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ABSTRACT

The validity of the Bardeen-Cooper-Schrieffer variational method is reexamined for two nuclear model cases, one resembling the system of deformed nuclei and the other spherical nuclei. For simplicity, a constant-pairing-force approximation is adopted. The projected BCS wave functions compare badly with the exact wave functions at pairing force strength around the critical force strength, and only for sufficiently strong pairing forces, does the BCS method seem to approach the exact. For the spherical case, the average value of the pair operator $(\frac{N}{2})$ is also calculated over a wide range of force strength, and the general behavior is found to be consistent with the results obtained on the wave function components. Finally the errors in eigenvalues are computed, and discussions are given as to the possible sources of the deviations.

I. INTRODUCTION

There has been a considerable amount of work devoted to the examination of the superconductivity theory of Bardeen, Cooper and Schrieffer (BCS),[1] and of Bogoliubov[2] applied to nuclear structure problems. The BCS variational approach (or equivalently Bogoliubov lowest-order "compensation" method) seems the best for larger pairing-force strength and large number of particles. It is well known that the ordinary BCS wave functions fail to conserve the number of particles. Attention has been given to the improved wave functions obtained by taking only those components of the BCS wave function which conserve the particle number.[3] There is generally a lowering in eigenvalue accompanying the projection procedure.

We will be mainly concerned here with an examination of the errors remaining after projecting the proper particle number components from lowest BCS solutions of some simple systems. Comparison is made with exact solutions over a wide range of pairing-force strength. We use only a simple constant pairing-force Hamiltonian and do not consider higher-order corrections to BCS solutions such as admixture of 4-quasi-particle components.

First, we examine a half-filled system with the nucleon pairs in six equally spaced levels. Such a system has some similarity to those in deformed nuclei.

Second, we study in greater detail the case of two orbitals with the same pair degeneracy Ω, and with Ω pairs of nucleons. In particular we study the case of $\Omega = 5$ (we call this a "symmetric case"). We shall also examine an unsymmetric case where $\Omega_u \neq \Omega_\ell$. For example, $\Omega_u=3$, $\Omega_\ell=4$, with four pairs of nucleons.

These systems all have in common the feature that below a certain critical pairing force strength there is no non-trivial BCS solution. That is,

at low force strength the BCS approximation gives no configuration mixing whatsoever, obviously a serious defect. From simple perturbation theory it is clear that no matter how small the residual force is, there will always be some configuration mixing. This spurious "threshold" behavior is not exhibited by BCS solutions for systems where a partly-filled degenerate level lies at the Fermi surface. Thus the well-studied system of a single, partly filled degenerate orbital does not exhibit this "threshold" behavior.[4]

II. A REVIEW OF BCS SOLUTIONS

This section is intended to define the notations. Let us take the convention of writing a complete set of quantum numbers by Greek letters, and all except the magnetic quantum number by Roman letters, i.e., $\alpha = (\eta_a \ \ell_a \ j_a \ m_a \ldots)$, and $a = (\eta_a \ \ell_a \ j_a \ldots)$. In this notation, the BCS reduced Hamiltonian is given by (for constant force strength)

$$H_{red} = \sum_{\alpha} \epsilon_\alpha \ a^+_\alpha \ a_\alpha - \frac{G}{4} \sum_{\alpha \beta} \ a^+_\alpha \ a^+_{-\alpha} \ a_{-\beta} \ a_\beta \tag{1}$$

where the fermion operator a_α satisfies the usual anticommutation rule. Using the trial wave function

$$\Psi_0 = \prod_\alpha (u_\alpha + v_\alpha \ a^+_\alpha \ a^+_{-\alpha}) \ |0\rangle \tag{2}$$

a variational calculation yields equations for determining the parameters u and v

$$\frac{G}{2} \sum_\alpha \ \frac{1}{[(\epsilon_\alpha - \lambda)^2 + \Delta^2]^{1/2}} = 1 \tag{3}$$

$$\Delta = G \sum_\alpha u_\alpha v_\alpha \tag{4}$$

$$\begin{pmatrix} v_\alpha^2 \\ u_\alpha^2 \end{pmatrix} = \frac{1}{2}\left[1 \mp \frac{\epsilon_\alpha - \lambda}{[(\epsilon_\alpha - \lambda)^2 + \Delta^2]}\right] \tag{5}$$

with

$$N = \sum_\alpha n_\alpha = 2\sum_{\alpha>0} v_\alpha^2 = \sum_{\alpha>0}\left\{1 - \frac{\epsilon_\alpha - \lambda}{[(\epsilon_\alpha - \lambda)^2 + \Delta^2]^{1/2}}\right\}. \tag{6}$$

In spherical representation, the summation index α is replaced by a Roman index, while multiplying the summand by $\Omega_a = j_a + \frac{1}{2}$. All the subscripts should then be in Roman letters.

The non-linear equation (3) with Eqs. (4), (5) and (6) can be solved analytically only for exceptional cases (an example is given later); however the solutions can be easily obtained by an electronic computer for more general cases.

III. UNIFORM SPACING (6-LEVEL) CASE

We consider here a system with three pairs of nucleons in six doubly degenerate levels; this is a case rather similar to those in deformed nuclei. The BCS equations then yield six independent parameters v_α's. The exact solution, which amounts to diagonalizing the reduced Hamiltonian (1) exactly, has twenty components. The wave function then has the form

$$\Psi_{ex} = \sum_{\alpha\beta\gamma} C_{\alpha\beta\gamma} \; A^+_{\alpha\beta\gamma} \; |0\rangle \tag{7}$$

with $A^+_{\alpha\beta\gamma\cdots} = a^+_\alpha a^+_{-\alpha} a^+_\beta a^+_{-\beta} a^+_\gamma a^+_{-\gamma} \cdots$.

If we label the levels as 1, 2,..., 6 in increasing order, then C_{123} is the lowest amplitude, C_{124} the amplitude with one pair excited and so on.

In order to compare the amplitude (7) with the BCS wave function (2), we need to project the appropriate component from the BCS wave function. The remaining parts in the BCS wave function are spurious, but necessary to make the wave function easy to handle. Defining a projection operator by

$$P(\mu\nu\epsilon) \; \Psi_0 = \left(\prod_{\lambda \neq \mu,\nu,\epsilon} u_\lambda \right) \; v_\mu v_\nu v_\epsilon \; A^+_{\mu\nu\epsilon} \; |0\rangle \tag{8}$$

we have

$$\frac{\langle 0|A_{124} P(124)|\Psi_0\rangle}{\langle 0|A_{123} P(123)|\Psi_0\rangle} = \frac{v_1 v_2 u_3 v_4 u_5 u_6}{v_1 v_2 v_3 u_4 u_5 u_6} = \frac{u_3 v_4}{v_3 u_4} \tag{9}$$

which may be compared with $\dfrac{C_{124}}{C_{123}}$ of the exact solution.

