the orthogonality relations (4). One way to make sure that they are satisfied is to construct the trial ρ and κ from a set of A 's and B 's which are themselves solutions of some HB equations with arbitrary potentials.

The point of this general formalism is that, in addition to their spherically symmetric solution, which is the one for which the usual BCS theory is suitable, the HB equations may also have deformed solutions, i.e., solutions for which the potentials Γ and Δ are not spherically symmetric.¹¹ If the value of \mathcal{H}_1 for such a solution is lower than that of the spherical solution, the corresponding nucleus will be deformed. Then, the HB equations give us the intrinsic excitations of this deformed nucleus. The moment of inertia may be obtained by the cranking formula¹² and the collective excitations by the method of linearized equations of motion.⁶ Thus, this formalism is capable of giving a unified description of spherical and deformed nuclei, the same shell-model Hamiltonian being used as starting point in both cases.

¹⁰ L. P. Gor'kov, J. Exptl. Theoret. Phys. (U.S.S.R.) **34**, 735 (1958) [translation: Soviet Phys.—JETP **34**(7), 505 (1958)]. See also footnote 17.

¹¹ The situation is similar to that pointed out by A. W. Overhauser [Phys. Rev. Letters **4**, 415, 462 (1960)]; namely, for an infinite system, the Hartree-Fock equations may have solutions which are not translationally invariant.

¹² D. R. Inglis, Phys. Rev. **96**, 1059 (1954).

3. APPLICATION TO PAIRING PLUS QUADRUPOLE FORCES

The rotational invariance of the interaction \mathcal{V} will now be explicitly exhibited. There are two ways of proceeding,⁶ one being in terms of a rotationally invariant particle-particle matrix element G ,

$$\mathcal{V}_{\alpha\beta\gamma\delta} = -\frac{1}{2} \sum_{JM} G(abcdJ) C(j_a j_b J; m_\alpha m_\beta M) \times C(j_c j_d J; m_\gamma m_\delta M), \quad (15a)$$

the other in terms of an invariant particle-hole matrix element F ,

$$\mathcal{V}_{\alpha\beta\gamma\delta} = -\frac{1}{2} \sum_{J'M'} F(acdbJ') s_\gamma C(j_a j_c J'; m_\alpha - m_\gamma M') \times s_\beta C(j_d j_b J'; m_\delta - m_\beta M'), \quad (15b)$$

with

$$s_\gamma = (-)^{j_\gamma - m_\gamma}. \quad (16)$$

The relation between G and F involves a Racah coefficient. It is immediately seen that form (15a) is the convenient one to use in Eq. (10a), because the summation there is over γ and δ , while form (15b) is suitable for Eq. (10b) where the sum is over β and δ . Our two potentials Γ and Δ are thus decomposed into their tensor components.

The assumed force has two parts. The pairing part is given by

$$G(abcdJ) = g \delta_{ab} \delta_{cd} \delta_{J0} (j_a + \frac{1}{2})^{\frac{1}{2}} (j_c + \frac{1}{2})^{\frac{1}{2}}. \quad (17)$$

To this value of G , there corresponds also an F ; but the recoupling spreads the strength of the latter over many angular momenta and it can therefore be neglected whenever it appears. On the other hand, the quadrupole part of the force is

$$F(acdbJ) = \frac{1}{2} \chi \delta_{J2} Q_{ac} Q_{db}, \quad (18)$$

where Q is defined by

$$\langle \alpha | r^2 Y_{2M}(\theta, \varphi) | \gamma \rangle = Q_{ac} s_\gamma C(j_a j_c 2; m_\alpha - m_\gamma M), \quad (19)$$

and satisfies

$$Q_{ac} = (-)^{j_a + j_c + 1} Q_{ca}. \quad (20)$$

If relations (2) are to be satisfied, there must actually be an additional part to F . But this will again be neglected, together with the whole quadrupole part of G , because the recoupling makes these terms small.¹³ Therefore, we use Eqs. (15a) and (17) in the expression (10a) for Δ , but Eqs. (15b) and (18) in Eq. (10b) for Γ .

These approximations make both G and F separable, and therefore the form of the two self-consistent potentials becomes immediately apparent. The pairing potential can be written¹⁴

$$\Delta_{\alpha\beta} = \delta_{\alpha, -\beta} s_\alpha \Delta, \quad (21)$$

with

$$\Delta = -\frac{1}{2} g \sum_\gamma s_\gamma \kappa_{\gamma, -\gamma}. \quad (22)$$

¹³ Those are the same approximations that were made in Sec. 4A of reference 6.

¹⁴ The state $-\beta$ is defined as having the same quantum numbers as β , except for the magnetic quantum number which is opposite.

