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Comparisons of BCS Nuclear Wave Functions with Exact Solutions

II Particle Number Conserving Method*

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ABSTRACT

It is shown that in a symmetric two-level model, a sudden transition from configuration-mixing to non-configuration-mixing state at a critical strength G_c is an artificial feature of the theory arising mainly from the number fluctuation in the wave function. The variational method taking the components of the BCS wave function with correct particle number shows that such a sudden transition should not occur. The effect of a 4-quasi-particle component in the number-conserving method is to improve higher order amplitudes of the wave function, to necessitate a reduction of Δ, and to modify the roles of the u and v parameters. The absence of a sudden transition is expected to have some bearing on the question of whether a discontinuous "Mottelson-Valatin effect" in the nuclear rotational spectra does exist in nature.

I. INTRODUCTION

Dietrich, Mang and Pradal[1] developed a variational method in the pairing model which should give the best possible solutions of the BCS form with projection of terms of proper particle number. This method (designated FBCS) was applied extensively to the actinide proton and neutron systems by Mang, Poggenburg, and Rasmussen[2]. The FBCS method consists of performing the variation on the u_i and v_i parameters after projection of fixed particle components rather than before. This method differs from the usual projection method (PBCS)[3] in the order in which projection and variation are performed.

It is well known that the conventional BCS method gives only trivial solutions (no configuration mixing) for pairing force strength below a critical force strength (denoted by G_c) determined by Belyaev's inequality[4]. Two of the authors (Rho and Rasmussen)[5] earlier studied two-level model systems by means of the BCS and exact methods to gain insight into the approximations and validity of the BCS method. We now wish to extend that study to include the FBCS method.

In I, we made the remark that the existence of G_c below which the BCS equation has only the trivial solutions might be an artificial feature of the theory, and might be due to fluctuation of number of particles. We show in the following that indeed the FBCS method in the two level case gives a non-trivial (or configuration mixing) solution for all attractive pairing force strengths. Nogami[6] has independently shown the same result by a different method and Dietrich[7] has provided in an unpublished paper an argument that the same conclusion should hold for general cases provided interaction is attractive.

In comparing the FBCS solutions with the exact ones, we find that the two methods yield in low-G limit exactly the same ratio c_1/c_o where c_i are the amplitudes with i-pair promoted to the upper level, but they deviate in c_i/c_o for $i \geq 2$. In order to match one more ratio c_2/c_o, one is tempted to introduce an additional (independent) variational parameter, say β, by adding a 4-quasi-particle component. We demonstrate, however, that it is not possible in the present model and framework to match exactly the two quantities simultaneously (though c_2/c_o may be improved). We show further by a generalized variational calculation that c_1/c_o can always be made to match with the exact value independently of what the parameter v turns out to be. As a consequence, the ground state energy in the low-G limit does not depend on the v-parameter up to third power of the coupling constant G. Thus unlike the FBCS method where the v-parameter (and hence Δ) is closely related to configuration mixing, v^2 and Δ do not play significant roles in the generalized FBCS method (GFBCS). This point is also discussed in a paper of Vautherin and Rho[8] where the same phenomenon occurs in an extended BCS theory without projection.

II. EXISTENCE OF NON-TRIVIAL SOLUTIONS

Let us consider the system with two levels of identical degeneracy Ω and with $N = 2\Omega$ nucleons or Ω pairs. This system seems sufficiently complex to bring out the superfluidity properties of a real nuclear system, but it is simple enough (owing to special symmetry) to yield exact analytic solutions for the BCS equations and approximate analytic solutions for the FBCS equations in the low-G limit.

Taking the separation of the two levels (denoted by h for the higher level and ℓ for the lower level) to be ϵ, we write the Hamiltonian in two forms:

$$H = \frac{\epsilon}{2} \sum_{\substack{r=h,\ell \\ m}} a^{+}_{rm} a_{rm} - G \sum_{\substack{r,s=h,\ell \\ m,m'>0}} a^{+}_{rm} a^{+}_{r-m} a_{s-m'} a_{sm'}$$

$$= \epsilon \left[S_z(h) - S_z(\ell) \right] - G \left[S_+(\ell) S_-(\ell) + S_+(h) S_-(h) \right.$$

$$\left. + S_+(\ell) S_-(h) + S_+(h) S_-(\ell) \right] \qquad (1)$$

where a^{+} and a are the fermion creation and annihilation operators respectively, and

$$S_+(i) = \sum_{m>0} a^{+}_{im} a^{+}_{i-m}$$

$$S_-(i) = \left[S_+(i) \right]^{+}$$

and

$$S_z(i) = \frac{1}{2} \sum_{m>0} \left\{ a^{+}_{im} a_{im} - a_{i-m} a^{+}_{i-m} \right\}$$

are the quasi-spin operators introduced in I.

