

electron-neutrino angular correlation coefficient,¹³ which set upper limits on $\langle\sigma\rangle$.

We now compare our experimental results with preliminary calculations based on Nilsson's rotational model.¹⁴ Using the experimental value of $\langle\sigma\rangle$, Eq. (9), we find that the deformation parameter is

$$\eta(\text{Ar}^{35}) = -2.3. \tag{10}$$

Mehta and Warke¹⁵ have studied the angular distribution of protons from the reaction Cl³⁵(*d,p*)Cl³⁶. The value of the deformation parameter of Cl³⁵ which they obtained by fitting the experimental angular distribution is $\eta(\text{Cl}^{35}) = -2.8$. As expected, the mirror nuclei Ar³⁵ and Cl³⁵ have nearly the same deformation. The experimental magnetic moments and the magnetic moments predicted from Nilsson's model are compared in Table II. Possibly the large discrepancies between measured and calculated magnetic moments are due in

¹³ W. B. Hermannsfeldt, R. L. Burman, P. Stähelin, J. S. Allen, and T. H. Braid, *Bull. Am. Phys. Soc.* **4**, 77 (1959).
¹⁴ S. G. Nilsson, *Kgl. Danske Videnskab. Selskab, Mat. Fys. Medd.* **29**, No. 16 (1955).
¹⁵ M. L. Mehta and C. S. Warke, *Nucl. Phys.* **13**, 451 (1959).

TABLE II. Experimental and theoretical values for the nuclear moments of Ar³⁵ and Cl³⁵. The theoretical values are computed from the rotational model using a deformation parameter $\eta = -2.3$.

	Experimental	Theoretical
$\mu(\text{Ar}^{35})$	+0.632 nm	+0.48 nm
$\mu(\text{Cl}^{35})$	+0.821 nm ^a	+0.98 nm
$\mu(\text{Cl}^{36}) + \mu(\text{Ar}^{36})$	+1.453 nm	+1.46 nm

^a See Ref. 5, p. 615.

part to pion exchange currents. The sum of the magnetic moments of mirror nuclei should be independent of such currents, however. In addition, there should be a spin orbit correction of about 0.2 nm to the Cl³⁵ moment.¹⁶ The corrected theoretical sum is then about 1.7 nm.

We plan to determine the asymmetries of Ne¹⁹ and Ar³⁵ more precisely in future experiments.

We are happy to thank the 90-in. cyclotron staff for their cooperation. In particular we thank Edward Ambrose and David Moyer for their help.

¹⁶ D. F. Zaretskii, *Zh. Eksperim. i Teor. Fiz.* **36**, 869 (1959) [English transl.: *Soviet Phys.—JETP* **9**, 612 (1959)].

The Number Problem in Bardeen-Cooper-Schrieffer and Random-Phase-Approximation Nuclear Calculations*

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(Received 18 September 1964)

Use is made of the quasiboson method to study the problem arising from number nonconservation in applications of BCS methods to nuclear problems. This method neglects higher orders in $1/\Omega$, where Ω is an average number of available shell-model single-particle states. A method is given which identifies and removes number-dispersion spurious effects. The relation of this method to the prescriptions of Nogami and of Nilsson is discussed. An illustration of the method is given in an explicit calculation for the energy of a two-shell system in order Ω^2 and order Ω . It is shown that the projected BCS wave function method gives the leading order Ω^2 exactly and results in a good approximation to order Ω . Variation of the parameters of the projected wave function affords zero improvement in either order Ω^2 or Ω .

I. INTRODUCTION

In this paper use is made of the quasiboson method to consider the problems arising from the non-conservation of particle number in applications of Bardeen-Cooper-Schrieffer (BCS) solutions to nuclear problems. Considerations are limited to spherical systems of even numbers of nucleons.

The first step in many nuclear calculations is made by use of the BCS method,^{1,2} which takes into account the most important parts of the pairing interactions. The remaining parts of the pairing interaction together with other, longer range, interactions remain as per-

* Work performed under the auspices of the U. S. Atomic Energy Commission.

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¹ J. Bardeen, L. N. Cooper, and J. R. Schrieffer, *Phys. Rev.* **108**, 1175 (1957); N. N. Bogoliubov, *Zh. Eksperim. i Teor. Fiz.* **34**, 58 and 73 (1958) [English transl.: *Soviet Phys.—JETP* **7**, 41 and 51 (1958)]; N. N. Bogoliubov, *Nuovo Cimento* **7**, 794 (1958); and J. G. Valatin, *Nuovo Cimento* **7**, 843 (1958).

² S. T. Beliaev, *Kgl. Danske Videnskab. Selskab, Mat. Fys. Medd.* **31**, No. 11 (1959).

turbations. These have been treated by the random-phase or quasiboson approximation (RPA).³ The use of the RPA constitutes the lowest order of a perturbation treatment, and higher order corrections should be considered. Beliaev and Zelevinsky⁴ have attempted a specific expansion in powers of a smallness parameter in order to treat systematically the lowest order, the RPA, and the higher order corrections. In this paper we use only the lowest terms of their expansions, and, therefore, only the quasiboson approximation. The Beliaev-Zelevinsky method is used only in providing a belief that the neglected terms are higher order in a parameter, which will be explained below. These higher order terms have not yet been systematically explored, nor are they explored here. Nevertheless the lowest order, quasiboson, approximation is widely believed to be a good approximation.

This procedure permits one to consider the number problem correspondingly. The number problem arises in the first step, which is the application of the BCS method. In this procedure, the number of particles is not an exact eigenvalue, and only the average number of particles N is fixed. The dispersion in the number is of the order of \sqrt{N} , which for nuclear applications is not inconsiderable. Recently, Nogami⁵ and Nilsson⁶ have given prescriptions for removal of the spurious effects of the number dispersion. Here, it is possible to write explicitly the dependence on the number dispersion, and so to remove explicitly any spurious contributions.

Another approach to the removal of the effects of number dispersion uses projected wave functions. Kerman, Lawson, and Macfarlane⁷ (KLM) projected out of the BCS wave function the part corresponding to exactly N particles, dropping all parts corresponding to

different populations. These projected wave functions are used to calculate the average value of the pairing-force Hamiltonian. Comparison with the ground-state energy calculated by an exact diagonalization of this same Hamiltonian showed that the use of the projected functions gave much better numerical agreement than the results with the BCS. Part of this improvement is due to the removal of the number dispersion.^{5,6} The rest of the improvement, as will be shown below, comes from the inclusion of part of the interactions omitted in the BCS treatment. The part still omitted will be given explicitly in terms of the expansion method. Its smallness can then be estimated for the particular physical problem. While it is, indeed, small for the KLM cases, this is not a general rule. A variation of the parameters of the projected wave function is shown to lead to no better results in the two leading orders.

II. REVIEW OF THE BCS, QUASIBOSON, AND BELIAEV-ZELEVINSKY METHODS

The popularly used Hamiltonian, consisting of a pairing-force interaction and a quadrupole-quadrupole interaction, can be written in the somewhat unorthodox form⁸

$$H = \sum_{\nu} \epsilon_{\nu} g_{\nu} \bar{B}_0(\nu) - \frac{f}{2} \sum_{\nu, \nu'} g_{\nu} g_{\nu'} \bar{A}_0^{\dagger}(\nu, \nu) \bar{A}_0(\nu', \nu') - \frac{\chi}{2} \sum_{\alpha\beta\gamma\delta, M} Q_{\alpha\beta} Q_{\gamma\delta} \bar{B}_{2M}^{\dagger}(\alpha, \beta) \bar{B}_{2M}(\gamma, \delta), \quad (1)$$

where the \bar{A}_{JM} , \bar{B}_{JM} are bilinear combinations of the annihilation and creation operators coupled to angular momentum J , M by the usual Clebsch-Gordan coefficients

$$\bar{A}_{JM}(\nu, \nu') = \sum_{m, m'} C(j_{\nu} j_{\nu'} J; m, m', M) a_{\nu' m'} a_{\nu m}, \quad (2)$$

$$\bar{B}_{JM}(\nu, \nu') = \sum_{m, m'} (-1)^{j_{\nu'} - m'} C(j_{\nu} j_{\nu'} J; m, -m', M) a_{\nu' m'}^{\dagger} a_{\nu m}, \quad (3)$$

ϵ_{ν} = single-particle energies,

$$g_{\nu} = (2j+1)^{1/2} = \Omega_{\nu}^{1/2},$$

f = pairing-force coupling constant,

χ = quadrupole-quadrupole coupling constant, and

$$Q_{\alpha\beta} = (\alpha || r^2 Y_2 || \beta) / \sqrt{5}.$$

³ M. Baranger, Phys. Rev. **120**, 957 (1960); R. Arvieu and M. Vénéroni, Compt. Rend. **250**, 992, 2155 (1960); T. Marumori, Progr. Theoret. Phys. (Kyoto) **24**, 331 (1960). Actually the equations of the RPA described in the above papers mix orders. The "quasiboson approximation" picks out only the leading order. In this paper, as in popular misuse, we do not distinguish in nomenclature between the two.

⁴ S. T. Beliaev and V. G. Zelevinsky, Nucl. Phys. **39**, 582 (1962).

⁵ Y. Nogami, Phys. Rev. **134**, B313 (1964).

⁶ S. G. Nilsson, Nucl. Phys. **55**, 97 (1964).