In Figs. 1 through 3 are given the ratios of amplitudes for both the BCS and exact solutions. We have taken six equally spaced levels each separated by 100 keV. Figure 1 shows the comparison for two of the nine amplitudes that involve a single pair promotion from the lowest levels 1, 2, 3 across the Fermi energy to 4, 5 or 6. The limiting slope in the weak-force limit is unity, corresponding to the first power dependence on G from first-order perturbation theory. For the ratio C_{124}/C_{123} the BCS value crosses the exact for a force strength just above critical. For the other ratio plotted, the BCS ratio only very slightly ever exceeds the exact. The second order amplitudes plotted in Fig. 2 do not cross until about three times critical force strength, while for the third order amplitude of Fig. 3 the BCS always lies below the exact.

In Fig. 4 are plotted the errors in eigenvalues of ordinary and projected BCS solutions of the system in question, as deduced by comparison with exact solutions of the 20×20 matrix. Notice that the curves are superimposed up to the critical force strength and thereafter the projected solution shows much less error. The maximum error for the projected solution comes at a force less than twice critical strength, and this error is about 17 keV, or one sixth the single-particle level spacing of 100 keV. The ordinary BCS eigenvalue may show an error of as much as half the single particle level spacing.

IV. SYMMETRIC TWO-DEGENERATE-LEVEL CASE

In this section, we examine the case of Ω pairs of nucleons in two levels of pair degeneracy Ω, separated by an energy difference of ϵ. In this case, the BCS equation can be solved analytically, and interesting features emerge from the comparison of the BCS and exact solutions. In order to be more general, a parallel calculation with two levels of different degeneracy ($\Omega_\ell = 4, \Omega_\mu = 3, N = 8$) is also performed. In the later case no such simple analytical BCS solution is available and hence the solutions are obtained by iterative numerical solution of the Belyaev equations.

What we will examine here are the following: first we calculate $\langle \frac{N}{2} \rangle$ for the upper level and compare the BCS and exact wave functions, second we compare the ratios of amplitudes in a manner analogous to Sec. III, and lastly make a comparison of ground state energy.

A. Quasi-Spin Method

For the system with large magnetic degeneracy, the Hamiltonian (1) can be easily diagonalized by the spin-wave method introduced by Anderson,[6] and later applied to nuclear problem by Kerman et al.[7] Let us use this method to calculate explicitly the Hamiltonian matrix of the system.

Following Kerman et al., we introduce the quasi-spin operators

$$\mathcal{S}_+ = \sum_a S_+(a) = \sum_{\alpha > 0} a_\alpha^+ a_{-\alpha}^+$$
$$\mathcal{S}_- = \sum_a S_-(a) = \sum_{\alpha > 0} a_{-\alpha} a_\alpha \qquad (10)$$

$$\mathcal{S}_z = \frac{1}{2} \sum_{\alpha > 0} \{a_\alpha^+ a_\alpha - a_{-\alpha} a_{-\alpha}^+\} = \sum_a S_z(a) = \frac{1}{2} \sum_\alpha a_\alpha^+ a_\alpha - \frac{1}{2} \sum_a \Omega(a)$$

where $\Omega(a) = j_a + 1/2$, and $\alpha > 0$ restricts the summation over only positive magnetic quantum numbers ($\sum_{\alpha>0} = \sum_{a,m_a>0}$) while α goes over both positive and negative values. In the operators of (10), we have for (1)

$$H_{red} = 2\sum_a \epsilon_a S_z(a) + \sum_a \epsilon_a \Omega(a) - G\, \mathcal{S}_+ \mathcal{S}_- \quad . \tag{11}$$

In the strong-coupling limit ($\frac{G}{\bar{\epsilon}} \gg 1$, where $\bar{\epsilon}$ is an average level spacing)

$$H^S_{red} \approx - G\, \mathcal{S}_+ \mathcal{S}_- \tag{12}$$

and in the weak-coupling limit, only the kinetic energy term remains

$$H^W_{red} \approx 2\sum_a \epsilon_a (S_z(a) + \Omega(a)/2) \quad . \tag{13}$$

Thus one could take a state that is diagonal in either H^W_{red} or H^S_{red} for a zero-order wave function. Let us introduce the quantum numbers σ, σ_0 as follows: since the operators defined in (10) obey the usual angular momentum commutation rules,

$$\begin{aligned} \mathcal{S}^2 |\sigma_1\sigma_2\ldots;\ \sigma\sigma_0\rangle &= \sigma(\sigma+1)|\sigma_1\sigma_2\ldots;\ \sigma\sigma_0\rangle \\ \mathcal{S}_z |\sigma_1\sigma_2\ldots;\ \sigma\sigma_0\rangle &= \sigma_0|\sigma_1\sigma_2\ldots;\ \sigma\sigma_0\rangle \end{aligned} \tag{14}$$

and

$$S_z(a)|\sigma_1\sigma_0^1,\ \sigma_2\sigma_0^2,\ \ldots,\ \sigma_a\sigma_0^a,\ldots\rangle = \sigma_0^a|\sigma_1\sigma_0^1,\ \sigma_2\sigma_0^2,\ \ldots,\ \sigma_a\sigma_0^a,\ \ldots\rangle$$

$$S^2(a)|\sigma_1\sigma_0^1,\ \sigma_2\sigma_0^2,\ \ldots,\ \sigma_a\sigma_0^a,\ \ldots\rangle = \sigma_a(\sigma_a+1)|\sigma_1\sigma_0^1,\ \sigma_2\sigma_0^2,\ \ldots,\ \sigma_a\sigma_0^a,\ \ldots\rangle \tag{15}$$

Here σ is the total quasi-spin quantum number, σ_0 the projection of σ on z axis, σ_1 the quasi-spin quantum number of state labelled by 1, and so on. The representation given in (14) is a "coupled representation" (equivalent to "J-representation" in shell model notation); that in (15) is a "m-representation."[8] For our purpose, it is more convenient to choose the m-representation and assign the quantum numbers as following: suppose we have a configuration given by

$$[a^{n_1}b^{n_2}c^{n_3}\ldots] \ . \tag{16}$$

Then

$$\begin{aligned}
\sigma_K &= \max|\ n_K-\Omega_K|/2 \\
\sigma_0^K &= (n_K - \Omega_K)/2 \\
\sigma &= \sum_K \Omega_K\ /2 \\
\sigma_0 &= \sum_K\ (n_K-\Omega_K)/2 \\
K &= a,b,\ \ldots
\end{aligned} \tag{17}$$

which yields for (16) wave function of the form

$$|\sigma_a \sigma_0^a , \sigma_b \sigma_0^b, \ldots\rangle \quad .$$

The seniority quantum number is related to the quantity given above by

$$\nu_a = \Omega_a - 2\sigma_a \quad .$$

Thus the ground state of even-particle system is given by

$$\sigma_a = \frac{\Omega_a}{2} \quad ,$$

which implies that we have to construct the wave functions with $\sigma_a = \frac{\Omega_a}{2}$. Thus an empty shell is denoted by $| \frac{\Omega_a}{2} , - \frac{\Omega_a}{2} \rangle$, and hence a state with p pairs in a may be generated by

$$(S_+(a))^p \; | \frac{\Omega_a}{2} , - \frac{\Omega_a}{2} \rangle = \left(p! \; \Omega_a(\Omega_a-1)\ldots(\Omega_a-p+1) \right)^{1/2} \left| \frac{\Omega_a}{2}, - \frac{\Omega_a}{2} + p \right\rangle \quad . \quad (18)$$