The set of BCS equations with the Hamiltonian given above was solved in I and the "critical force strength" was found to be

$$G_c = \epsilon / 2\Omega \, . \qquad (2)$$

Now using Eq. (2.9) of Dietrich et. al[1], the expression for total energy for Eq. (1) in FBCS method can be written as

$$E_0 = \frac{1}{R_0^0}\left\{ \sum_\alpha (2\epsilon_\alpha - G) v_\alpha^2 R_1^1(\alpha) - G \sum_{\substack{\alpha,\beta \\ \alpha \neq \beta}}' u_\alpha v_\alpha u_\beta v_\beta R_1^2(\alpha\beta) \right\} \tag{3}$$

where the "residuum function" R is defined by[9]

$$R_0^n = \oint \frac{dz}{z^{n+1}} \prod_K \left(u_K^2 + z v_K^2 \right),$$

$$R_1^1(\gamma) = \oint \frac{dz}{z^{n}} \prod_{K \neq \gamma} \left(u_K^2 + z v_K^2 \right) \tag{4}$$

and where the contour of integration may be any path around the origin. In Eqs. (3) and (4), n is the number of pairs and N the total number of orbitals (magnetic substates).

The trial wave function corresponding to Eq. (3) is given by

$$\phi_0 = \frac{C}{2\pi i} \oint \frac{dz}{z^{n+1}} \prod_{\substack{K \\ m>0}} \left(1 + z \frac{v_K}{u_K} a_{K,m}^\dagger a_{K,-m}^\dagger \right) |0\rangle$$

$$= C \hat{P}_n \left\{ \prod_K \exp\left[v_K S_+(K)/u_K \right] |0\rangle \right\}$$

$$= C \hat{P}_n \left\{ \prod_K \sum_{\lambda=0}^{\Omega_K} \left(\frac{v_K}{u_K} \right)^\lambda \left(\frac{\Omega_K!}{(\Omega_K - \lambda)!\, \lambda!} \right)^{1/2} |K^\lambda\rangle \right\} \tag{5}$$

where C is the normalization constant proportional to R_o^o . We have replaced the contour integral by an equivalent operation P_n projecting out the components with n pair. In the last line of Eq. (5), we have made use of the relation

$$\left[S_+(K)\right]^\lambda |0\rangle = \left[\lambda!\, \Omega_K(\Omega_K-1)\cdots(\Omega_K-\lambda+1)\right]^{1/2} |K^\lambda\rangle \tag{6}$$

where $|k^\lambda\rangle$ is an eigenstate of $[S(k)]^2$.

Using the symmetry properties of the system (same degeneracy etc.) and Eq. (4), one can verify that the condition

$$(\phi_o | N | \phi_o) = 2\Omega$$

implies

$$u_k = v_k = u$$

and

$$v_\ell = u_\ell = v. \tag{7}$$

This relation holds exactly even when a four quasi-particle component is added.

With the relations of Eq. (7), Eq. (3) becomes

$$E_o = \frac{1}{R_o^o}\Big\{\Omega(\epsilon - 3G\Omega)u^2 R_1'(k) - \Omega(\epsilon + G\Omega)v^2 R_1'(\ell) - 2G\Omega^2 u^2(v^2-u^2)\, R_1^2(k\ell)\Big\}. \tag{8}$$

We are mainly interested in the limit $G \to 0$, and hence we can expand the R functions in powers of $x \equiv u^2/v^2$. Keeping terms up to quadratic in x, we have

$$E_o = 2\Omega^2 \left\{ \epsilon - G(\Omega-1) \right\} x^2 - 2G\Omega^2 x - (\epsilon + G)\Omega \Big\} \tag{9}$$

The minimization of E_o determines the x:

$$\frac{1}{2\Omega^2} \frac{\delta E_o}{\delta x} = 2 \left\{ \epsilon - G(\Omega-1) \right\} x - G = 0$$

or

$$x = G/2\{\epsilon - G(\Omega-1)\} \tag{10}$$

First we notice that x is linear in G and consequently the energy Eq. (9) is valid up to third power in G,

$$E_o = -\epsilon\Omega \left\{ 1 + 2\zeta + 2\Omega\zeta^2 + 4\Omega(\Omega-1)\zeta^3 \right] + O(\zeta^4)$$

where

$$\zeta \equiv G/2\epsilon \tag{11}$$

Next Eq. (10) shows that a non-trivial solution with $x > 0$ obtains in the FBCS method for all $G > 0$. The solution also has the proper perturbation theoretical limiting dependence of configuration mixture on pairing force strength. The apparent singularity in the solution at $\epsilon = G(\Omega-1)$ is a consequence of our retaining only terms quadratic in x for Eq. (9). Equation (10) is valid only if $G \ll \frac{\epsilon}{\Omega}$. The FBCS solution which minimizes Eq. (8) behaves properly in the limit of large G where both PBCS and FBCS approach the exact solutions.