⁷ A. K. Kerman, R. D. Lawson, and M. H. Macfarlane, Phys. Rev. **124**, 162 (1961).

The Bogoliubov-Valatin transformation introduces the quasiparticle operators $\alpha_{\nu m}$ by

$$\alpha_{\nu m} = u_{\nu} a_{\nu m} - (-1)^{j_{\nu} - m} v_{\nu} a_{\nu - m}^{\dagger}, \quad (4)$$

together with the inverse transformation

$$a_{\nu m} = u_{\nu} \alpha_{\nu m} + (-1)^{j_{\nu} - m} v_{\nu} \alpha_{\nu - m}^{\dagger}. \quad (5)$$

The usual treatment^{1,2} of BCS will not be repeated here, since we will give an alternate demonstration in terms of the methods to be discussed. It will be recalled that a

⁸ The quadrupole-quadrupole interaction of (1) is in the same form as that written by L. S. Kisslinger and R. A. Sorenson, Rev. Mod. Phys. **35**, 853 (1963). The differences between this and the usual form in which the a , a^{\dagger} are written in normal form can be expressed as an addition to the single-particle energies, ϵ_{ν} . This added part is of order 1, compared to the ϵ_{ν} which will be taken to be of order g^2 .

term $-\lambda\hat{N}$, where \hat{N} is the number operator, is added to H , and u, v are chosen so as to eliminate the terms of the form $\alpha^\dagger\alpha^\dagger, \alpha\alpha$ from

$$H - \lambda\hat{N}. \quad (6)$$

Further, λ is chosen so as to satisfy the average number condition

$$N = \langle 0 | \hat{N} | 0 \rangle, \quad (7)$$

where the expectation of \hat{N} is taken in the quasiparticle

vacuum. This transformation does not completely diagonalize H ; even the quasiparticle vacuum is not an exact eigenfunction of H . Further, there remains a residual interaction between the quasiparticles.

Instead of proceeding directly from this point, it is somewhat more convenient in this particular problem to begin with the form of the Bogoliubov-Valatin transformation, Eqs. (4) and (5), but to specify the u 's and v 's below. With this transformation the $\bar{A}_{JM}(\nu, \nu')$ and $\bar{B}_{JM}(\nu, \nu')$ are expressed in terms of the analogous quasipair operators

$$A_{JM}(\nu, \nu') = \sum C(j_\nu j_{\nu'} J; m, m' M) \alpha_{\nu' m'} \alpha_{\nu m}, \quad (8)$$

$$B_{JM}(\nu, \nu') = \sum_{mm'} (-1)^{j_{\nu'} - m'} C(j_\nu j_{\nu'} J; m, -m', M) \alpha_{\nu' m'}^\dagger \alpha_{\nu m}. \quad (9)$$

Instead of the $A_{JM}(\nu, \nu')$, $B_{JM}(\nu, \nu')$, further work is made somewhat easier if the linear combinations

$$A_{JM}^{(\pm)}(\nu, \nu') = \frac{1}{2} [A_{JM}(\nu, \nu') \pm (-1)^{J+M} A_{J-M}^\dagger(\nu, \nu')], \quad (10)$$

$$B_{JM}^{(\pm)}(\nu, \nu') = \frac{1}{2} [B_{JM}(\nu, \nu') \pm (-1)^{J+M} B_{J-M}^\dagger(\nu, \nu')], \quad (11)$$

together with the analogous definitions for $\bar{A}_{JM}^{(\pm)}(\nu, \nu')$, $\bar{B}_{JM}^{(\pm)}(\nu, \nu')$, are used. The relation between the particle and quasiparticle pair operators is

$$\bar{A}_{JM}^{(\pm)}(\nu, \nu') = \xi_{\nu\nu'}^{(\pm)} A_{JM}^{(\pm)}(\nu, \nu') - \eta_{\nu\nu'}^{(\pm)} B_{JM}^{(\pm)}(\nu, \nu') + \frac{1}{2} (\frac{1}{2} \pm \frac{1}{2}) g_\nu \eta_{\nu\nu}^{(+)} \delta_{J0} \delta_{\nu\nu'}, \quad (12)$$

$$\bar{B}_{JM}^{(\pm)}(\nu, \nu') = \eta_{\nu\nu'}^{(\pm)} A_{JM}^{(\pm)}(\nu, \nu') + \xi_{\nu\nu'}^{(\pm)} B_{JM}^{(\pm)}(\nu, \nu') + \frac{1}{2} (\frac{1}{2} \pm \frac{1}{2}) g_\nu (1 - \xi_{\nu\nu}^{(+)} \delta_{J0} \delta_{\nu\nu'}), \quad (13)$$

where

$$\xi_{\nu\nu'}^{(\pm)} = u_\nu u_{\nu'} \mp v_\nu v_{\nu'}, \quad (14)$$

$$\eta_{\nu\nu'}^{(\pm)} = u_\nu v_{\nu'} \pm v_\nu u_{\nu'}. \quad (15)$$

The transformation of the $\bar{A}_{JM}(\nu, \nu')$ into $A_{JM}(\nu, \nu')$, $B_{JM}(\nu, \nu')$ is a trivial consequence. In terms of these quasiparticle operators H takes the temporarily formidable form

$$\begin{aligned} H = & \sum_\nu \epsilon_\nu g_\nu^2 v_\nu^2 - \frac{1}{8} \sum_{\nu\nu'} g_\nu^2 g_{\nu'}^2 \eta_{\nu\nu}^{(+)} \eta_{\nu'\nu'}^{(+)} + \sum_\nu \epsilon_\nu g_\nu \eta_{\nu\nu}^{(+)} A_0^{(+)}(\nu, \nu) - \frac{1}{2} f \sum_{\nu\nu'} g_\nu g_{\nu'}^2 \xi_{\nu\nu}^{(+)} \eta_{\nu'\nu'}^{(+)} A_0^{(+)}(\nu, \nu) \\ & + \frac{1}{2} f \sum_\nu g_\nu^2 \xi_{\nu\nu}^{(+)} + \sum_\nu \epsilon_\nu g_\nu \xi_{\nu\nu}^{(+)} B_0^{(+)}(\nu, \nu) + \frac{1}{2} f \sum_{\nu\nu'} g_\nu g_{\nu'}^2 \eta_{\nu\nu}^{(+)} \eta_{\nu'\nu'}^{(+)} B_0^{(+)}(\nu, \nu) \\ & + \frac{1}{2} f \sum_{\nu\nu'} g_\nu g_{\nu'} A_0^{(-)}(\nu, \nu) A_0^{(-)}(\nu', \nu') - \frac{1}{2} f \sum_{\nu\nu'} g_\nu g_{\nu'} \xi_{\nu\nu}^{(+)} \xi_{\nu'\nu'}^{(+)} A_0^{(+)}(\nu, \nu) A_0^{(+)}(\nu', \nu') \\ & + \frac{1}{2} f \sum_{\nu\nu'} g_\nu g_{\nu'} \xi_{\nu\nu}^{(+)} \eta_{\nu'\nu'}^{(+)} [A_0^{(+)}(\nu, \nu) B_0^{(+)}(\nu', \nu') + B_0^{(+)}(\nu', \nu') A_0^{(+)}(\nu, \nu)] - f \sum_\nu g_\nu \eta_{\nu\nu}^{(+)} A_0^{(+)}(\nu, \nu) \\ & - \frac{1}{2} f \sum_{\nu\nu'} g_\nu g_{\nu'} \eta_{\nu\nu}^{(+)} \eta_{\nu'\nu'}^{(+)} B_0^{(+)}(\nu, \nu) B_0^{(+)}(\nu', \nu') - f \sum_\nu g_\nu \xi_{\nu\nu}^{(+)} B_0^{(+)}(\nu, \nu) \\ & - \frac{1}{2} \chi \sum_{\alpha\beta\gamma\delta, M} Q_{\alpha\beta} Q_{\gamma\delta} \eta_{\alpha\beta}^{(+)} \eta_{\gamma\delta}^{(+)} (-1)^M A_{2-M}^{(+)}(\alpha, \beta) A_{2M}^{(+)}(\gamma, \delta) \\ & - \frac{1}{2} \chi \sum_{\alpha\beta\gamma\delta, M} Q_{\alpha\beta} Q_{\gamma\delta} \eta_{\alpha\beta}^{(+)} \xi_{\gamma\delta}^{(+)} (-1)^M [A_{2-M}^{(+)}(\alpha, \beta) B_{2M}^{(+)}(\gamma, \delta) + B_{2M}^{(+)}(\gamma, \delta) A_{2-M}^{(+)}(\alpha, \beta)] \\ & - \frac{1}{2} \chi \sum_{\alpha\beta\gamma\delta, M} Q_{\alpha\beta} Q_{\gamma\delta} \xi_{\alpha\beta}^{(+)} \xi_{\gamma\delta}^{(+)} (-1)^M B_{2-M}^{(+)}(\alpha, \beta) B_{2M}^{(+)}(\gamma, \delta). \quad (16) \end{aligned}$$

We will briefly discuss this Hamiltonian in terms of the Beliaev-Zelevinsky⁴ expansion.