One can say that the pairing potential is a constant and that every state is paired with its time-reversed. This is the same simple situation as in the BCS theory. As for the Hartree potential, it becomes

$$\Gamma_{\alpha\gamma} = -Q_{ac} \sum_M s_\gamma C(j_a j_c 2; m_\alpha - m_\gamma M) D_M^* = \Gamma_{\gamma\alpha}^* = s_\alpha s_\gamma \Gamma_{-\gamma, -\alpha}, \quad (23)$$

where the D_M 's are 5 parameters describing the quadrupolar deformation and defined by

$$D_M = \chi \sum_{\beta\delta} Q_{bd} s_\delta C(j_b j_d 2; m_\beta - m_\delta M) \rho_{\beta\delta} = (-)^M D_{-M}^*. \quad (24)$$

With the further substitution

$$C_\alpha^i = s_\alpha B_{-\alpha}^i, \quad (25)$$

the HB equations (9) become

$$E_i A_\alpha^i = (\epsilon_\alpha - \lambda) A_\alpha^i + \sum_\gamma \Gamma_{\alpha\gamma} A_\gamma^i + \Delta C_\alpha^i, \quad (26a)$$

$$E_i C_\alpha^i = -(\epsilon_\alpha - \lambda) C_\alpha^i - \sum_\gamma \Gamma_{\alpha\gamma} C_\gamma^i + \Delta^* A_\alpha^i. \quad (26b)$$

One can take Δ real and positive without loss of generality. Then the solution is

$$E_i = (q_i^2 + \Delta^2)^{\frac{1}{2}}, \quad (27)$$

$$A_\alpha^i = u_i W_\alpha^i, \quad C_\alpha^i = v_i W_\alpha^i, \quad (28)$$

$$u_i = [\frac{1}{2}(1 + q_i/E_i)]^{\frac{1}{2}}, \quad v_i = [\frac{1}{2}(1 - q_i/E_i)]^{\frac{1}{2}}, \quad (29)$$

where q_i and W_α^i (normalized) are solutions of the eigenvalue equation

$$q_i W_\alpha^i = (\epsilon_\alpha - \lambda) W_\alpha^i + \sum_\gamma \Gamma_{\alpha\gamma} W_\gamma^i, \quad (30)$$

which involves only the Hartree potential.

It is clear that, if there exists a solution with $D_M \neq 0$, it must have the appropriate degeneracy to contain all possible orientations of the nucleus in space. Therefore, we can require that the axes of the deformation be the coordinate axes, i.e., assume $D_1 = D_{-1} = 0$ and $D_2 = D_{-2}$ (real). Then our solution contains three parameters: Δ , D_0 , and D_2 . To determine these parameters, we have three self-consistency conditions, obtained from Eqs. (22) and (24), namely,

$$\sum_i E_i^{-1} = 4/g, \quad (31)$$

$$D_M = \chi \sum_i v_i^2 \langle W^i | r^2 Y_{2M} | W^i \rangle. \quad (32)$$

Of course, the problem is complicated by the fact that we have to solve Eq. (30), i.e., find the energy levels of a particle in a deformed well. A fourth parameter, the chemical potential, is determined by Eq. (13) which takes the form

$$n = \sum_i v_i^2. \quad (33)$$

Instead of trying to solve the self-consistency conditions directly, it is probably easier to minimize \mathcal{H}_1 with assumed values of Δ , D_0 , and D_2 . Expression (12) for \mathcal{H}_1 becomes in the present case

$$\mathcal{H}_1 = \sum_i \langle W^i | \epsilon - \lambda | W^i \rangle v_i^2 - (g\Delta^2/16) (\sum_i E_i^{-1})^2 - \frac{1}{2} \chi \sum_M (\sum_i v_i^2 \langle W^i | r^2 Y_{2M} | W^i \rangle)^2, \quad (34)$$

where W^i , v_i^2 , and E_i must be considered as functions of Δ , D_0 , and D_2 through Eqs. (30), (29), (27), (23). If one uses the self-consistency conditions, \mathcal{H}_1 takes the simpler form

$$\mathcal{H}_1 = \sum_i \langle W^i | \epsilon - \lambda | W^i \rangle v_i^2 - D^2/2\chi - \Delta^2/g, \quad (35)$$

with

$$D^2 = D_0^2 + 2D_2^2, \quad (36)$$

but expression (34), not (35), is the one that must be minimized.

Numerical calculations based on this method are in progress. Even away from the minimum, one can still interpret the variational expression (34) as giving the energy of the nucleus when a certain deformation and a certain pairing potential have been imposed upon it. This energy is the same as that derived by Belyaev² and Kisslinger and Sorensen⁵ using a Lagrange multiplier.