Now a matrix element of the Hamiltonian given by Eq. (11) can be easily written down. Let us specialize in two-level case; we get

$$\langle \sigma_1 \sigma_1^0, \sigma_2 \sigma_2^0 \; | H_{red} | \sigma_1' \sigma_1^{0'}, \sigma_2' \sigma_2^{0'} \rangle = 2[\epsilon_1(\sigma_1^0 + \frac{\Omega_1}{2})$$

$$+ \epsilon_2(\sigma_2^0 + \frac{\Omega_2}{2})] \; \delta_{\sigma_1 \sigma_1'} \; \delta_{\sigma_2 \sigma_2'} \; \delta_{\sigma_1^0 \sigma_1^{0'}} \; \delta_{\sigma_2^0 \sigma_2^{0'}}$$

$$- G \sum_{\sigma} C(\sigma_1 \sigma_2 \sigma \; ; \; \sigma_1^0 \sigma_2^0 \sigma_0) \; C(\sigma_1' \sigma_2' \sigma \; ; \; \sigma_1^{0'} \sigma_2^{0'} \sigma_0) \; (\sigma(\sigma+1) - \sigma_0(\sigma_0-1)) \quad . \quad (19)$$

Furthermore one can easily check that (since $\sigma_1^0 + \sigma_2^0 = \sigma_1^{0'} + \sigma_2^{0'}$)

$$\langle \sigma_1^0 \sigma_1^0,\ \sigma_2^0 \sigma_2^0 \,|H_{red}|\, \sigma_1^0 \sigma_1^{0\prime},\ \sigma_2^0 \sigma_2^{0\prime} \rangle \neq 0 \qquad (20)$$

only if

$$\sigma_1^0 - \sigma_1^{0\prime} = 0, \pm 1$$

$$\sigma_2^0 - \sigma_2^{0\prime} = 0, \mp 1 \quad .$$

This is, of course, physically rather obvious, since one knows that the two states (in the bra and ket) could differ by at most two particles.

If we put $\Omega_a = \Omega_b = 5$, $N = 10$, $\epsilon_a - \epsilon_b \equiv \epsilon$ in the "symmetric" example we get a matrix of the form

$$H_{red} = \begin{bmatrix} -5G & -5G & 0 & 0 & 0 & 0 \\ -5G & 2\epsilon-13G & -8G & 0 & 0 & 0 \\ 0 & -8G & 4\epsilon-17G & -9G & 0 & 0 \\ 0 & 0 & -9G & 6\epsilon-17G & -8G & 0 \\ 0 & 0 & 0 & -8G & 8\epsilon-13G & -5G \\ 0 & 0 & 0 & 0 & -5G & 10\epsilon-5G \end{bmatrix} \qquad (21)$$

For a slightly "non-symmetric" case with $\Omega_a = 4$, $\Omega_b = 3$, $N = 8$, we have

$$H_{red} = \begin{bmatrix} -4G & -2\sqrt{3}G & 0 & 0 \\ -2\sqrt{3}G & 2\epsilon-9G & -2\sqrt{6}G & 0 \\ 0 & -2\sqrt{6}G & 4\epsilon-10G & -3\sqrt{2}G \\ 0 & 0 & -3\sqrt{2}G & 6\epsilon-7G \end{bmatrix} \qquad (22)$$

Let us consider the behavior at large and small G of the lowest state eigenfunction of Eq. (11). For small G (i.e., $\frac{G}{\epsilon} \ll 1$), we get by first order perturbation theory

$$\left\langle \frac{N_u}{2} \right\rangle \approx \frac{G^2}{4\epsilon^2} \left[\sum_{\sigma} C\left(\frac{\Omega}{2}\ \frac{\Omega}{2}\ \sigma\ ;\ \frac{\Omega}{2} - \frac{\Omega}{2}\ 0\right) C\left(\frac{\Omega}{2}\ \frac{\Omega}{2}\ \sigma\ ;\ \frac{\Omega}{2} - 1,\right.\right.$$

$$\left.\left. - \frac{\Omega}{2} + 1\ 0\right) \sigma\ (\sigma + 1) \right]^2 \equiv \frac{G^2}{4\epsilon^2}\ \zeta\ (\Omega) \qquad (23)$$

for the case of $\Omega_\ell = \Omega_u = \Omega$, $\epsilon_u - \epsilon_\ell = \epsilon$, the subscripts ℓ, and u denoting lower and upper levels respectively. For $\Omega = 5$, $\zeta\ (\Omega=5) = 25$, and hence the slope of (23) as a function of G goes as $\frac{25G}{2\epsilon^2}$ (for the non-symmetric example, it goes as $\frac{6G}{\epsilon^2}$). The ratio of amplitude $\frac{C_1}{C_0}$ (where the subscript denotes the number of pairs excited) behaves like $\frac{5G}{2\epsilon}$ for low G values.

In the strong-pairing-force limit ($\frac{G}{\epsilon} \gg 1$), the "J-scheme" diagonalizes the matrix and hence we have

$$\left\langle \frac{N_u}{2} \right\rangle = \sum_{\sigma_1^0 \sigma_2^0} \left[C\left(\frac{\Omega}{2}\ \frac{\Omega}{2}\ \Omega;\ \sigma_1^0 \sigma_2^0\ 0\right)\right]^2\ \left(\sigma_2^0 + \frac{1}{2}\ \Omega\right) = \frac{1}{2}\ \Omega \qquad (24)$$

As we shall see later, this high-G limit coincides with the BCS method.

B. The BCS Solutions

In the case where $\Omega_\ell = \Omega_u = \Omega$ and the number of particles makes the system half filled, the chemical potential λ lies exactly half way between upper and lower levels. If we measure the single-particle energy from $\lambda = 0$, obviously $-\epsilon_\ell = \epsilon_u = \frac{\epsilon}{2}$. Therefore the solutions of the set of BCS equations are readily obtained.

$$u_\ell^2 = v_u^2 = u_\ell v_u = (1 - \frac{\epsilon}{2G\Omega})/2,$$

$$u_u^2 = v_\ell^2 = u_u v_\ell = (1 + \frac{\epsilon}{2G\Omega})/2,$$

$$\Delta^2 = (G\Omega)^2 - \frac{\epsilon^2}{4} \quad . \tag{25}$$

From Eq. (25), we see that in order for Δ to be real, the condition should hold

$$G \geq \frac{\epsilon}{2\Omega} \quad . \tag{26}$$

Thus the BCS solution breaks down for pairing force smaller than $\frac{\epsilon}{2\Omega}$. It is instructive to notice that the "critical" pairing force strength given by $G_c = \frac{\epsilon}{2\Omega}$ is proportional to $\frac{\epsilon}{\Omega}$; thus the requirement that $\frac{\epsilon}{\Omega}$ should be small for the validity of BCS solutions is in fact related to the size of G_c.

Using Eq. (25), we obtain

$$\langle \frac{N_u}{2} \rangle = \Omega\, v_u^2 = \frac{\Omega}{2} [1 - \frac{\epsilon}{2G\Omega}] \quad . \tag{27}$$

Thus the behavior of the BCS solution at small pairing-force strength is drastically different from the exact solution. One can see that the BCS value of $\langle \frac{N_u}{2} \rangle$ falls much faster than the exact value for small G.