The heart of their method lies in the expansion of the $A_{JM}(\nu, \nu')$, $B_{JM}(\nu, \nu')$ as a series in powers of other operators, $\bar{A}_{JM}(\nu, \nu')$, that obey exact boson commutation rules,

$$[\bar{A}_{JM}(\mu, \mu'), \bar{A}_{J'M'}^\dagger(\nu, \nu')] = \delta_{JJ'} \delta_{MM'} (\delta_{\mu\nu} \delta_{\mu'\nu'} + (-1)^{j_\mu - j_{\mu'} + J} \delta_{\mu\nu'} \delta_{\mu'\nu}). \quad (17)$$

The coefficients of the expansion are determined by the requirement that the $A_{JM}(\nu, \nu')$ and $B_{JM}(\nu, \nu')$ obey their exact commutation rules

$$[A_{J_1 M_1}(\nu_1, \nu_1'), A_{J_2 M_2}^\dagger(\nu_2, \nu_2')] = \delta_{J_1 J_2} \delta_{M_1 M_2} (\delta_{\nu_1 \nu_2} \delta_{\nu_1' \nu_2'} + (-1)^{j_{\nu_1} - j_{\nu_1'} + J_1} \delta_{\nu_1 \nu_2'} \delta_{\nu_1' \nu_2}) \\ - \sum_{J_3, \nu_3 \nu_3'} (1 + \hat{P}_1)(1 + \hat{P}_2) Y(1, 2, 3) B_{J_3 M_3}(\nu_3, \nu_3'), \quad (18)$$

$$[B_{J_3 M_3}(\nu_3, \nu_3'), A_{J_1 M_1}^\dagger(\nu_1, \nu_1')] = \sum_{J_2, \nu_2 \nu_2'} (1 + \hat{P}_1) Y(1, 2, 3) A_{J_2 M_2}^\dagger(\nu_2, \nu_2'), \quad (19)$$

$$[B_{J_1 M_1}(\nu_1, \nu_1'), B_{J_2 M_2}^\dagger(\nu_2, \nu_2')] = \sum_{J_3 \nu_3 \nu_3'} (1 - \hat{P}_1 \hat{P}_2 \hat{P}_3) Y(1, 3, 2) B_{J_3 M_3}(\nu_3, \nu_3'), \quad (20)$$

where \hat{P}_1 is an operator that permutes ν_1 with ν_1' and multiplies the result by the phase factor $(-1)^{j_{\nu_1} - j_{\nu_1'} + J}$, j_{ν_1} , $j_{\nu_1'}$ being coupled to J . The function $Y(1, 2, 3)$ is given by

$$Y(1, 2, 3) = \delta_{\nu_1 \nu_2'} \delta_{\nu_1 \nu_3} \delta_{\nu_2 \nu_3'} [(2J_2 + 1)(2J_3 + 1)]^{1/2} W(j_3 j_1' J_3 J_2; J_1 j_2) C(J_2 J_3 J_1; M_2 M_3 M_1). \quad (21)$$

In the simplest RPA everything except the first, the δ , term in Eq. (18) is dropped, so that the $A_{JM}(\nu, \nu')$ are treated as boson operators, the $B_{JM}(\nu, \nu') J \neq 0$ are neglected, and $B_0(\nu, \nu)$ is replaced by

$$(1/g_\nu) \sum_{JM\nu'} A_{JM}^\dagger(\nu, \nu') A_{JM}(\nu, \nu').$$

Instead, Beliaev and Zelevinsky give an expansion in boson operators. As an example we consider the simplest case, $A_0(\nu, \nu)$; the expansion is

$$A_0(\nu, \nu) = A_0(\nu, \nu) - \frac{1}{2g_\nu^2} \sum_{\nu' \nu'', J_1 J_2 J_3, M_1 M_2 M_3} [(2J_1 + 1)(2J_2 + 1)]^{1/2} g_\nu W(j_\nu j_\nu J_1 J_2; J_3 j_\nu \nu') \\ \times (-1)^{J_1 + J_3 + M_2} C(J_1 J_2 J_3; -M_1 M_2 - M_3) A_{J_1 M_1}^\dagger(\nu'', \nu') A_{J_2 M_2}(\nu, \nu'') A_{J_3 M_3}(\nu, \nu') \\ + (\text{terms involving } \hat{A}^5 \text{ terms and higher odd powers}). \quad (22)$$

The point is that the coefficient of the \hat{A}^3 term is of order $1/g^2$, where g is an average over the g_ν . This follows from the fact that the Racah coefficient is of order $1/g$, for large g . Thus, the \hat{A}^3 term involving $J_3 = 0$ is easily evaluated, and is just

$$(-1/2g_\nu^2) \sum_{JM\nu'} \hat{A}_{JM}^\dagger(\nu, \nu') \hat{A}_{JM}(\nu, \nu') A_0(\nu, \nu). \quad (23)$$

The smallness parameter of Beliaev-Zelevinsky is measured by the small factor $(1/g_\nu^2)$. Similar arguments are given by them for cases more complicated than the simple one shown above. The general expansion is given as

$$A_{JM}(\nu, \nu') = \hat{A}_{JM}(\nu, \nu') + (\hat{A}^3 \text{ terms of order } 1/g^2) \\ + (\text{higher order } \hat{A}^5 \text{ terms}). \quad (24)$$

Similarly $B_0(\nu, \nu)$ is expanded as

$$B_0(\nu, \nu) = 1/g_\nu \sum_{JM\nu'} \hat{A}_{JM}^\dagger(\nu, \nu') A_{JM}(\nu, \nu'). \quad (25)$$

For this special case the series terminates, and a simple closed form results. The more general case, $B_{JM}(\nu, \nu')$ has an expansion

$$B_{J_1 M_1}(\nu_1, \nu_1') = \sum_{\nu_2 \nu_3 \nu_2' \nu_3' J_2 J_3 M_2 M_3} Y(2, 3, 1) \\ \times \hat{A}_{J_3 M_3}^\dagger(\nu_3, \nu_3') \hat{A}_{J_2 M_2}(\nu_2, \nu_2') \\ + (\text{higher order terms beginning with } \hat{A}^4). \quad (26)$$

In Eq. (26) the first term is of order $1/g$, and the higher terms begin with order $1/g^3$. In the work below we use only the first, the *quasiboson*, terms. We take from Beliaev-Zelevinsky the description of "higher orders" as higher orders in $1/g^2$.

III. PERTURBATION PROGRAM

By use of these expansions, the Hamiltonian can be written as an expansion in powers of the parameters, $1/g$. The subsequent solution in powers of $1/g^2$ by perturbation theory, then, amounts to a corresponding diagonalization of the Hamiltonian to the order considered. Since the number operator, \hat{N} , commutes with H , this implies a corresponding diagonalization of \hat{N} .

To examine this point it is useful to write the number operator \hat{N}

$$\hat{N} = \sum_\nu g_\nu \bar{B}_0(\nu, \nu) = \sum_\nu \{g_\nu^2 v_\nu^2 + g_\nu \eta_{\nu\nu}^{(+)} A_0^{(+)}(\nu, \nu) \\ + g_\nu \xi_{\nu\nu}^{(+)} B_0(\nu, \nu)\}, \quad (27)$$

in its expansion:

$$\hat{N} = \sum_\nu g_\nu^2 v_\nu^2 + \sum_\nu g_\nu \eta_{\nu\nu}^{(+)} A_0^{(+)}(\nu, \nu) \\ + \sum_{\nu\nu', JM} \xi_{\nu\nu'}^{(+)} A_{JM}^\dagger(\nu, \nu') A_{JM}(\nu, \nu') \\ + (\text{terms in order } 1/g \text{ and higher}), \quad (28)$$

where $\hat{A}_0^{(+)}(\nu, \nu)$ has a definition analogous to that appearing in Eq. (10). The leading term is a constant equal to the BCS value for $\langle 0 | \hat{N} | 0 \rangle = N$. In order to diagonalize \hat{N} , up to and including order 1, it is useful to introduce the self-motivating notation

$$\pi(\nu) \equiv \hat{A}_0^{(+)}(\nu, \nu), \quad x(\nu) \equiv i\hat{A}_0^{(-)}(\nu, \nu), \quad (29)$$

$$[\pi(\nu), x(\nu)] = 1/i. \quad (30)$$

Then, to this order,

$$\begin{aligned} \hat{N} = & \sum_{\nu} g_{\nu}^2 v_{\nu}^2 + \sum_{\nu} \{ g_{\nu} \eta_{\nu\nu}^{(+)} \pi(\nu) \\ & + \xi_{\nu\nu}^{(+)} [\pi(\nu)^2 + x(\nu)^2 - 1] \} \\ & + \sum_{\nu', J \neq 0, M} \xi_{\nu\nu}^{(+)} \hat{A}_{JM}^{\dagger}(\nu, \nu') \hat{A}_{JM}(\nu, \nu'). \end{aligned} \quad (31)$$

The diagonalization is now easily seen. The $\hat{A}_{JM}(\nu, \nu')$, $\hat{A}_{JM}^{\dagger}(\nu, \nu)$, $J \neq 0$, commute with the $\pi(\nu)$, $x(\nu)$ and also with those of different J , M as seen in Eq. (17); the last term is, therefore, in diagonal form. The second term has the form of a harmonic oscillator whose center has been shifted. It is diagonalized by the displacement transformation

$$\pi(\nu) + g_{\nu} \eta_{\nu\nu}^{(+)} / 2\xi_{\nu\nu}^{(+)} = \pi'(\nu). \quad (32)$$

However, since this shift is of order g_{ν} , all matrix elements of $\pi(\nu)$ and of $x(\nu)$ will be of the order g_{ν} . This, in turn, means that the matrix elements of $\hat{A}_0(\nu, \nu)$ are of order g_{ν} . This can also be seen directly from the easily derived result for the unexpanded $A_0(\nu, \nu)$

$$\langle N_{\nu} - 2 | A_0(\nu, \nu) | N_{\nu} \rangle = u_{\nu}^2 \left(\frac{N_{\nu}(g_{\nu}^2 + 2 - N_{\nu})}{g_{\nu}^2} \right)^{1/2} \sim (N_{\nu})^{1/2}, \quad (33)$$

where $|N_{\nu}\rangle$ denotes the state with N_{ν} particles in the ν shell. However, the whole expansion has meaning only if the matrix elements of all \hat{A} are at most of order 1. Further, this difficulty with \hat{A} is not confined to the expansion of $A_0(\nu, \nu)$ or of \hat{N} , but would appear in the higher order terms of $A_{JM}(\nu, \nu')$, $J \neq 0$.