III. COMPARISONS WITH EXACT SOLUTIONS

Exact solutions are obtained by the quasi-spin method as described in I and come from the diagonalization of a tri-diagonal matrix of dimensionality $(\Omega+1)$. We have obtained variational solutions to the complete FBCS energy expression of Eq. (8) using the computer program of Mang, Poggenburg, and Rasmussen[2].

Specifically we study the system with $\Omega_p = \Omega_n = 5$ and orbital separation $\epsilon = 1$ MeV. The error in the ground state energy is plotted in Fig. 1 against pairing force strength for several variational methods. There are the ordinary BCS, PBCS and FBCS which also have been studied numerically on large systems, but without benefit of knowing the exact solutions, by Mang, Poggenburg and Rasmussen. A fourth method is a PBCS retaining a v^4 self-energy term, which has been often dropped but carefully examined in some calculations of Lande.[10] Note that all methods except FBCS make the same error below the critical pairing strength $G_c = \frac{\epsilon}{2\Omega} = 0.1$ MeV; this results because projection of fixed particle component from a trivial solution does not modify the wave functions.

In Fig. 2 is plotted v_h^2 vs. G. Notice that FBCS method always gives a larger v_h^2 than BCS (more properly PBCS) with the v^4 terms. The BCS method without the v^4 terms gives a rapidly rising v_h^2 which crosses slightly over FBCS at $G \approx 0.14$. Thus the curious cusp in the error curve for PBCS in Fig. 1 occurs near this cross-over, and, of course, FBCS and PBCS solutions and energy value errors are identical at the cross-over.

Let us now see how well the various amplitudes of the exact wave function are matched by the FBCS method. There are $\Omega+1$ (=6) amplitudes c_0 through c_Ω in the wave function, corresponding to components with zero through Ω (=5) pairs in the upper level and, respectively, Ω through zero pairs in the lower. In I we showed that the ratio c_i/c_o are easiest to compare with BCS-type wave functions. In Fig. 3 is plotted the comparison of c_1/c_o for FBCS and exact solutions. The two solutions are indistinguishable below $G \approx 1.5\ G_c$ but for higher G values the FBCS slightly overshoots the exact solution. Figure 4 shows the "second-order" amplitude ratio c_2/c_o. Here there is a slight overshoot by FBCS for $G \gtrsim 1.5\ G_c$, but the second order amplitude is progressively underestimated as one goes to weaker G than $1.5\ G_c$. The error is about 50% at $G = G_c$ and a factor of two at $G = 0.5\ G_c$. We do not plot the higher-order ratios c_3/c_o, c_4/c_o, etc., but we have checked c_3/c_o and find it a few percent low at $G = 1.9\ G_c$ and almost a factor of four low at $G = G_c$.

Let us examine briefly the nature of the error in c_2/c_o by using a simple perturbation theory. From Eq. (20) of I, we derive generally that the first two off-diagonal matrix elements in the Hamiltonian matrix for degeneracies Ω in higher and lower level are $-\Omega G$ and $-2(\Omega-1)G$. Thus by first order perturbation theory the ratio of amplitude of one pair promoted to the higher level (c_1) to the amplitude of zero pairs promoted (c_o) is

$$\lim_{G\to 0} \left(\frac{c_1}{c_o}\right)_{exact} = \Omega\mathcal{G} + O(\mathcal{G}^2) \qquad (12)$$

where ζ is defined by $\zeta = G/2\epsilon$. By second order perturbation method, we have the ratio c_2/c_o,

$$\lim_{G\to 0}\left(\frac{c_2}{c_0}\right)_{exact} = -\Omega(\Omega-1)\zeta^2 + O(\zeta^3) . \tag{13}$$

From Eq. (10), we have

$$\lim_{G\to 0}\left(\frac{u^2}{v^2}\right) = \lim_{G\to 0} x = \zeta . \tag{14}$$

Now using Eq. (5) and (13), we obtain for the FBCS theory

$$\lim_{G\to 0}\left(\frac{c_1}{c_0}\right)_{FBCS} = -\Omega\zeta \tag{15}$$

in agreement with the exact result Eq. (12). However, for the second order ratio, we get

$$\lim_{G\to 0}\left(\frac{c_2}{c_0}\right)_{FBCS} = \frac{1}{2}\Omega(\Omega-1)\zeta^2 . \tag{16}$$

Thus in the low-vorce limit the FBCS variational wave function gets c_1/c_o correct and is a factor of two low on the second order amplitude.