As was mentioned before, as G becomes large, $\langle \frac{N_u}{2} \rangle$ approaches $\frac{\Omega}{2}$, and the BCS and exact solutions approach each other at large force strength G.

For the purpose of comparing the amplitudes, a slightly different representation of the BCS wave function is needed. The BCS wave function, Eq. (2), has to be rewritten in the quasi-spin operators introduced in Eq. (10), since the exact wave function is expanded in the basis vectors of the type

$$|a^{2p}\rangle \equiv \left|\frac{\Omega_a}{2}, -\frac{\Omega_a}{2}+p\right\rangle = \left[p!\Omega_a(\Omega_a-1)\ldots(\Omega_a-p+1)\right]^{-1/2}(S_+(a))^p|0_a\rangle \quad (28)$$

where

$$|0_a\rangle = \left|\frac{\Omega_a}{2}, -\frac{\Omega_a}{2}\right\rangle$$

denotes an empty a-orbital, and p denotes the number of pairs in the a-shell. A rather straightforward manipulation of Eq. (2) easily gives

$$\Psi_0 = \prod_{K=a,b,\ldots} u_K^{\Omega_K}\left[\sum_{\lambda=0}\frac{1}{\lambda!}\left(\frac{v_K}{u_K}\right)^{\lambda}(S_+(K))^{\lambda}\right]|0_K\rangle \quad . \quad (29)$$

In the representation of Eq. (28),

$$\Psi_0 = \prod_{K=a,b,\ldots} u_K^{\Omega_K}\left[|K^0\rangle + \sum_{\lambda=1}^{\Omega_K}\sqrt{\lambda!}\left(\frac{v_K}{u_K}\right)^{\lambda}\binom{\Omega_K}{\lambda}|K^{2\lambda}\rangle\right] \quad (30)$$

where we have used the usual binomial-coefficient notation $\binom{n}{m} = \frac{n!}{(n-m)!\,m!}$. Now we designate the amplitude of the lowest zero-order configuration by C_0, the next by C_1, and so on. In the absence of interaction, the lowest configuration with p pairs is then $|a^p b^0 c^0\ldots\rangle$, where a is the lowest j-shell, the next $|a^{p-2}b^2c^0\ldots\rangle$ a state with a pair excited from a to b.

From Eq. (30), we have (for the case of $p = \Omega_a$)

$$C_0 = v_a^{\Omega_a}\prod_{K=b,c,\ldots} u_K^{\Omega_K}$$

$$C_1 = \Omega_a\Omega_b\, u_a^{\Omega_a-1}v_a\,u_b\,v_b^{\Omega_b-1}\prod_{K=c,d,\ldots} u_K^{\Omega_K} \quad (31)$$

etc.

If we specialize with the symmetric two-level case, the result becomes simple. Letting $\Omega_a = \Omega_b = \Omega$, and $P_a + P_b = \Omega$ ($P_a + P_b$ is the total number of pairs).

$$C_0 \equiv C[a^{2\Omega}] = (v_a\, u_b)^{\Omega}$$

$$C_1 \equiv C[a^{2\Omega-2}\, b^2] = \Omega\, u_a\, v_a^{\Omega-1}\, u_b^{\Omega-1}\, v_b$$

$$C_2 \equiv C[a^{2\Omega-4}\, b^4] = \frac{1}{2}\Omega\,(\Omega-1)\, u_a^2\, v_a^{\Omega-2}\, u_b^{\Omega-2}\, v_b^2\,,$$

$$\vdots$$

$$C_p \equiv C[a^{2\Omega-2p}\, b^{2p}] = \binom{\Omega}{p} u_a^p\, v_a^{\Omega-p}\, u_b^{\Omega-p}\, v_b^p \qquad (32)$$

where p is number of pairs promoted from a to b. The ratio of a higher order amplitude to the lowest order one is then given by

$$\frac{C_p}{C_0} = \binom{\Omega}{p} \left(\frac{u_a\, v_b}{v_a\, u_b} \right)^p . \qquad (33)$$

Substituting Eqs. (25) into Eq. (33), we finally have

$$\frac{C_p}{C_0} = \binom{\Omega}{p} \left[\frac{2G\Omega-\epsilon}{2G\Omega+\epsilon} \right]^p \qquad (34)$$

Thus for very large pairing-force strength, the ratio approaches just $\binom{\Omega}{p}$, the number of ways of distributing p pairs in Ω places.

C. Numerical Solutions

Here we make a detailed comparison of the BCS and exact solutions for the symmetric (and the unsymmetric) example, computed over a range of pairing-force strength. The separation between the a and b levels is taken to be 1 MeV. In Figs. 5 and 6 are given the $\langle \frac{N_u}{2} \rangle$ values vs. G for the symmetric and unsymmetric cases respectively. Notice that both cases exhibit a similar appearance. We shall now look more closely at the symmetric case. In this case, the critical pairing-force strength $G_c = 0.1$ MeV. The average number of pairs in the upper level $\langle \frac{N_u}{2} \rangle$ coincides for BCS and exact solution

at a force just above critical, and thereafter the BCS solution remains above the exact solution. At larger G the two methods approach asymptotically. The exact wave funtion here has six components and we now wish to compare BCS and exact solutions with respect to all components. In Figs. 7 through 9, are plotted the ratios of amplitudes for the symmetric, degenerate case analogous to Figs. 1 through 3. It is to be noted that there always occurs a cross-over of the two ratios, and also that the largest error is made in the amplitude for promotion of a single pair, the error being smaller in the higher order components. The cross-over points do not all occur at exactly the same force strength, but there is actually a region of maximum accuracy of the projected BCS wave function just above threshold.

One other point to be noted is the existence of inflection points in the ratios of amplitudes in the exact solution. In the absence of an analytical solution for the exact case the precise force strength G where the inflection point occurs is not sharply determined; however, it appears to occur very close to G_c, that is, just where the configuration mixing ceases to be present in the BCS method. The configuration mixing in the exact solution drops rapidly at G_c; however, whereas the BCS solution goes down all the way to zero, there always remains configuration mixing of the pair-promotion type in the more correct solution. Thus the breakdown of the BCS method at G_c is probably an exaggerated manifestation of such a change of configuration mixing. The sharp transition between superfluid and normal states of nuclear matter is clearly an artificial feature of the BCS approximation, for the size of our system is comparable to those in real nuclei.

The errors in energy are plotted in Fig. 10. The general trend is similar to Fig. 4 for the non-degenerate example with one anomaly in Fig. 10. As was seen before, the amplitudes of the wave functions from the two methods

cross over in a narrow range of pairing-strength. As Fig. 10 shows, the G value where the first order amplitudes cross is about the same G value at which the error plot from the projected solution shows a strange dip. The projected solution has the maximum error very near the critical pairing-strength, a somewhat different feature from the non-degenerate case.