To remove this difficulty the use of exact eigenfunctions of $\pi(\nu)$ or of the oscillator, $[\pi'(\nu)]^2 + [x(\nu)]^2$,

must be replaced by averaging in a packet in $\pi(\nu)$, $x(\nu)$ space such that both $\pi(\nu)$ and $x(\nu)$ are confined to a spread of order 1 about a magnitude of order 1. This will guarantee that such quantities as $\pi(\nu)^2$ and $x(\nu)^2$, for example, will be of order 1. This packet, then, through the connection with the number operator, Eq. (31), results in a weighted average over different number eigenfunctions and eigenvalues. Different packets in $\pi(\nu)$ and $x(\nu)$ may or may not correspond to different averages over the number eigenvalues. There is *not* a one-to-one correspondence between the $\pi(\nu)$, $x(\nu)$ averaging and the number averaging. However, it will be explicitly shown that it is only the number averaging that determines all physical results. For this reason it will be sufficient to specify only the number-packet: the way in which systems with different numbers of particles appear in the weighted average. Further, since the number dependence will be made manifest it will be easy to keep the number averaging the same for all states, and so remove all possible spurious contributions.

In passing, it is worth noting that the BCS vacuum is a number packet that fulfills the above requirements.

The use of the packet introduces contributions to the energy of the form $\langle (\hat{N} - N)^2 \rangle$ as well as higher powers of the number dispersion. These are spurious effects of the number averaging. However, since they will be made explicit they will be removable. In addition, since the degree of freedom associated with the number dispersion is explicitly fixed by the packet the spurious states based on ψ such as $(\hat{N} - N)\psi$ no longer appear. The point is that ψ corresponds to a given weighting of different numbers; schematically it can be written as

$$\psi = \sum w_N \psi(N). \quad (34)$$

However, $(\hat{N} - N)\psi$, in general, corresponds to a different set of weights, w_N , and is, therefore, excluded by the necessity of keeping the number packet fixed.

These considerations are made clearer by the simple example in the next section.

IV. THE TWO-SHELL PROBLEM IN ORDER g^2

Using the above expansions, the Hamiltonian of Eq. (1) can be written, up to and including order g^2 , as

$$\begin{aligned} H = & \sum_{\nu} \epsilon_{\nu} g_{\nu}^2 v_{\nu}^2 - \frac{1}{8} f \sum_{\nu\nu'} g_{\nu}^2 g_{\nu'}^2 \eta_{\nu\nu}^{(+)} \eta_{\nu'\nu'}^{(+)} + \sum_{\nu} \epsilon_{\nu} g_{\nu} \eta_{\nu\nu}^{(+)} \hat{A}_0^{(+)}(\nu, \nu) - \frac{1}{2} f \sum_{\nu\nu'} g_{\nu} g_{\nu'}^2 \xi_{\nu\nu}^{(+)} \eta_{\nu'\nu'}^{(+)} \hat{A}_0^{(+)}(\nu, \nu) \\ & + \frac{1}{2} f \sum_{\nu} g_{\nu}^2 \xi_{\nu\nu}^{(+)} + \sum_{\nu\nu', JM} \epsilon_{\nu} \xi_{\nu\nu}^{(+)} \hat{A}_{JM}^{\dagger}(\nu, \nu') \hat{A}_{JM}(\nu, \nu') + \frac{1}{2} f \sum_{\nu\nu'', JM} g_{\nu} g_{\nu'}^2 \eta_{\nu\nu}^{(+)} \eta_{\nu'\nu''}^{(+)} \hat{A}_{JM}^{\dagger}(\nu, \nu'') \hat{A}_{JM}(\nu, \nu') \\ & + \frac{1}{2} f \sum_{\nu\nu'} g_{\nu} g_{\nu'} \hat{A}_0^{(-)}(\nu, \nu) \hat{A}_0^{(-)}(\nu', \nu') - \frac{1}{2} f \sum_{\nu\nu'} g_{\nu} g_{\nu'} \xi_{\nu\nu}^{(+)} \xi_{\nu'\nu'}^{(+)} \hat{A}_0^{(+)}(\nu, \nu) \hat{A}_0^{(+)}(\nu', \nu') \\ & - \frac{1}{2} \chi \sum_{\alpha\beta\gamma\delta, M} Q_{\alpha\beta} Q_{\gamma\delta} \eta_{\alpha\beta}^{(+)} \eta_{\gamma\delta}^{(+)} (-1)^M \hat{A}_{2-M}^{(+)}(\alpha, \beta) \hat{A}_{2M}^{(+)}(\gamma, \delta). \end{aligned} \quad (35)$$

It is worth noting that the ϵ_{ν} , the single-particle energies, and $\chi Q_{\alpha\beta} Q_{\gamma\delta}$, the quadrupole interaction energy, have been taken of order $(g^2 f)$ to reflect the practical choice of parameters. It is useful to rewrite this expanded Hamiltonian (35) in terms of the canonical variables $\pi(\nu)$, $x(\nu)$ introduced in Eq. (29), together with the additional

definition Δ , whose obvious significance will be discussed below :

$$\Delta = -\frac{f}{2} \sum_{\nu} g_{\nu}^2 \eta_{\nu\nu}^{(+)} = f \sum_{\nu} g_{\nu}^2 u_{\nu} v_{\nu}. \quad (36)$$

Since the $\eta_{\nu\nu}^{(+)}$ are of order 1, Δ is of order g^2 . In this new notation H takes the form

$$\begin{aligned} H = & \sum_{\nu} \epsilon_{\nu} g_{\nu}^2 v_{\nu}^2 - \frac{1}{2} \Delta^2 / f + \sum_{\nu} g_{\nu} (\epsilon_{\nu} \eta_{\nu\nu}^{(+)} - \Delta \xi_{\nu\nu}^{(+)}) \pi(\nu) + \sum_{\nu} (\epsilon_{\nu} \xi_{\nu\nu}^{(+)} + \Delta \eta_{\nu\nu}^{(+)}) [\pi(\nu)^2 + x(\nu)^2 - 1] \\ & + \frac{1}{2} f \sum_{\nu} g_{\nu}^2 \xi_{\nu\nu}^{(+)} - \frac{1}{2} f \sum_{\nu\nu'} g_{\nu} g_{\nu'} x(\nu) x(\nu') - \frac{1}{2} f \sum_{\nu\nu'} g_{\nu} g_{\nu'} \xi_{\nu\nu}^{(+)} \xi_{\nu'\nu'}^{(+)} \pi(\nu) \pi(\nu') + \sum_{\nu} (\epsilon_{\nu} \xi_{\nu\nu}^{(+)} + \Delta \eta_{\nu\nu}^{(+)}) \\ & \times \sum_{J \neq 0, M, \nu'} A_{JM}^{\dagger}(\nu, \nu') A_{JM}(\nu, \nu') - \frac{1}{2} \chi \sum_{\alpha\beta\gamma\delta, M} Q_{\alpha\beta} Q_{\gamma\delta} \eta_{\alpha\beta}^{(+)} \eta_{\gamma\delta}^{(+)} (-1)^M A_{2-M}^{(+)}(\alpha, \beta) A_{2M}^{(+)}(\gamma, \delta). \quad (37) \end{aligned}$$

This Hamiltonian contains both real effects and spurious effects arising from the number dispersion. We give here an analysis that allows these spurious terms to be uniquely identified. For simplicity of presentation this is first done in the simple special case of two shells.