In fact, no wave function of projected BCS product type can simultaneously match both c_1/c_o and c_2/c_o in the low-G region. The FBCS method in this case minimizes the energy of the system by using its single degree of freedom to closely match c_1/c_o, which is larger than c_2/c_o and more significant in determing the total energy. Chasman,[11] for instance, has been able to obtain lower energy values in his iterative-variational approach by introducing more degrees of freedcm than in the BCS methods in the form of factors correcting on the average the higher-order amplitudes with respect to lower-order amplitudes. Thus in order to improve on the second-order component, we are tempted to introduce one more variational parameter β in addition to v by adding a four-quasi-particle (projected) wave function to the FBCS function.

IV. EFFECT OF 4-QUASI-PARTICLE COMPONENTS

There has been considerable study of improvements to BCS wave functions via the random-phase approximation (RPA) treatment of interactions between quasiparticles.[12] The emphasis has been mainly on the effect of ground state correlations on excited states. Frequently the RPA method is applied to quadrupole-quadrupole force component, admixing, 4, 8, 12 etc. quasi-particle components into the ground state. In our work here, we shall not consider effects of force components in addition to the pairing force in Hamiltonian. Even with the pure pairing force alone, there remain the residual terms H_{40}, H_{22}, and H_{31} in the quasi-particle Hamiltonian. It seems worth exploring whether introduction of terms of 4-quasi-particle forms might naturally provide extra variational parameters to improve further the FBCS wave functions in the low G region. So far

as we know, such higher order corrections to fixed-particle-number (projected) wave functions have not been studied heretofore, although a few studies[13] have been made to incorporate such corrections to ordinary BCS wave function in infinite systems, as well as in finite systems. The latter studies have been primarily concerned with their effect on the energy gap.

Let us first construct a trial wave function for our two-level system. A generalization to more realistic cases will be obvious. We consider the 4-quasi-particle component built up by creating two quasiparticles each in the upper and lower levels.[14] The wave function for such a state looks like

$$\alpha^+_{\ell m_1}\alpha^+_{\ell -m_1}\alpha^+_{h m_2}\alpha^+_{h -m_2}\prod_{\substack{K\\ m_K>0}}\left(u_K + v_K\, a^+_{K m_K} a^+_{K -m_K}\right)|0\rangle$$

$$= \left(u_\ell a^+_{\ell m_1} a^+_{\ell -m_1} - v_\ell\right)\left(u_h\, a^+_{h m_2} a^+_{h -m_2} - v_h\right)\prod_{\substack{K\\ m_K\neq m_1,m_2}}\left(u_K + v_K a^+_{K m_K} a^+_{K -m_K}\right)|0\rangle \tag{17}$$

where α's are here quasi-particle operators. For our calculation, it is more appropriate to write the wave function Eq. (17) in a coupled representation where each of the pair of quasiparticles is coupled to total angular momentum zero. From the second form of Eq. (5), we have (unnormalized)

$$\Phi_4 = \frac{(uv)^\Omega}{\Omega}\left\{\frac{1}{u^2}S_+(\ell) - \frac{v}{u}\Omega\right\}\left\{\frac{1}{v^2}S_+(h) - \frac{u}{v}\Omega\right\}\sum_{\lambda\lambda'=0}^{\Omega} q_\lambda(\ell)\, q_{\lambda'}(h)\,|0\rangle$$

$$= \frac{(uv)^{\Omega-2}}{\Omega}\sum_{\lambda,\lambda'=0}^{\Omega}\left(\lambda\lambda' - \lambda\Omega u^2 - \lambda'\Omega v^2 + \Omega^2 u^2 v^2\right) q_\lambda(\ell)\, q_{\lambda'}(h)\,|0\rangle \tag{18}$$

where

$$q_\lambda(a) \equiv \frac{1}{\lambda!}\left(\frac{v_a}{u_a}\right)^\lambda [S_+(a)]^\lambda$$

and where use has been made of the relations (7). For convenience, we also write down Eq. (5) in the same notation

$$\phi_0 = C\,(uv)^\Omega \sum_{\lambda\lambda'=0}^{\Omega} q_\lambda(\ell)\, q_{\lambda'}(k)\,|0) \,. \tag{19}$$