It is important to keep in mind two distinct types of error associated with BCS energies. The first arises from the presence of wave function components with spurious numbers of particles, and projecting out the spurious components from a BCS solution, we see, results in a considerable decrease in error above critical force strength. The remaining error is associated with the spurious phenomenon of the sharp superfluid-normal phase transition. The projected BCS solution simply has fewer variational parameters than the degrees of freedom in the system. Further marked improvements without an increase in the number of variational parameters have been achieved by Dietrich, Mang, and Pradal[3] through performing the variation with the fixed-particle Hamiltonian expression, rather than first wolving the BCS equations. Also Bang, Mihailov, and Soloviev[9] have achieved improved solutions by inserting a renormalized G_{eff} (increasing over G more as G decreases in magnitude) into the BCS equations. Both these methods give non-trivial solutions, no matter how weak the pairing-force strength. Such new methods appear to be of great importance in pairing-force calculations where small or zero Δ-values would appear in the ordinary BCS solutions.

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REFERENCES AND FOOTNOTES

1. J. Bardeen, L. N. Cooper, and J. R. Schrieffer, Phys. Rev. 108, 1175 (1959).
2. N. N. Bogoliubov, Nuovo Cimento 7, 794 (1958); J. G. Valatin, Nuovo Cimento 7, 843 (1958).
3. See for example, B. F. Bayman, Nucl. Phys. 15, 33 (1960); A. K. Kerman, R. D. Lawson, and M. H. Macfarlane, Phys. Rev. 124, 162 (1961); K. Dietrich, H. J. Mang, and J. Pradal, UCRL-11083, Phys. Rev. (to be published).
4. B. R. Mottelson, in The Many Body Problem (Dunod, Paris, 1959).
5. S. T. Belyaev, Kgl. Danske Videnskab. Selskab, Mat.-Fys. Medd. 31, No. 11 (1959).
6. P. W. Anderson, Phys. Rev. 112, 1900 (1958).
7. See Kerman et al., reference 3.
8. A. de-Shalit and I. Talmi, Nuclear Shell Theory (Academic Press, New York and London, 1963).
9. Bang, Mihailov, and Soloviev, Private communication (1964).

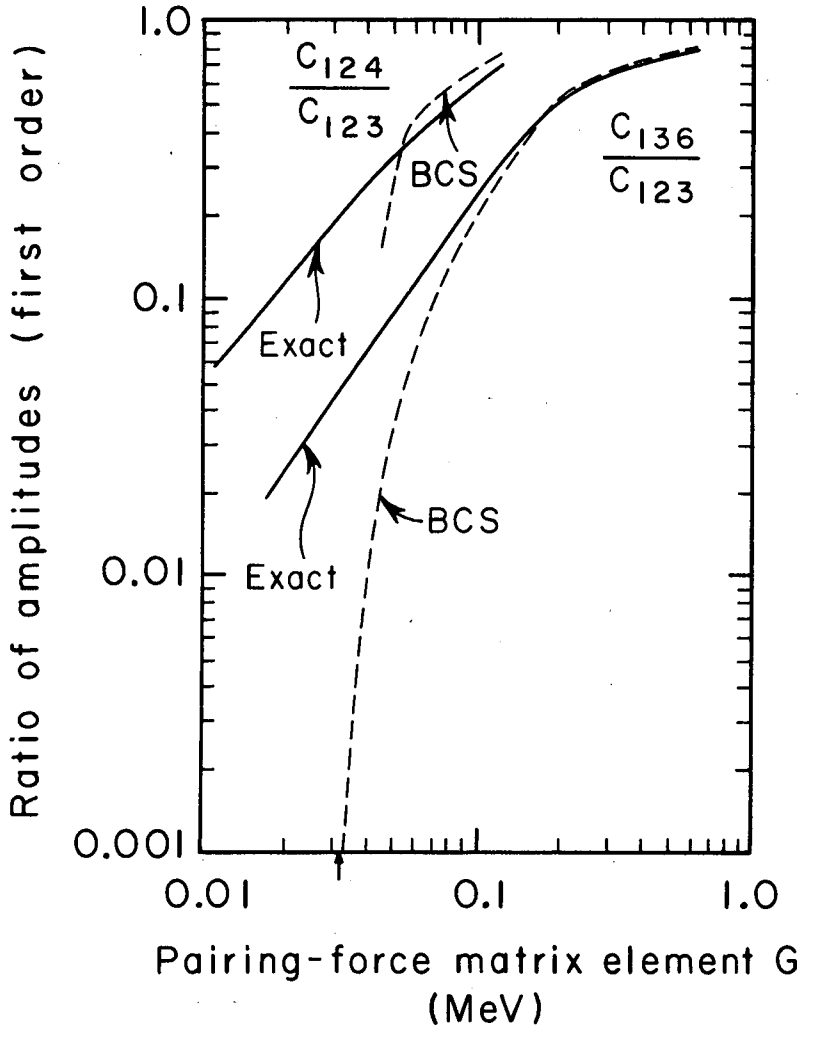

Fig. 1. The ratios of amplitudes, C_{124}/C_{123} and C_{136}/C_{123} in the six-level, three-pair non-degenerate model with ϵ=100 KeV. The arrow indicates the critical force strength.

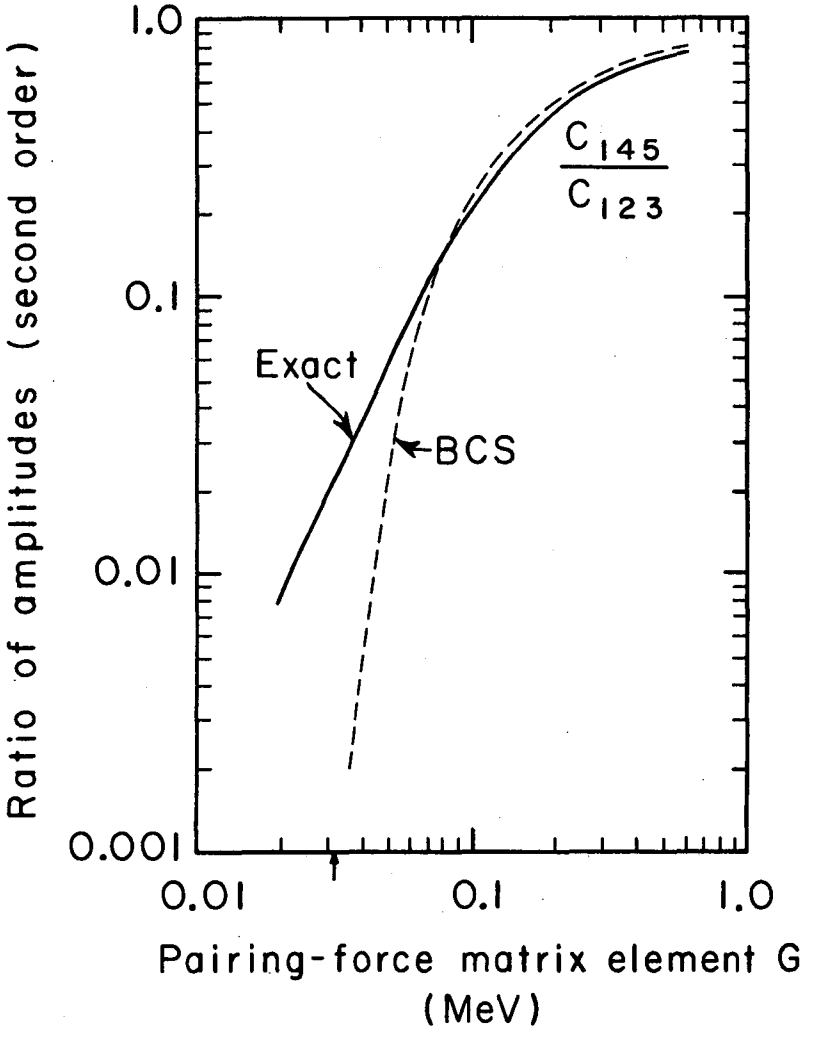

Fig. 2. The ratio of amplitude (2nd order) C_{145}/C_{123} in the six-level, three-pair non-degenerate model with ϵ=100 KeV.