The leading g^4 terms in the Hamiltonian, Eq. (37), are just the first two constant terms. The third term in the Hamiltonian, for example, which is of order g^3 , contains both a number dispersion part as well as real parts. The number operator is

$$\begin{aligned} \hat{N} = & [g_1^2 v_1^2 + g_2^2 v_2^2] + [g_1 \eta_{11}^{(+)} \pi(1) + g_2 \eta_{22}^{(+)} \pi(2)] + [\xi_{11}^{(+)} (\pi(1)^2 + x(1)^2 - 1) + \xi_{22}^{(+)} (\pi(2)^2 + x(2)^2 - 1)] \\ & + \xi_{11}^{(+)} \sum_{J \neq 0, M} \hat{A}_{JM}^{\dagger}(1, 1) \hat{A}_{JM}(1, 1) + \xi_{22}^{(+)} \sum_{J \neq 0, M} \hat{A}_{JM}^{\dagger}(2, 2) \hat{A}_{JM}(2, 2) + (\xi_{11}^{(+)} + \xi_{22}^{(+)}) \\ & \times \sum_{J \neq 0, M} \hat{A}_{JM}^{\dagger}(1, 2) \hat{A}_{JM}(1, 2) + (\text{terms of order } 1/g \text{ and lower}). \quad (38) \end{aligned}$$

The v_1 and v_2 are chosen, as in BCS, so that

$$N = g_1^2 v_1^2 + g_2^2 v_2^2. \quad (39)$$

The remainder of Eq. (38) is the number dispersion, $(\hat{N} - N)$. The leading term in this dispersion is the second term of Eq. (38), of order g , which can be compactly written in terms of a new variable π_N

$$(g_1^2 \eta_{11}^{(+2)} + g_2^2 \eta_{22}^{(+2)})^{1/2} \pi_N, \quad (40)$$

where π_N is defined by

$$\pi_N = \frac{g_1 \eta_{11}^{(+)} \pi(1) + g_2 \eta_{22}^{(+)} \pi(2)}{(g_1^2 \eta_{11}^{(+2)} + g_2^2 \eta_{22}^{(+2)})^{1/2}}. \quad (41)$$

It is convenient, then, to further define a complete canonical set of variables⁹

$$\begin{aligned} \pi_N &= \frac{g_1 \eta_{11}^{(+)} \pi(1) + g_2 \eta_{22}^{(+)} \pi(2)}{(g_1^2 \eta_{11}^{(+2)} + g_2^2 \eta_{22}^{(+2)})^{1/2}}, \\ x_N &= \frac{g_1 \eta_{11}^{(+)} x(1) + g_2 \eta_{22}^{(+)} x(2)}{(g_1^2 \eta_{11}^{(+2)} + g_2^2 \eta_{22}^{(+2)})^{1/2}}, \\ \pi_R &= \frac{g_2 \eta_{22}^{(+)} \pi(1) - g_1 \eta_{11}^{(+)} \pi(2)}{(g_1^2 \eta_{11}^{(+2)} + g_2^2 \eta_{22}^{(+2)})^{1/2}}, \\ x_R &= \frac{g_2 \eta_{22}^{(+)} x(1) - g_1 \eta_{11}^{(+)} x(2)}{(g_1^2 \eta_{11}^{(+2)} + g_2^2 \eta_{22}^{(+2)})^{1/2}}, \end{aligned} \quad (42)$$

which have the simple commutation rules

$$[\pi_R, x_R] = [\pi_N, x_N] = \frac{1}{i}, \quad (43)$$

$$[\pi_R, \pi_N] = [\pi_R, x_N] = [x_R, \pi_N] = [x_R, x_N] = 0.$$

Since the R and N variables commute with each other, the R degree of freedom has indeed no part of π_N . To the order in g in which π_N represents the number dispersion, π_R and x_R will give rise to real excitations, free of spurious contributions. The real $0+$ excitation in even systems is, in this order, describable entirely in π_R, x_R .

With this notation, the Hamiltonian can be written,

⁹ A similar procedure is described and used by D. R. Bes, Nucl. Phys. 49, 544 (1963). See also D. J. Thouless and J. G. Valatin, Nucl. Phys. 31, 211 (1962).

to order g^3 , as

$$H = (\text{constant in } g^4) + \frac{g_1 g_2 \eta_{22}^{(+)} (\epsilon_1 \eta_{11}^{(+)} - \Delta \xi_{11}^{(+)}) - g_1 g_2 \eta_{11}^{(+)} (\epsilon_2 \eta_{22}^{(+)} - \Delta \xi_{22}^{(+)})}{(g_1^2 \eta_{11}^{(+)^2} + g_2^2 \eta_{22}^{(+)^2})^{1/2}} \pi_R$$

$$+ \frac{g_1^2 \eta_{11}^{(+)} (\epsilon_1 \eta_{11}^{(+)} - \Delta \xi_{11}^{(+)}) + g_2^2 \eta_{22}^{(+)} (\epsilon_2 \eta_{22}^{(+)} - \Delta \xi_{22}^{(+)})}{(g_1^2 \eta_{11}^{(+)^2} + g_2^2 \eta_{22}^{(+)^2})^{1/2}} \pi_N + (\text{terms in order } g^2 \text{ and lower}). \quad (44)$$

The diagonalization of the R part of the Hamiltonian would present a familiar problem, since in order g^3 it would result in a continuous spectrum; the inclusion of order g^2 terms would make the spectrum discrete, but π_R, x_R would be of order g , thereby invalidating the expansion. To avoid this we choose the u 's and v 's entering into $\Delta, \eta^{(+)}$ and $\xi^{(+)}$ to make the coefficient of π_R in Eq. (44) zero; that is, we choose them so that

$$\frac{\epsilon_1 \eta_{11}^{(+)} - \Delta \xi_{11}^{(+)}}{\eta_{11}^{(+)}} = \frac{\epsilon_2 \eta_{22}^{(+)} - \Delta \xi_{22}^{(+)}}{\eta_{22}^{(+)}} = \lambda, \quad (45)$$

where λ is a constant. These two equations combined with the requirement (39) completely determine the three parameters v_1, v_2 , and λ . In terms of the original u 's and v 's these equations are seen to be just the BCS equations without the Hartree-Fock contribution to the single-particle energies:

$$\begin{aligned} (\epsilon_1 - \lambda) u_1 v_1 - \frac{1}{2} \Delta (u_1^2 - v_1^2) &= 0, \\ (\epsilon_2 - \lambda) u_2 v_2 - \frac{1}{2} \Delta (u_2^2 - v_2^2) &= 0, \\ N &= g_1^2 v_1^2 + g_2^2 v_2^2, \end{aligned} \quad (46)$$

together with the definition of the gap parameter Δ ,

$$\Delta = f[g_1^2 u_1 v_1 + g_2^2 u_2 v_2].$$

The omitted Hartree-Fock single-particle energy contributions are of order $1/g^2$ smaller than the terms in Eq. (46). Incidentally, the arbitrary inclusion of such terms would not have changed any of the energies up to and including order g^2 .

With this choice of u 's, v 's, the Hamiltonian in order g^3 , Eq. (44) takes the very simple form

$$H = (\text{constant in } g^4) + \lambda [g_1^2 \eta_{11}^{(+)^2} + g_2^2 \eta_{22}^{(+)^2}]^{1/2} \pi_N$$

$$+ (\text{terms in order } g^2 \text{ and lower})$$

$$= (\text{constant in } g^4) + \lambda (\hat{N} - N)$$

$$+ (\text{terms in order } g^2 \text{ and lower}). \quad (47)$$

In the BCS procedure the second term $\lambda(\hat{N} - N)$ is removed by the special procedure of working not with H , but with $(H - \lambda \hat{N})$. Since in both the BCS procedure and here $\langle \pi_N \rangle = 0$, this term does not contribute anyhow. This completes the discussion of order g^3 .

To proceed in order g^2 , the RPA order, it is not sufficient to identify $(\hat{N} - N)$ with

$$(g_1^2 \eta_{11}^{(+)^2} + g_2^2 \eta_{22}^{(+)^2})^{1/2} \pi_N;$$

the next order terms in the expansion of \hat{N} , Eq. (38), must also be considered. To do this most expeditiously it is very convenient to have all the contributions to $(\hat{N} - N)$ lumped together. This is carried out by a canonical transformation, which is defined by

$$e^{-iS} \frac{\hat{N} - N}{(g_1^2 \eta_{11}^{(+)^2} + g_2^2 \eta_{22}^{(+)^2})^{1/2}} e^{iS} = \pi_N; \quad (48)$$

here $(\hat{N} - N)$ is taken up to and including order 1, Eq. (38). The explicit solution for S is easily constructed and turns out to be

$$S = -\frac{\xi_{11}^{(+)}}{2g_1 \eta_{11}^{(+)}} [\pi(1)^2 x(1) + x(1)^3/3 - x(1) + x(1) \sum_{J \neq 0, M} (A_{JM}^\dagger(1,1) A_{JM}(1,1) + A_{JM}^\dagger(1,2) A_{JM}(1,2))]$$

$$- \frac{\xi_{22}^{(+)}}{2g_2 \eta_{22}^{(+)}} [\pi(2)^2 x(2) + x(2)^3/3 - x(2) + x(2) \sum_{J \neq 0, M} (A_{JM}^\dagger(2,2) A_{JM}(2,2) + A_{JM}^\dagger(2,1) A_{JM}(2,1))]$$

$$+ \text{Hermitian conjugate}. \quad (49)$$

The same canonical transformation, Eq. (48), is then applied to the Hamiltonian, and the result again expressed in the original variables π_N, x_N, π_R, x_R and the $A_{JM}, J \neq 0$. The entire number dispersion now occurs only via π_N . Since π_R, x_R commute with π_N exactly, we are sure that the spurious effects are separated and confined to the π_N dependence. Of course, there is a simpler procedure possible to avoid worrying about the identification of those g^2 terms which, together with the g^3 term in Eq. (47), combine in making up $\lambda(\hat{N} - N)$. This consists of simply adding, at the beginning, the exact $-\lambda \hat{N}$ to the Hamiltonian. We have chosen the other canonical transformation procedure to illustrate that which becomes necessary in the higher orders.