Now introducing $x = \frac{u^2}{v^2}$, and projecting out the components $\lambda + \lambda' = \Omega$, we get

$$\Psi_0 = N P_\Omega(\phi_0 + \beta\phi_1) = N \sum_{\lambda=0}^{\Omega} K_\lambda\,|\lambda) \tag{20}$$

where

$$N^{-2} = \sum_{\lambda=0}^{\Omega} K_\lambda^2 \,,$$

$$K_\lambda \equiv K_\lambda(x,\beta) = \left\{\Omega x - \beta(\lambda x + \lambda - \Omega)^2\right\} x^{-\lambda}\binom{\Omega}{\lambda}$$

and $|\lambda)$ is defined by

$$\begin{aligned}
&|\lambda) \equiv |\Omega,\lambda) \,,\\
&[S(\ell)]^2\,|\lambda) = [S(k)]^2\,|\lambda) = \tfrac{1}{2}\Omega(\tfrac{1}{2}\Omega+1)\,|\lambda) \,,\\
&S_z(\ell)\,|\lambda) = (-\tfrac{1}{2}\Omega+\lambda)\,|\lambda) \,,\\
&S_z(k)\,|\lambda) = (\tfrac{1}{2}\Omega-\lambda)\,|\lambda) \,.
\end{aligned} \tag{21}$$

Now if we designate as $c_n^{(4)}$ the amplitude of n pairs promoted in $P_\Omega \Phi_4$, we obtain from Eq. (20)

$$\frac{C_0^{(4)}}{C_0} = -X \ ,$$

$$\frac{C_1^{(4)}}{C_0} = -\left[1-(\Omega-1)X\right]^2 ,$$

and

$$\frac{C_2^{(4)}}{C_0} = -2(\Omega-1)X\left[1-\frac{\Omega-2}{2}X\right]^2 . \tag{22}$$

On the other hand, we obtain from $P_\Omega \Phi_0$

$$\frac{C_1}{C_0} = \Omega X \ ,$$

and

$$\frac{C_2}{C_0} = \frac{1}{2}\Omega(\Omega-1)X^2 . \tag{23}$$

Thus explicitly

$$\Psi_0 = N\left\{(1-\beta X)|\Omega\rangle + \left[\Omega X - \beta(1-(\Omega-1)X)^2\right]|\Omega-1\rangle \right.$$

$$\left. + \left[\frac{\Omega(\Omega-1)}{2}X^2 - 2\beta(\Omega-1)X\left(1-\frac{\Omega-2}{2}X\right)^2\right]|\Omega-2\rangle + \cdots\right\} . \tag{20a}$$

A standard variational treatment minimizing the energy with respect to x and β will be presented in the next section. Let us see whether, given the two degrees of freedom x and β, we can find x and β values to match in the low G limit the amplitude ratios c_1/c_o and c_2/c_o to the exact values.

The conditions to be satisfied are for the first order amplitude ratio

$$\frac{\Omega x - \beta\left[1-(\Omega-1)x\right]^2}{1-\beta x} = \Omega\zeta + \cdots \tag{24}$$

and for the second-order amplitude ratio

$$\frac{\frac{\Omega(\Omega-1)}{2}x^2 - 2\beta(\Omega-1)x\left[1-\frac{\Omega-2}{2}x\right]^2}{1-\beta x} = \Omega(\Omega-1)\zeta^2 + \cdots . \tag{25}$$

In Eqs. (24) and (25), we have neglected higher order terms on the right hand side. Thus retaining only the lowest power terms in x and β on the left (for $G \to 0$), we obtain

$$\Omega x - \beta \approx \Omega\zeta \tag{24a}$$

and

$$\frac{\Omega(\Omega-1)}{2}x^2 - 2\beta x(\Omega-1) \approx \Omega(\Omega-1)\zeta^2 . \tag{25a}$$

By a trivial computation, one can see that there exists no real and non-negative x satisfying Eqs. (24) and (25) (x is in fact complex). Therefore the extra degree of freedom is not sufficient to fix c_1/c_o and c_2/c_o simultaneously. However a variational calculation with the addition of the 4-quasi-particle component improves the ratio c_2/c_o. This improvement can be seen in the following way: the left hand side of Eq. (25) as a function of x [with β satisfying Eq. (24)] has the maximum $\frac{2}{3}\Omega(\Omega-1)\zeta^2$ for the value $x = \frac{2}{3}\zeta$. Now if β satisfies Eq. (24), the ground state energy E_4 (and its derivative) is expected to be a smooth function of x in the neighborhood of the extremum point, and to satisfy from the variational principle

$$E_4(x) \geqslant E_{exact} \text{ for all } x \ , \tag{26a}$$

$$\left(\frac{dE_4(x)}{dx}\right)_{x\approx\frac{2}{3}\zeta} = 0 \ , \tag{26b}$$

$$E_4(x\approx\tfrac{2}{3}\zeta) \lesssim E_o \ . \tag{26c}$$

We shall see in the next section that Eq. (24) follows from the condition $\frac{\partial E_4(x,\beta)}{\partial\beta} = 0$. Thus we expect that $c_2/c_o \approx \frac{2}{3}\Omega(\Omega-1)\zeta^2$ which is certainly an improvement over the FBCS value Eq. (16) .