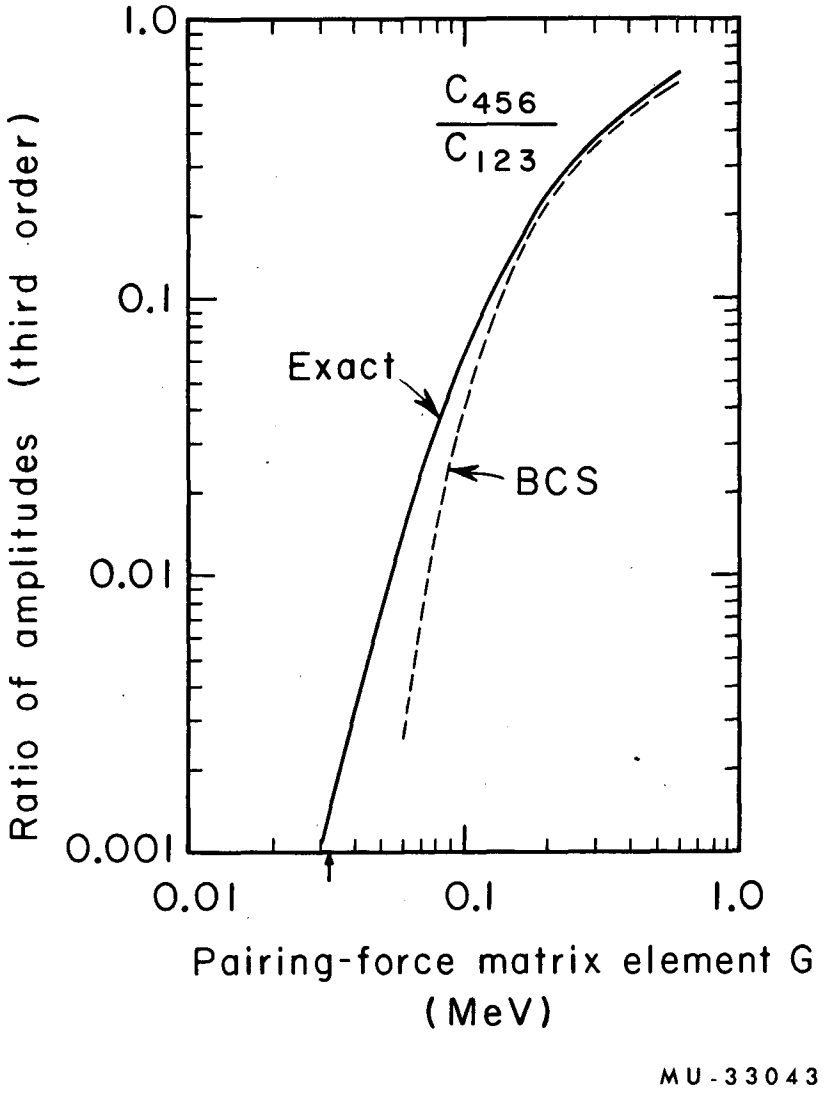

Fig. 3. The ratio of amplitude (3rd order) C_{456}/C_{123} in the six-level, three-pair non-degenerate model with ϵ=100 KeV.

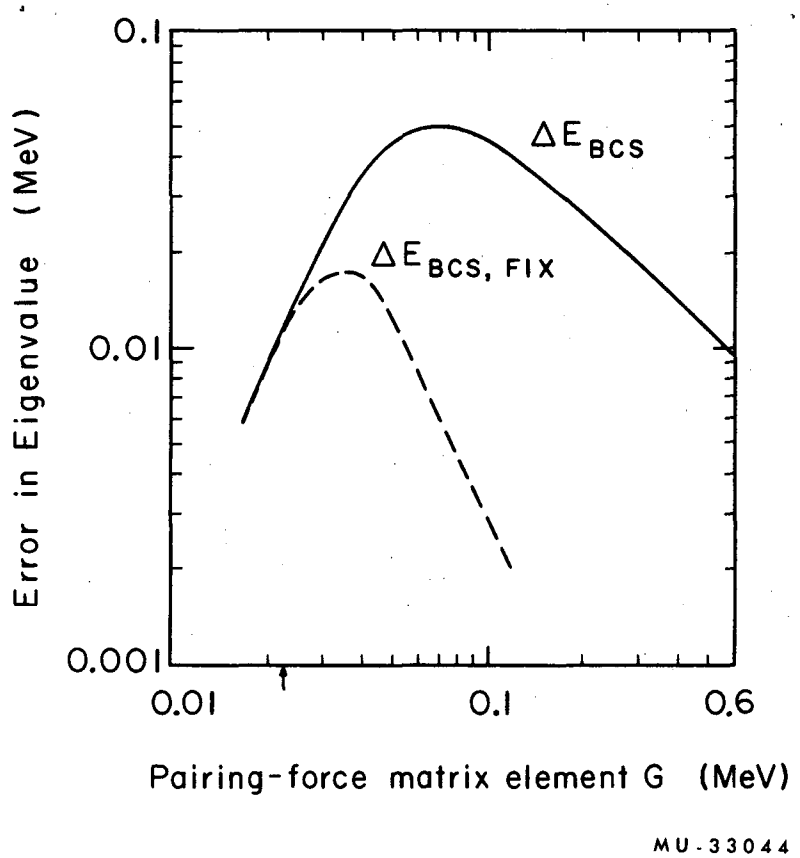

Fig. 4. Error in eigenvalues for the ordinary and projected BCS solutions of the six-level, three-pair model as deduced by comparison with exact solutions of 20 × 20 matrix.