After the canonical transformation the Hamiltonian becomes, up to and including order g^2 ,

$$\begin{aligned}
H = & \epsilon_1 g_1^2 v_1^2 + \epsilon_2 g_2^2 v_2^2 - \frac{1}{2} \Delta^2 / f + \lambda (g_1^2 \eta_{11}^{(+2)} + g_2^2 \eta_{22}^{(+2)})^{1/2} \pi_N \\
& + E_1 \sum_{J \neq 0, M} [\dot{A}_{JM}^\dagger(1,1) \dot{A}_{JM}(1,1) + A_{JM}^\dagger(1,2) \dot{A}_{JM}(1,2)] \\
& + E_2 \sum_{J \neq 0, M} [\dot{A}_{JM}^\dagger(2,2) \dot{A}_{JM}(2,2) + A_{JM}^\dagger(2,1) \dot{A}_{JM}(2,1)] \\
& - \frac{1}{2} \chi \sum_M (-1)^M [Q_{11} \eta_{11}^{(+)} \dot{A}_{2-M}^{(+)}(1,1) + 2Q_{12} \eta_{12}^{(+)} \dot{A}_{2-M}^{(+)}(1,2) + Q_{22} \eta_{22}^{(+)} \dot{A}_{2-M}^{(+)}(2,2)] \\
& \times [Q_{11} \eta_{11}^{(+)} \dot{A}_{2M}^{(+)}(1,1) + 2Q_{12} \eta_{12}^{(+)} \dot{A}_{2M}^{(+)}(1,2) + Q_{22} \eta_{22}^{(+)} \dot{A}_{2M}^{(+)}(2,2)] \\
& - fN + \frac{1}{2} f (g_1^2 \eta_{11}^{(+2)} + g_2^2 \eta_{22}^{(+2)}) \pi_N^2 + \frac{1}{2} f \frac{g_1^2 \eta_{11}^{(+2)} + g_2^2 \eta_{22}^{(+2)}}{\eta_{11}^{(+)} \eta_{22}^{(+)}} [\pi_R^2 + x_R^2 - 1] \\
& + 2f g_1^2 g_2^2 \frac{\eta_{12}^{(-2)} \eta_{11}^{(+)} \eta_{22}^{(+)}}{g_1^2 \eta_{11}^{(+2)} + g_2^2 \eta_{22}^{(+2)}} \pi_N^2 - 2f g_1 g_2 \eta_{12}^{(-2)} \frac{g_1^2 \eta_{11}^{(+2)} - g_2^2 \eta_{22}^{(+2)}}{g_1^2 \eta_{11}^{(+2)} + g_2^2 \eta_{22}^{(+2)}} \pi_N \pi_R \\
& - 2f g_1^2 g_2^2 \frac{\eta_{12}^{(-2)} \eta_{11}^{(+)} \eta_{22}^{(+)}}{g_1^2 \eta_{11}^{(+2)} + g_2^2 \eta_{22}^{(+2)}} \pi_R^2. \quad (50)
\end{aligned}$$

Here

$$E_\nu = \Delta / \eta_{\nu\nu}^{(+)} = [(\epsilon_\nu - \lambda)^2 + \Delta^2]^{1/2} \quad (51)$$

denotes the usual BCS quasiparticle energy, again without the Hartree-Fock contribution to the single-particle energy; E_ν is of order g^2 . It is worth noting that x_N does not appear anywhere; this is, of course, because \hat{N} , and therefore, π_N commutes with H . It is also worth noting that the Hamiltonian in order g^2 , Eq. (50), is the part of the whole Hamiltonian that is diagonalized by the RPA.

The π_N^2 terms appearing in order g^2 would give a spurious contribution if they were included; they must be subtracted out. This can be done by subtracting from H a term proportional to \hat{N}^2 . This is the procedure of Nogami⁵; the determination of the correct proportionality constant is, however, not immediate. The Nilsson method⁶ assumes that the energy depends quadratically on N ; knowing the N and N^2 dependence

of the BCS result together with the BCS number dispersion permits solving for the corrected energy. In the procedure outlined in this paper the π_N^2 terms can be dropped either by inspection or by subtraction of an $(\hat{N} - N)^2$ term; the coefficient in the subtraction term is completely defined in this order. The $\pi_N \pi_R$ term can be removed by a canonical transformation leaving only an additional π_N^2 term which is handled as other π_N^2 terms. It can also be dropped on inspection since it can only result in an energy contribution involving π_N , and all such terms are to be dropped in any case. It should be remarked that higher powers of π_N appear in higher order. For this reason the prescriptions of Nogami and of Nilsson based on an \hat{N}^2 dependence are no better than the simple prescription based on order g^2 .

Had we not had the aid of the canonical transformation in identifying all parts of $(\hat{N} - N)$ to the desired order, a portion of H , Eq. (37),

$$\sum_\nu \frac{\epsilon_\nu \eta_{\nu\nu}^{(+)} - \Delta \xi_{\nu\nu}^{(+)}}{\eta_{\nu\nu}^{(+)}} \xi_{\nu\nu}^{(+)} \sum_{\nu', J \neq 0, M} A_{JM}^\dagger(\nu, \nu') \dot{A}_{JM}(\nu, \nu') = \lambda \sum_\nu \xi_{\nu\nu}^{(+)} \sum_{\nu', J \neq 0, M} A_{JM}^\dagger(\nu, \nu') A_{JM}(\nu, \nu'), \quad (52)$$

might not have looked spurious. In fact this g^2 term is entirely spurious, since it goes with a g^3 part to form $\lambda(\hat{N} - N)$. In earlier work this spurious contribution was avoided because it was not H that was used, but $H - \lambda \hat{N}$, which just subtracts out this spurious term. Since it would seem, at first glance, more natural to use H in the RPA, the use of $(H - \lambda \hat{N})$ was very fortunate and correct.

We now have a Hamiltonian free of spurious contributions:

$$\begin{aligned}
H = & \epsilon_1 g_1^2 v_1^2 + \epsilon_2 g_2^2 v_2^2 - \frac{1}{2} fN (g_1^2 + g_2^2 + 2 - N) + \frac{1}{2} f g_1^2 g_2^2 \eta_{12}^{(-2)} \\
& + E_1 \sum_{J \neq 0, M} [\dot{A}_{JM}^\dagger(1,1) \dot{A}_{JM}(1,1) + \dot{A}_{JM}^\dagger(1,2) \dot{A}_{JM}(1,2)] \\
& + E_2 \sum_{J \neq 0, M} [\dot{A}_{JM}^\dagger(2,2) \dot{A}_{JM}(2,2) + \dot{A}_{JM}^\dagger(2,1) \dot{A}_{JM}(2,1)] \\
& - \frac{1}{2} \chi \sum_M (-1)^M [Q_{11} \eta_{11}^{(+)} \dot{A}_{2-M}^{(+)}(1,1) + 2Q_{12} \eta_{12}^{(+)} \dot{A}_{2-M}^{(+)}(1,2) + Q_{22} \eta_{22}^{(+)} \dot{A}_{2-M}^{(+)}(2,2)] \\
& \times [Q_{11} \eta_{11}^{(+)} \dot{A}_{2M}^{(+)}(1,1) + 2Q_{12} \eta_{12}^{(+)} \dot{A}_{2M}^{(+)}(1,2) + Q_{22} \eta_{22}^{(+)} \dot{A}_{2M}^{(+)}(2,2)] \\
& + \frac{1}{2} f \frac{g_1^2 \eta_{11}^{(+2)} + g_2^2 \eta_{22}^{(+2)}}{\eta_{11}^{(+)} \eta_{22}^{(+)}} [\pi_R^2 + x_R^2 - 1] - 2f g_1^2 g_2^2 \frac{\eta_{12}^{(-2)} \eta_{11}^{(+)} \eta_{22}^{(+)}}{g_1^2 \eta_{11}^{(+2)} + g_2^2 \eta_{22}^{(+2)}} \pi_R^2. \quad (53)
\end{aligned}$$

It is easily diagonalized. The $J \neq 0$ parts are handled separately since they commute with the $J=0$ or π_R, x_R parts; this results in the usual RPA equations and results. The π_R, x_R part of the Hamiltonian is even more easily handled. For later purposes we will need the ground-state energy. This is

$$E = \epsilon_1 g_1^2 v_1^2 + \epsilon_2 g_2^2 v_2^2 - \frac{1}{2} f N (g_1^2 + g_2^2 + 2 - N) + \frac{1}{2} f g_1^2 g_2^2 \eta_{12}^{(-)2} \\ + \frac{1}{2} f \frac{g_1^2 \eta_{11}^{(+)} + g_2^2 \eta_{22}^{(+)}}{\eta_{11}^{(+)} \eta_{22}^{(+)}} \left\{ \left[\frac{1 - 4\eta_{12}^{(-)}}{(g_1^2 \eta_{11}^{(+)} + g_2^2 \eta_{22}^{(+)})^2} \right]^{1/2} - 1 \right\} + \frac{5}{2} \sum_{\sigma} \omega_{\sigma} - \frac{15}{2} (E_1 + E_2), \quad (54)$$

where ω_{σ} are the solutions of the usual dispersion equation arising from diagonalization of the $J=2$ part in Eq. (53). It is worth noting that $\eta^{(-)}$ is zero for the degenerate case and Eq. (54) goes over to the well-known result. It should also be noted that the last two terms cancel each other in the case of vanishing quadrupole-quadrupole interaction ($\chi=0$), since the three ω_{σ} 's appearing in the first of these terms become in that case equal to $2E_1$, $(E_1 + E_2)$ and $2E_2$, respectively.