Note that an improvement on c_2/c_o necessitates a renormalization of u and v and in fact reduces x by about 30% (therefore a reduction of Δ). This is consistent with the nuclear matter calculation, though the reduction is less drastic than in nuclear matter.[13] It should be emphasized that while configuration mixing is effectively increased, $v_h^2 = u^2$ is decreased. In fact we shall show later that the expectation value of the

number operator N_i is independent of v^2 in the low G region, differing thus from the ordinary FBCS method.

V. VARIATIONAL METHOD

In this section, we show that in the low-G limit, the stationarity condition of E_4 with respect to β is equivalent to the condition necessary for matching c_1/c_o to the exact value, and that the energy $E_4(x)$ is independent of x up to the third power in ζ. In so doing, we assume that x behaves linearly in ζ in the low-G limit.

The trial wave function is given by Eq. (20), and the relevant matrix elements of the Hamiltonian Eq. (1) are given by[15]

$$
\begin{aligned}
&(\lambda|[S_z(k)-S_z(\ell)]|\lambda) = -2\lambda+\Omega, \\
&(\lambda|S_+(\ell)S_-(\ell)|\lambda) = \Omega\lambda+\lambda-\lambda^2, \\
&(\lambda|S_+(k)S_-(k)|\lambda) = \Omega\lambda+\Omega-\lambda^2-\lambda, \\
&\sum_{\lambda\lambda'} K_\lambda K_{\lambda'}(\lambda'|S_+(\ell)S_-(k)|\lambda) = \sum_\lambda K_\lambda K_{\lambda+1}(\Omega-\lambda)(\lambda+1), \\
&\sum_{\lambda,\lambda'} K_\lambda K_{\lambda'}(\lambda'|S_+(k)S_-(\ell)|\lambda) = \sum_\lambda K_\lambda K_{\lambda-1}(\lambda\Omega-\lambda^2+\lambda)
\end{aligned}
\tag{27}
$$

Consequently we have

$$
\begin{aligned}
E_4(x,\beta) = -\Big[\sum_\lambda K_\lambda^2\Big]^{-1} \sum_{\lambda=0}^{\Omega} \Big\{ &\big[\epsilon(2\lambda-\Omega)+G(2\lambda\Omega+\Omega-2\lambda^2)\big]K_\lambda^2 \\
&+2G\lambda(\Omega-\lambda+1)K_\lambda K_{\lambda-1}\Big\}
\end{aligned}
\tag{28}
$$

with the understanding that $K_\lambda = 0$ for $\lambda < 0$.

Now varying Eq. (28) with respect to β and solving for it by expanding the resulting equation in powers of ζ and x, one finds

$$\beta = -\Omega\zeta + \Omega x - 2\Omega(\Omega-1)(\zeta^2 + \zeta x - x^2) + O(\zeta^3) . \tag{29}$$

Comparing with Eq. (24), we see that Eq. (29) is exactly the same as Eq. (24) except for one term proportional to ζ^2. The absence of such a term in Eq. (24) is obviously due to taking only the term linear in ζ on the right hand side, and that term should be included in order to be consistent up to second order in ζ. Thus we have shown that c_1/c_o matches the exact value independently of x values. As a consequence of this result, the energy E_4 with β satisfying Eq. (29) is independent of x up to third power of ζ in low-G limit. The second order amplitude (two-pair promoted component) contributes in $(\underline{\Phi}_o | H | \underline{\Phi}_o)$ only the terms of $O(\zeta^4)$ and hence up to $O(\zeta^3)$, only the first and second components in Eq. (20a) contribute. But β satisfies Eq. (29) and therefore E_4 is a constant[16]: i.e.,

$$E_4(x) = \text{const} + O(x^3\zeta) + O(x^2\zeta^2) + \text{etc.} \tag{30}$$

Expanding in powers of ζ, we have

$$E_4(x) = a + b\zeta + c\zeta^2 + d\zeta^3 + O(x^2\zeta^2) + \ldots \tag{31}$$

It is clear from our discussion that if we neglect terms of $O(\zeta^4)$, E_o [Eq. (11)] and E_4 should be the same; i.e.,

$$\begin{aligned} a &= -\epsilon\Omega , \\ b &= -2\epsilon\Omega , \\ c &= -2\epsilon\Omega^2 , \\ d &= -4\epsilon\Omega^2(\Omega-1) . \end{aligned} \tag{32}$$

Let us consider the occupation probability of a pair for a magnetic substate ν (in the upper or lower level) which is defined by

$$f_\nu^2 = (\Psi_0 | (a_\nu a_{-\nu})^+ a_\nu a_{-\nu} | \Psi_0)$$

In the FBCS theory, it is given by[1]

$$f_\nu^2 = v_\nu^2 \frac{R_1'(\nu)}{R_0^0} \tag{33}$$

where the R function is used for compactness and also to exhibit the similarity in form to the ordinary BCS theory. The coefficient v_ν^2 is a function of u and v factors, and thus f_ν^2 is a function of x. Therefore x is closely related to configuration mixing. But in GFBCS [analogously to $(\Psi_0 | H | \Psi_0)$] f_ν^2 does not depend upon x (up to the third power in ζ) due to the condition Eq. (29). Therefore here x does not play the same role (the amount of configuration mixing) as in the FBCS.