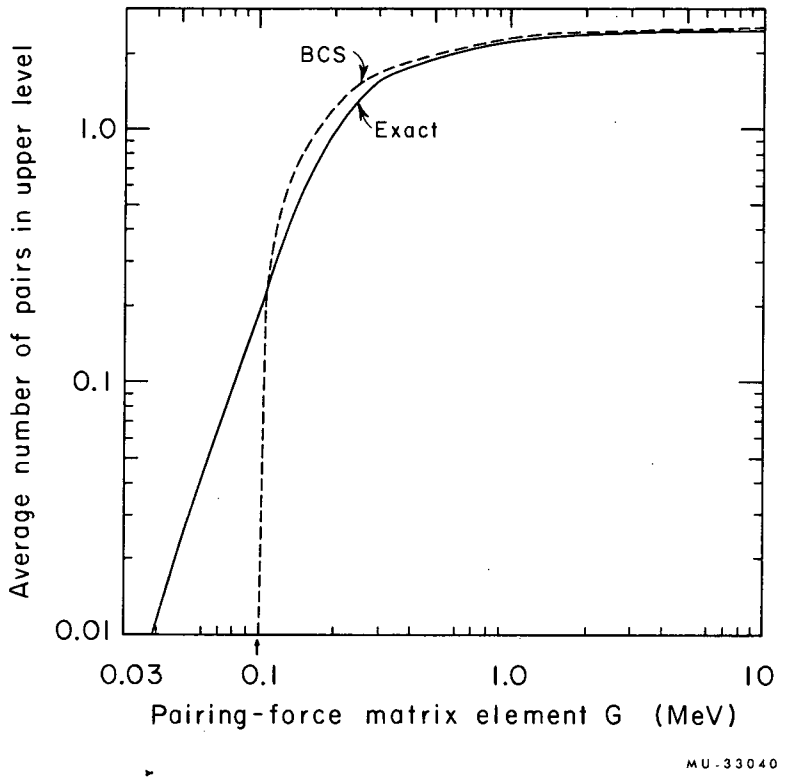

Fig. 5. Average number of pairs in the upper level $\langle \frac{N_u}{2} \rangle$, where $j_u = j_\ell = 9/2$, N=10, ϵ=1 MeV.

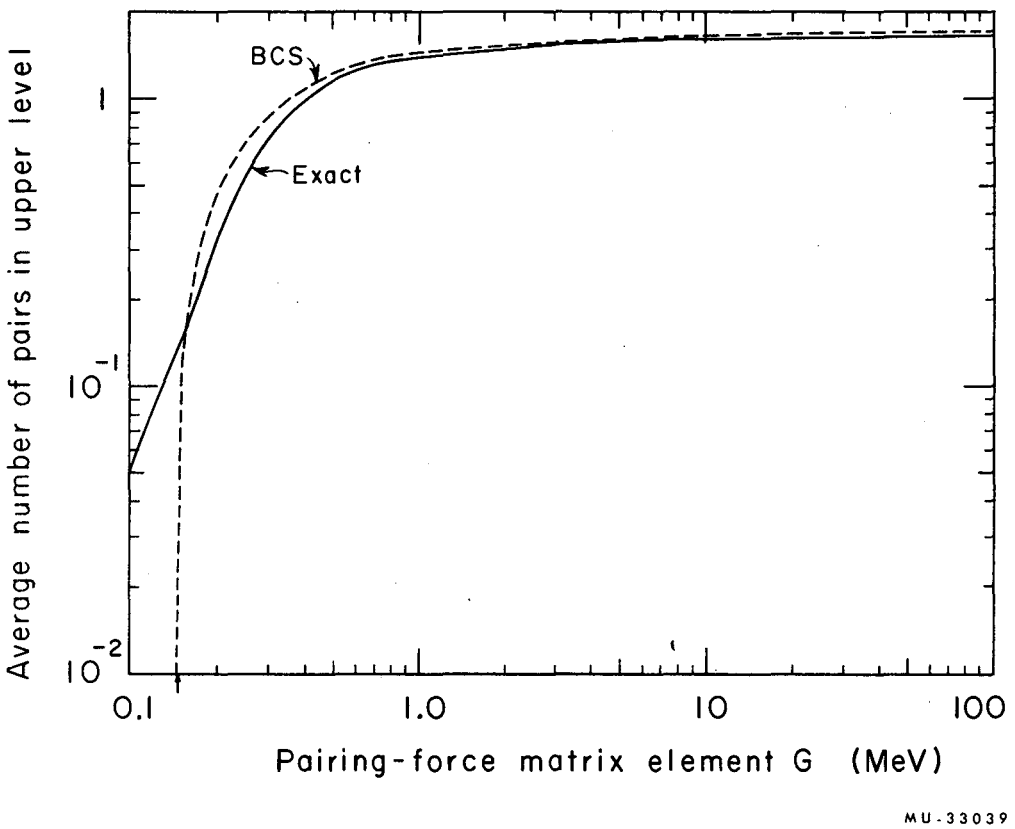

Fig. 6. Average number of pairs in the upper level $\langle \frac{N_u}{2} \rangle$, where $j_u=5/2$, $j_\ell=7/2$, N=8, ϵ=1 MeV.

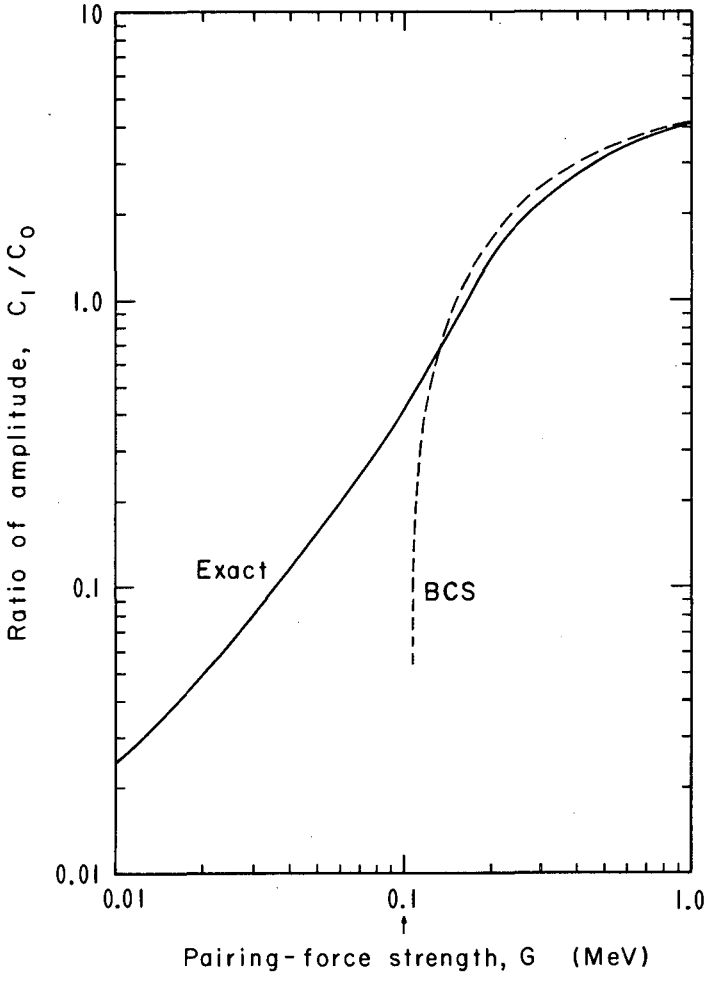

Fig. 7. The ratio of amplitudes C_1/C_0 in the symmetric case with $\Omega_u=\Omega_\ell=5$, N=10, ϵ=1 MeV.