The procedures are immediately generalized to the case of more than two shells. For m shells ($m-1$) different operators $\pi_{R_1}, \dots, \pi_{R_{m-1}}$, and $x_{R_1}, \dots, x_{R_{m-1}}$ can be constructed so that they have the canonical commutation rules, and so that all commute with corresponding π_N and x_N

$$\pi_N = \frac{1}{\left(\sum_{\nu=1}^m g_{\nu}^2 \eta_{\nu\nu}^{(+)} \right)^{1/2}} \sum_{\nu=1}^m g_{\nu} \eta_{\nu\nu}^{(+)} \pi(\nu), \\ x_N = \frac{1}{\left(\sum_{\nu=1}^m g_{\nu}^2 \eta_{\nu\nu}^{(+)} \right)^{1/2}} \sum_{\nu=1}^m g_{\nu} \eta_{\nu\nu}^{(+)} x(\nu). \quad (55)$$

The condition that all terms in order g^3 , linear in $\pi_{R_{\nu}}$, vanish again leads to the BCS conditions

$$(\epsilon_{\nu} - \lambda) u_{\nu} v_{\nu} - \frac{1}{2} \Delta (u_{\nu}^2 - v_{\nu}^2) = 0, \quad \nu = 1, \dots, m \\ N = \sum_{\nu=1}^m g_{\nu}^2 v_{\nu}^2, \quad (56)$$

where

$$\Delta = f \sum_{\nu=1}^m g_{\nu}^2 u_{\nu} v_{\nu}.$$

To order g^3 the Hamiltonian takes the form analogous to Eq. (47)

$$H = (\text{constant in } g^4) + \lambda \left[\sum_{\nu} g_{\nu}^2 \eta_{\nu\nu}^{(+)} \right]^{1/2} \pi_N. \quad (57)$$

The canonical transformation S ,

$$e^{-iS} [\hat{N} - N] / \sum g_{\nu}^2 \eta_{\nu\nu}^{(+)} e^{iS} = \pi_N,$$

$$\mathcal{E} = \langle \Phi_N | H | \Phi_N \rangle = - (f/2) N (g_1^2 + g_2^2 + 2 - N)$$

$$+ \left[2\epsilon_1 + f g_2^2 \left(1 - \frac{u_1 v_2}{u_2 v_1} \right) \right] \mathfrak{N}_N^2 [(N/2)!]^2 \sum_{p+q=N/2} \binom{v_1}{u_1}^{2p} \binom{v_2}{u_2}^{2q} \frac{(g_1^2/2)!}{(g_1^2/2-p)! p!} \frac{(g_2^2/2)!}{(g_2^2/2-q)! q!} p \\ + \left[2\epsilon_2 + f g_1^2 \left(1 - \frac{u_2 v_1}{u_1 v_2} \right) \right] \mathfrak{N}_N^2 [(N/2)!]^2 \sum_{p+q=N/2} \binom{v_1}{u_1}^{2p} \binom{v_2}{u_2}^{2q} \frac{(g_1^2/2)!}{(g_1^2/2-p)! p!} \frac{(g_2^2/2)!}{(g_2^2/2-q)! q!} q \\ - 2f \left(2 - \frac{u_1 v_2}{u_2 v_1} - \frac{u_2 v_1}{u_1 v_2} \right) \mathfrak{N}_N^2 [(N/2)!]^2 \sum_{p+q=N/2} \binom{v_1}{u_1}^{2p} \binom{v_2}{u_2}^{2q} \frac{(g_1^2/2)!}{(g_1^2/2-p)! p!} \frac{(g_2^2/2)!}{(g_2^2/2-q)! q!} p q, \quad (61)$$

is also immediately generalized from its two-shell form (49). To this same order in g

$$S = - \sum_{\nu} \frac{\xi_{\nu\nu}^{(+)}}{2g_{\nu} \eta_{\nu\nu}^{(+)}} \left[\pi(\nu)^2 x(\nu) + x(\nu)^3 / 3 - x(\nu) \right. \\ \left. + x(\nu) \sum_{J \neq 0, M, \nu'} \hat{A}_{JM}^{\dagger}(\nu, \nu') \hat{A}_{JM}(\nu, \nu') \right] \\ + \text{Hermitian conjugate.} \quad (58)$$

V. COMPARISON WITH PROJECTED WAVE-FUNCTION METHODS

It is of interest to compare the results of the projected wave-function methods with those obtained above, that are complete in order g^2 . To do this, the projected wave-function results must be similarly expanded in powers of g . Since these projected wave functions have been considered most extensively for pairing forces alone, we do so here, putting the coefficient of the quadrupole-quadrupole force χ , equal to zero.

The BCS solution for the ground state of an even system, whose average number of particles is N , is

$$|0\rangle = \prod_{\nu, m > 0} (u_{\nu} + v_{\nu} (-1)^{j_{\nu} - m} a_{\nu m}^{\dagger} a_{\nu - m}^{\dagger}) |0\rangle_P, \quad (59)$$

where $|0\rangle_P$ is the particle vacuum. The part of $|0\rangle$ corresponding to exactly the N particles has the well-known form

$$|\Phi_N\rangle = \mathfrak{N}_N \left[\sum_{\nu, m > 0} v_{\nu} / u_{\nu} (-1)^{j_{\nu} - m} a_{\nu m}^{\dagger} a_{\nu - m}^{\dagger} \right]^{N/2} |0\rangle_P \\ = \mathfrak{N}_N \left[\sum_{\nu} (g_{\nu}/2) v_{\nu} / u_{\nu} \bar{A}_0^{\dagger}(\nu, \nu) \right]^{N/2} |0\rangle_P; \quad (60)$$

here \mathfrak{N}_N is the necessary normalization constant. The expectation value of the pairing Hamiltonian [Eq. (1), with $\chi=0$], can, then, be written out in a straightforward way. For the special case of the two-shell problem:

and the normalization condition becomes

$$1 = \mathfrak{N}_N^2 [(N/2)!]^2 \sum_{p+q=N/2} \left(\frac{v_1}{u_1}\right)^{2p} \left(\frac{v_2}{u_2}\right)^{2q} \frac{(g_1^2/2)!}{(g_1^2/2-p)!p!} \frac{(g_2^2/2)!}{(g_2^2/2-q)!q!}. \tag{62}$$

The evaluation of these sums, to the desired order, follows usual mathematical methods.¹⁰ The terms in these sums peak at $p \sim g_1^2 v_1^2/2$, $q \sim g_2^2 v_2^2/2$ and the sums get their main contributions from a region of the p, q variables whose spread about this peak is of order g . It is, therefore, useful to introduce the new variable, δ , $p = g_1^2 v_1^2/2 + \delta$, $q = g_2^2 v_2^2/2 - \delta$. Since the effective range of δ is an order g smaller than $g_1^2 v_1^2/2$ or $g_2^2 v_2^2/2$, it is possible to expand in $\delta/(g_1^2 v_1^2/2)$ and $\delta/(g_2^2 v_2^2/2)$. Further, the factorials can be sufficiently well approximated by the first term of Stirling's formula. Then, the weighting of terms in the sums turns out to be proportional to

$$\exp\left[-4\left(\frac{g_1^2 \eta_{11}^{(+)+2} + g_2^2 \eta_{22}^{(+)+2}}{g_1^2 g_2^2 \eta_{11}^{(+)+2} \eta_{22}^{(+)+2}}\right)\delta^2\right].$$

This, in turn, is an *a posteriori* justification of the procedures used up to here. Finally, the finite sums can be replaced by infinite integrals, the error being smaller by an order of g than the order of the present calculation. In this way we obtain

$$\mathcal{E} = -\frac{f}{2}N(g_1^2 + g_2^2 + 2 - N) + [\epsilon_1 g_1^2 v_1^2 + \epsilon_2 g_2^2 v_2^2] + \frac{1}{2} f g_1^2 g_2^2 \eta_{12}^{(-)2} - 8f \frac{\eta_{12}^{(-)2}}{\eta_{11}^{(+)} \eta_{22}^{(+)}} \langle \delta^2 \rangle_{\text{av}}, \tag{63}$$

where

$$\begin{aligned} \langle \delta^2 \rangle_{\text{av}} &= \int d\delta \delta^2 \exp\left[-4\left(\frac{g_1^2 \eta_{11}^{(+)+2} + g_2^2 \eta_{22}^{(+)+2}}{g_1^2 g_2^2 \eta_{11}^{(+)+2} \eta_{22}^{(+)+2}}\right)\delta^2\right] / \int d\delta \exp\left[-4\left(\frac{g_1^2 \eta_{11}^{(+)+2} + g_2^2 \eta_{22}^{(+)+2}}{g_1^2 g_2^2 \eta_{11}^{(+)+2} \eta_{22}^{(+)+2}}\right)\delta^2\right], \\ &= \frac{1}{8} \left(\frac{g_1^2 g_2^2 \eta_{11}^{(+)+2} \eta_{22}^{(+)+2}}{g_1^2 \eta_{11}^{(+)+2} + g_2^2 \eta_{22}^{(+)+2}}\right). \end{aligned} \tag{64}$$