VI. CONCLUDING REMARKS

Although the model we have studied is perhaps an oversimplified one, it has, however, many features that are relevant in realistic systems. In this paper, we have confined our attention mainly to low pairing-force strength region. We have seen in I that in the high-G region all the approximations (ordinary BCS, PBCS, and FBCS) approach the exact results. Physically important region is of course the intermediate region which has been neglected in our studies (though considered in our numerical calculations) for the sole reason that analytic solutions are not available.

There is nevertheless a justification for studying the low-G limit. Besides gaining an insight into the pairing theory per se, it has also a physical significance connected with the Mottelson-Valatin (MV) effect in the rotational spectra of nuclei.[17] The Mottelson-Valatin argument goes as follows: Coriolis forces in rotational nuclei act in opposite directions to the pairing force and tend to decouple the time-reversed pairs. This effectively reduces the pairing strength, and as the angular frequency ω increases, there is a certain critical point ω_c at which the BCS gap equations have only trivial solutions. The resulting discontinuity in rotational energy [$\Delta E = E(\omega_c - \delta) - E(\omega_c + \delta)$ where δ is an infinitesimal quantity] has been sought experimentally, and not found.

As calculated by Chan and Valatin[18], the solution of the BCS equations in the presence of Coriolis force gives a smaller discontinuity of the rotational energy than does the Mottelson-Valatin coupling constant argument. Though ω_c comes out to be higher than MV estimate, it still does exist; i.e., $\left(\frac{d\Delta(\omega)}{d\omega}\right)_{\omega = \omega_c} = \infty$. Qualitatively the two results are equivalent.

The decrease of pairing correlation with increasing rotational velocity undoubtedly occurs, but we would stress that there should be no discontinuity. On the basis of our studies, we clearly see that the discontinuity is an artificial feature of the BCS method, and that this unrealistic feature is removed in the FBCS procedures - a gradual continuous decrease of superfluidity with increasing rotational angular momentum would be reproduced by the FBCS variational method. This result was also obtained numerically in realistic systems by Mang, Poggenburg, and Rasmussen.[2]

The addition of 4-quasi-particle components in a generalized variational method (GFBCS) gives a further improvement, but does not qualitatively alter our conclusion. The latter feature is, however, not the case if the projection procedure is not employed. Vautherin and Rho[8] have studied the effect of adding a 4-quasi-particle component to the ordinary BCS wave function as a trial wave function. This is an extended BCS theory without projection (GBCS). They have found that Δ goes to zero at $G_c' \gtrsim G_c$, where G_c' and G_c are the critical-force constants in the GBCS and BCS methods respectively, and that in general $\Delta \lesssim \Delta_{BCS}$. However the configuration mixing in the upper level does not vanish completely at the critical point. For example, the occupation probability in the upper level $\langle N_h \rangle$ remains non-zero even though $\Delta = 0$, and goes to zero as $G \to 0$. There is a very small discontinuity of $\langle N_h \rangle$ at G_c', but it is almost smeared out. Thus even within the BCS framework, a more correct treatment will not exhibit as sharp a discontinuity in the MV effect as asserted by Mottelson, Valatin and Chan.[17, 18]

Finally we emphasize that Δ in an extended theory (i.e., GFBCS) is not directly related to odd-even mass differences or a physical energy gap (as it is in the BCS theory).

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FOOTNOTES AND REFERENCES

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14. The (projected) components with all four quasiparticles either in the upper or in the lower level can be expressed, if properly combined, as a linear combination of the (projected) zero-quasi-particle and the four-quasi-particle component used here.
15. We prefer to use quasi-spin operators here instead of R functions; they are, of course, equivalent. Though the quasi-spin operator method is convenient for our purpose, the R function method is more suitable for actual numerical computation.

16. By an explicit calculation substituting Eq. (29) into Eq. (28), one can verify that terms of the form x, $x\zeta$, $x^2\zeta$ and x^3 drop out exactly, with only constant terms and terms of $O(x^2\zeta^2)$, $O(x^3\zeta)$ etc. left behind.