To investigate the stability of the spherical solution, we can expand Eq. (34) in powers of D_M and $\delta = \Delta - \Delta_0$, where Δ_0 is the value taken by the pairing potential for the spherical solution. Since there must be no first-order terms, the expansion has the form

$$\mathcal{H}_1 = \mathcal{H}_{10} + aD^2 + b\delta^2 + \text{higher order terms.} \quad (37)$$

The sign of a tells us whether the spherical solution is stable against small deformations (b is always positive). If $a > 0$, we cannot guarantee that there does not exist a solution of energy lower than \mathcal{H}_{10} with a large deformation. But if $a < 0$, we are sure that the lowest solution is deformed. The calculation of a by the methods of perturbation theory is straightforward and one finds

$$a = \frac{1}{2}\Lambda(1 - \chi\Lambda), \quad (38)$$

with

$$\Lambda = \sum_{ab} (E_a + E_b)^{-1} Q_{ab}^2 (u_a v_b + v_a u_b)^2. \quad (39)$$

This result is actually identical with Eq. (29) of reference 5.

It is interesting to make a comparison with the equation giving the vibrational frequency ω of the spherical nucleus, as calculated with linearized equations of motion, which is¹⁵

$$\chi \sum_{ab} \frac{(E_a + E_b) Q_{ab}^2 (u_a v_b + v_a u_b)^2}{(E_a + E_b)^2 - \omega^2} = 1. \quad (40)$$

The vibrational frequency is that solution ω which is smaller than all combinations $(E_a + E_b)$. It exists only if χ is sufficiently small or the nucleus sufficiently near closed shells. Otherwise, the value of ω^2 may turn out to be negative, i.e., ω is imaginary. We see by comparing Eqs. (38) and (40) that the point at which ω vanishes to become imaginary is precisely the point

¹⁵ This is Eq. (88) of reference 6, with $L_{ab} = 20\pi Q_{ab}^2$.

where a becomes negative and the spherical solution becomes unstable against small deformations.

This semiclassical result, which we verified explicitly in the case of pairing plus quadrupole forces, is actually much more general and will hold whenever a many-fermion system is treated in the self-consistent field approximation. The proof is very simple^{16a}. The linearized equations of motion used on the spherical side are obtained by linearizing¹⁶

$$i\hbar d\rho_{op}/dt = [\rho_{op}, \mathcal{H}], \quad (41a)$$

$$i\hbar d\kappa_{op}/dt = [\kappa_{op}, \mathcal{H}], \quad (41b)$$

about the spherical solution. The HB equations, on the other hand, can be obtained from the equations¹⁷

$$[\rho_{op}, \mathcal{H}] = 0, \quad [\kappa_{op}, \mathcal{H}] = 0. \quad (42)$$

An additional approximation, Hartree factorization,¹⁸ is used in both cases. Clearly, if the linearized Eqs. (41) have a zero-frequency solution, there exist two small quantities that can be added to ρ and κ without destroying the validity of Eqs. (42). In other words, the energy surface (as a function of deformation and pairing potential, for instance) has an inflexion point there, which indicates the boundary between a stable and an unstable situation. Thus, the fact that a certain oscillation frequency reaches zero means that the ground state is about to become unstable against this particular kind of deformation, just as it would in a classical problem.

As we mentioned at the end of the introduction, the transition region between two different types of ground states is complicated by nonlinear effects and quantum mechanical zero-point motion. In nuclei, because of their small size, this region is particularly large, but a proper theory of it does not exist.¹⁹ At the moment, agreement must be restricted to rather stiff spherical nuclei and to strongly deformed ones and one has to be content if the transition calculated by the above methods falls somewhere in between the two. A sharp transition between two different kinds of nuclei does occur in nature, as evidenced by the systematics of collective levels,²⁰ but it is not clear that this is exactly the transition we have been talking about.

^{16a} Note added in proof. Further discussion of this point has now been published by D. J. Thouless, Nuclear Phys. **21**, 225 (1960); **22**, 78 (1960).

¹⁶ In the following, $(\rho_{op})_{\alpha\beta} = c_\alpha^* c_\beta$ and $(\kappa_{op})_{\alpha\beta} = c_\beta c_\alpha$.

¹⁷ This is one of the alternative ways of deriving the HB equations. Let us look upon Eqs. (9) as the eigenvalue equation for an operator \mathcal{H}' , whose number of lines and columns is twice the number of states. One finds that Eqs. (42), when factorized, state that a certain operator involving ρ and κ (the operator K of reference 3) must commute with \mathcal{H}' . To find this operator K , one must therefore diagonalize \mathcal{H}' , i.e., solve the HB equations.

¹⁸ H. Ehrenreich and M. H. Cohen, Phys. Rev. **115**, 786 (1959).

¹⁹ J. Sawicki (to be published) has drawn attention to the problems presented by a nonlinear theory of collective oscillations.

²⁰ G. S. Goldhaber and J. Weneser, Phys. Rev. **98**, 212 (1955).