Putting all these steps together, results in an expression for \mathcal{E} good up to and including order g^2

$$\mathcal{E} = -\frac{1}{2} f N (g_1^2 + g_2^2 + 2 - N) + [\epsilon_1 g_1^2 v_1^2 + \epsilon_2 g_2^2 v_2^2] + \frac{1}{2} f g_1^2 g_2^2 \eta_{12}^{(-)2} - f g_1^2 g_2^2 \eta_{11}^{(+)} \eta_{22}^{(+)} \eta_{12}^{(-)2} / (g_1^2 \eta_{11}^{(+)+2} + g_2^2 \eta_{22}^{(+)+2}). \tag{65}$$

Here the u 's and v 's obey the BCS conditions without Hartree-Fock additions to the single-particle energies, as given in Eq. (46). For these u 's and v 's the coefficient of the term involving $\langle \delta \rangle_{\text{av}}$ vanishes exactly. It should be noted that $\langle \delta \rangle_{\text{av}}$ itself does not vanish; also, the equation for $\langle \delta \rangle_{\text{av}}$ is not just the simple analog of Eq. (64) since there are additional terms in the distribution which can be described schematically as of the form δ/g^2 , δ^3/g^4 times the exponential. It is also worth mentioning that the mathematical conclusions about the (p, q) regions that contribute importantly to the sums (61) and (62) could have been guessed immediately from the BCS results. To see this we have only to note that $2p$ corresponds to the number of particles occupying shell 1, which we call N_1 ; $2q$ corresponds to the number occupying shell 2, which we correspondingly call N_2 . Now the BCS results for the average of N_1 and of N_2 and for their dispersions are

$$\begin{aligned} \bar{N}_1 &= g_1^2 v_1^2, \quad \bar{N}_2 = g_2^2 v_2^2 \\ \langle (N_1 - \bar{N}_1)^2 \rangle_{\text{av}}^{1/2} &= (1/2)^{1/2} g_1 \eta_{11}^{(+)} \\ \langle (N_2 - \bar{N}_2)^2 \rangle_{\text{av}}^{1/2} &= (1/2)^{1/2} g_2 \eta_{22}^{(+)}. \end{aligned}$$

Because of the connections between N_1 , N_2 and p, q

¹⁰ See, for example, W. Feller, *An Introduction to Probability Theory and its Applications* (John Wiley & Sons, Inc., New York, 1957), Vol. 1, 2nd ed., Sec. VII.2.

these relations imply that p, q are effectively confined in a region of order (g_1, g_2) about the mean $\frac{1}{2} g_1^2 v_1^2$, $\frac{1}{2} g_2^2 v_2^2$.

It should be remarked in passing that the use of BCS u 's and v 's with, rather than without, the Hartree-Fock single-particle energies would not change the energy in either order g^4 or g^2 . These single-particle energy shifts are of order $1/g^2$ with respect to the ϵ . Their inclusion would then change the u 's and v 's by order $1/g^2$. However, as will be seen below, the order g^4 terms are stationary with respect to a shift in the u 's and v 's. The effect of this shift would then first contribute to the energy in order 1, which is beyond the region of interest here.

The same result for \mathcal{E} , as that given in Eq. (65), can also be obtained very much more simply and elegantly by taking the expectation value of Eq. (53), with $\chi=0$, in the boson vacuum, so that

$$\langle x_R^2 \rangle = \langle \pi_R^2 \rangle = \frac{1}{2}.$$

The two results are the same because it can be shown that the boson vacuum and the BCS vacuum are equivalent. A difference might be thought to occur in the π_N^2 terms. However, on the one hand, they have been dropped in Eq. (53), while on the other they would contribute zero when the expectation is taken in $|\Phi_N\rangle$, the exact number eigenfunction. These number dis-

persion terms are in this way also handled equivalently.

Finally we can compare \mathcal{E} , Eq. (65), which results from using the projected wave functions, with the result obtained by exact diagonalization of Eq. (53) with $\chi=0$, E , given in Eq. (54). The E and \mathcal{E} are identical in order g^4 . They differ in order g^2 , the difference being

$$E - \mathcal{E} = \frac{1}{2} f \frac{g_1^2 \eta_{11}^{(+2)} + g_2^2 \eta_{22}^{(+2)}}{\eta_{11}^{(+)} \eta_{22}^{(+)}} \times \left\{ \left[1 - 4 \left(\eta_{12}^{(-2)} \frac{g_1^2 g_2^2 \eta_{11}^{(+2)} \eta_{22}^{(+2)}}{(g_1^2 \eta_{11}^{(+2)} + g_2^2 \eta_{22}^{(+2)})^2} \right) \right]^{1/2} - 1 + 2 \left(\eta_{12}^{(-2)} \frac{g_1^2 g_2^2 \eta_{11}^{(+2)} \eta_{22}^{(+2)}}{(g_1^2 \eta_{11}^{(+2)} + g_2^2 \eta_{22}^{(+2)})^2} \right) \right\}. \quad (66)$$

This is, of course, negative. It is immediately seen that when $\eta_{12}^{(-2)}$, $\eta_{12}^{(-2)} = (u_1 v_2 - v_1 u_2)^2$, is small, even the order g^2 difference is greatly reduced; $1-x/2$ is a very good approximation to $(1-x)^{1/2}$ for reasonably small x . In summary, then, the projected wave-function method gives the correct result in order g^4 , and a good approximation in order g^2 . This seems to provide a basis for understanding the excellent numerical agreement that Kerman, Lawson, and Macfarlane⁷ found between the projected wave-function result, and the result they obtained by an exact diagonalization of the whole Hamiltonian.

We can also easily discuss the possibility of improving the projected wave functions by varying the u 's and v 's after projecting. We call these "improved" projected wave functions Φ_N' . We again restrict ourselves to the two-shell problem. A glance at the form of the wave function, (60), makes it clear that the only parameter in this problem is the combination X ,

$$X = (v_2/u_2)(v_1/u_1)^{-1}; \quad (67)$$

that is, \mathcal{E}_v ,

$$\mathcal{E}_v = \langle \Phi_N' | H | \Phi_N' \rangle / \langle \Phi_N' | \Phi_N' \rangle, \quad (68)$$

is a function of the parameter X only. To make the calculations especially simple we add the additional constraint,

$$N = g_1^2 v_1^2 + g_2^2 v_2^2; \quad (69)$$

this costs us nothing, since, even with this constraint, X can still run over the whole range, $-\infty$ to $+\infty$. However, with this constraint the calculations for \mathcal{E}_v go through just as those for \mathcal{E} above, and the answer is just of the form given in Eqs. (63) and (64), except that one of the v 's, say v_1 , is now a variational parameter. It is trivial to verify that the g^4 contribution to the energy, which we call $\mathcal{E}_v^{(4)}$, is a minimum at the choice of variational parameters given by Eq. (46), the BCS values. This guarantees that minimizing both $\mathcal{E}_v^{(4)}$ and the g^2 contributions to the energy, $\mathcal{E}_v^{(2)}$ will produce changes in the u 's and v 's only of higher order in $1/g$. This, taken together with the vanishing of $(\partial \mathcal{E}_v^{(4)} / \partial v_1)$

at the BCS values of v , means that the variational minimum energy is the same both in order g^4 and g^2 as the projected BCS result, Eq. (65), and no lower. Finally, knowing that the result depends only on the X parameter we can drop the constraint, Eq. (69), and state that the result of the general variation is *zero* improvement over the projected BCS, in orders g^4 and g^2 , even though Eq. (66) implies that there is room for improvement in order g^2 .

Of course, such methods cannot be expected to give order g^2 correctly since they are based on BCS functions which do not contain quasiparticle correlations. However, such correlations contribute in order g^2 . In the weak-coupling case where the gap, Δ , as defined by the BCS equations (46), vanishes, the argument in orders of $1/g$ ceases to be valid. A considerable improvement may very well be obtained by varying the v 's in this case.¹¹

VI. HIGHER ORDERS

We have not considered terms beyond those of order g^2 in the Hamiltonian. However, an exploration of the higher orders is important both to establish the applicability of the lower orders and as a source of corrections.

The number operator can also be expanded to higher order and the transformation S can be produced to explicitly gather these higher order terms into π_N . The contributions of π_N , in turn are controlled by the packet. Up to order g^2 the π_N , π_N^2 dependence can be removed by subtraction of terms proportional to \hat{N} and \hat{N}^2 . In many applications it is sufficient to insure that the expectation values of the powers of π_N are equal in the ground and excited states. Thus, to calculate the anharmonicity to order $1/g^2$ in the ratio of energy spacings of vibrational nuclei, this constancy is sufficient. However, a bolder approach is also possible at the end. It will be recalled that a packet was required so that A_0 and A_0^+ would be of order 1 in order to validate the expansion. This in turn meant a packet that would keep both π_N and x_N of order 1. Since they do not commute, squeezing the packet so that the dispersion in π_N approaches zero would make the dispersion in x_N infinite. However, since x_N cannot appear in the final transformed form of the Hamiltonian this infinite dispersion of x_N has no consequences. We can then proceed to take the final packet so that $\pi_N \rightarrow 0$. Put more simply, we finally arrive at an effective *zero* number dispersion, up to the order considered.

ACKNOWLEDGMENTS

We wish to thank Dr. Guy Emery, Dr. J. O. Rasmussen, and Dr. M. Vénéronei for discussions. One of the authors (I.U.) wishes to thank Lawrence Radiation Laboratory for its hospitality during his summer visit.

¹¹ H. J. Mang, J. K. Poggenburg, and J. O. Rasmussen, University of California Radiation Laboratory Report No. UCRL 10939 (unpublished).