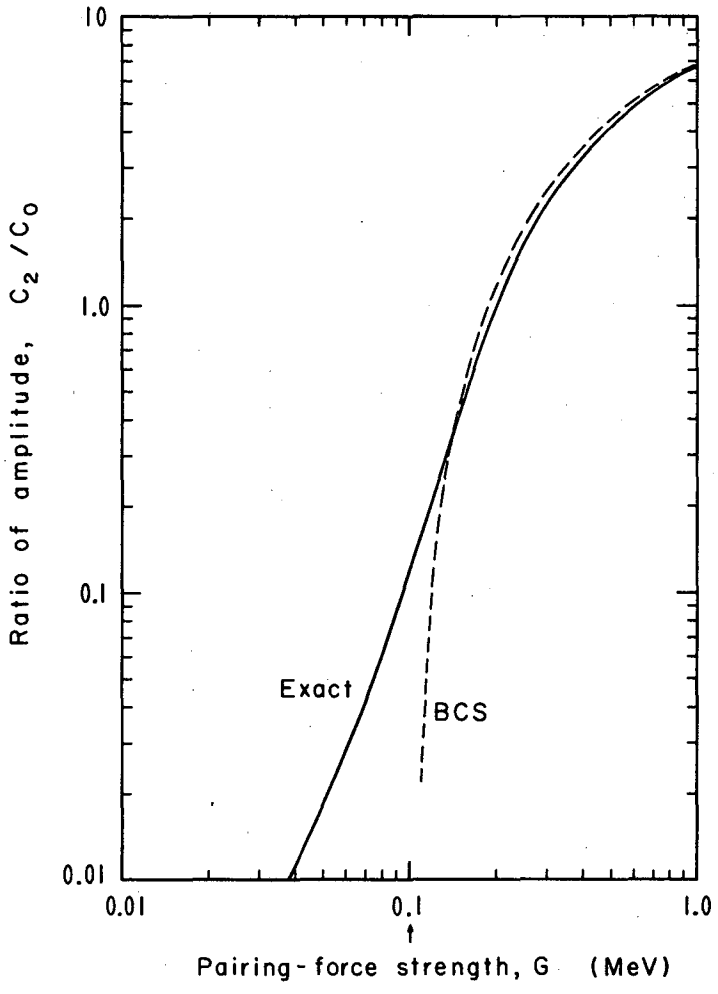

Fig. 8. The ratio of amplitude C_2/C_0 in the symmetric case with $\Omega_u=\Omega_\ell=5$, N=10, ϵ=1 MeV.

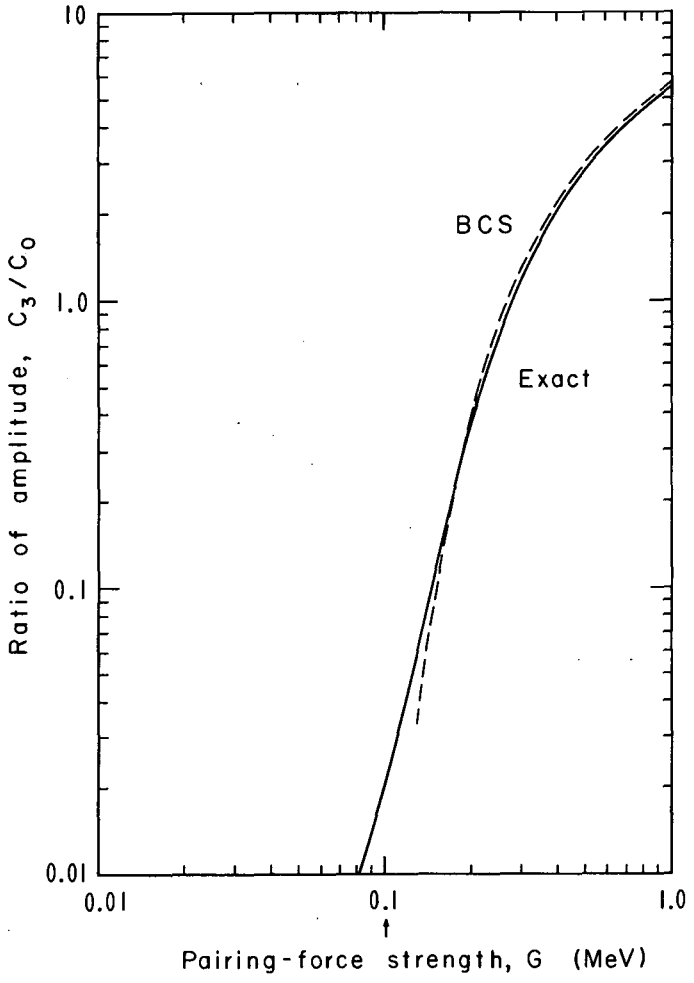

Fig. 9. The ratio of amplitude C_3/C_0 in the symmetric case with $\Omega_u=\Omega_\ell=5$, N=10, ϵ=1 MeV.

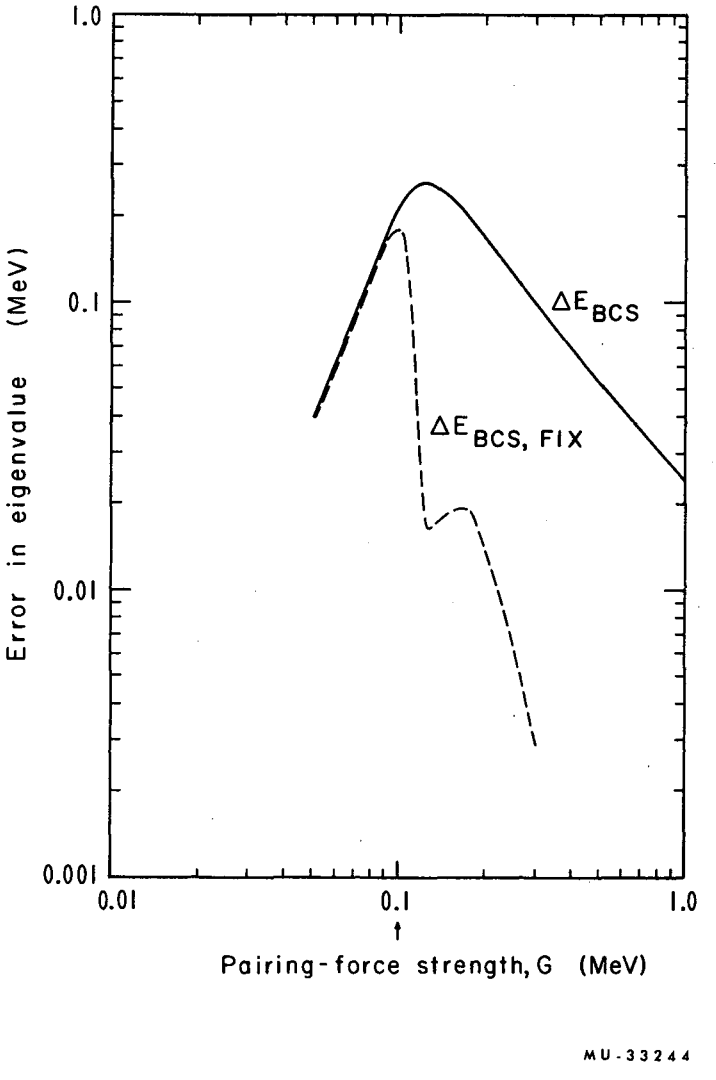

Fig. 10. Error in eigenvalues for the ordinary and projected BCS solutions of the symmetric case as deduced by comparison with exact solutions.