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FIGURE CAPTIONS

1. Error in the ground state energy for various variational methods, as deduced by comparison with exact solutions. The BCS critical force strength is indicated by an arrow. $\Omega_h = \Omega_\ell = 5$, N = 10, ϵ = 1MeV.
2. v^2 for the upper level (v_h^2) for the BCS and FBCS methods. $\Omega_h = \Omega_\ell = 5$, N = 10, ϵ = 1MeV.
3. The first order amplitude ratio c_1/c_o for the FBCS and exact solutions calculated with $\Omega_h = \Omega_\ell = 5$, N = 10, ϵ = 1MeV.
4. The second order amplitude ratio c_2/c_o for the FBCS and exact solutions calculated with $\Omega_h = \Omega_\ell = 5$, N = 10, ϵ = 1MeV.

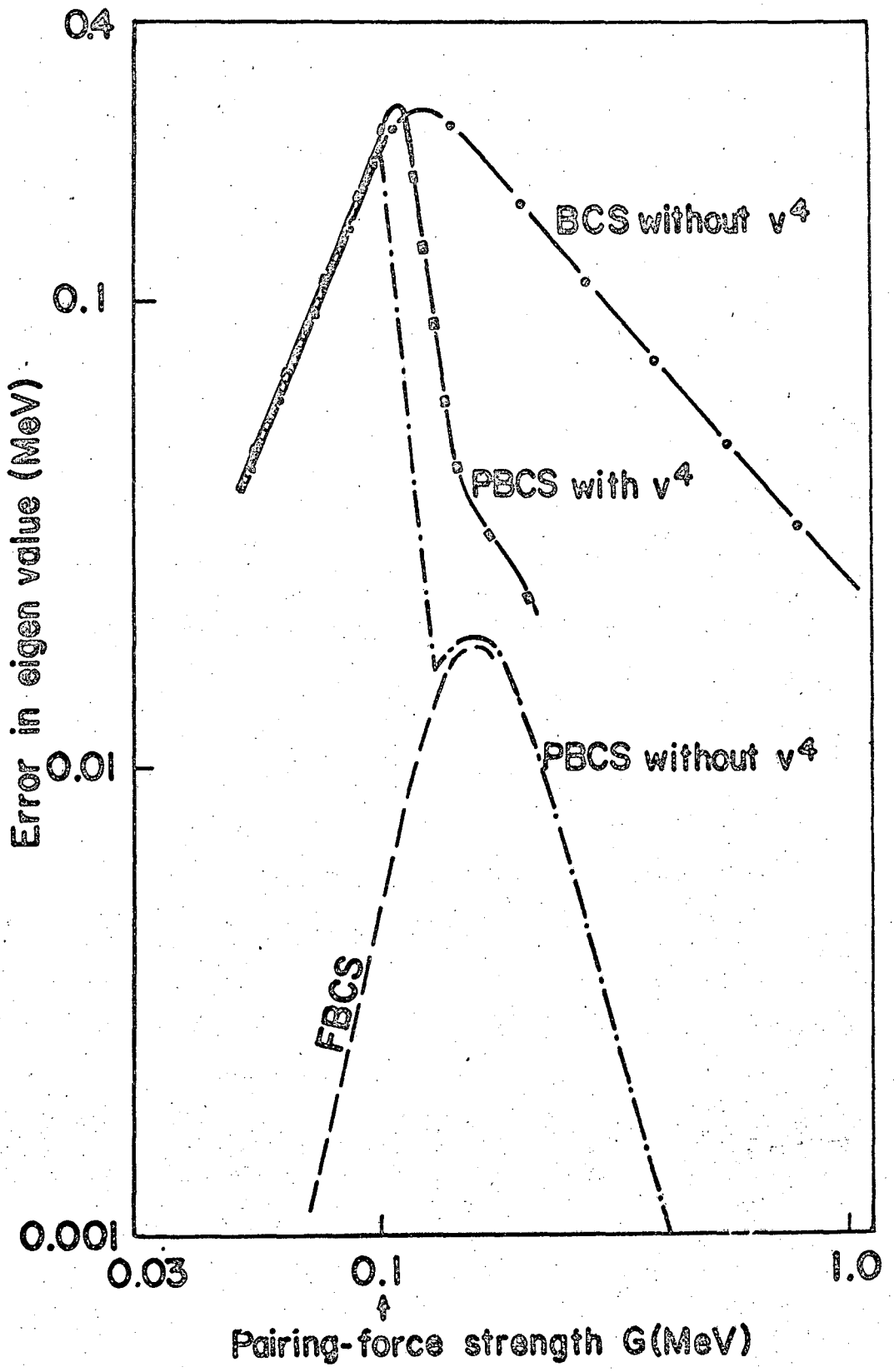
0.4
0.1
0.01
0.001
Error in eigen value (MeV)
BCS without v⁴
PBCS with v⁴
PBCS without v⁴
FBCS
0.03
0.1
1.0
Pairing-force strength G(MeV)

FIGURE 1.

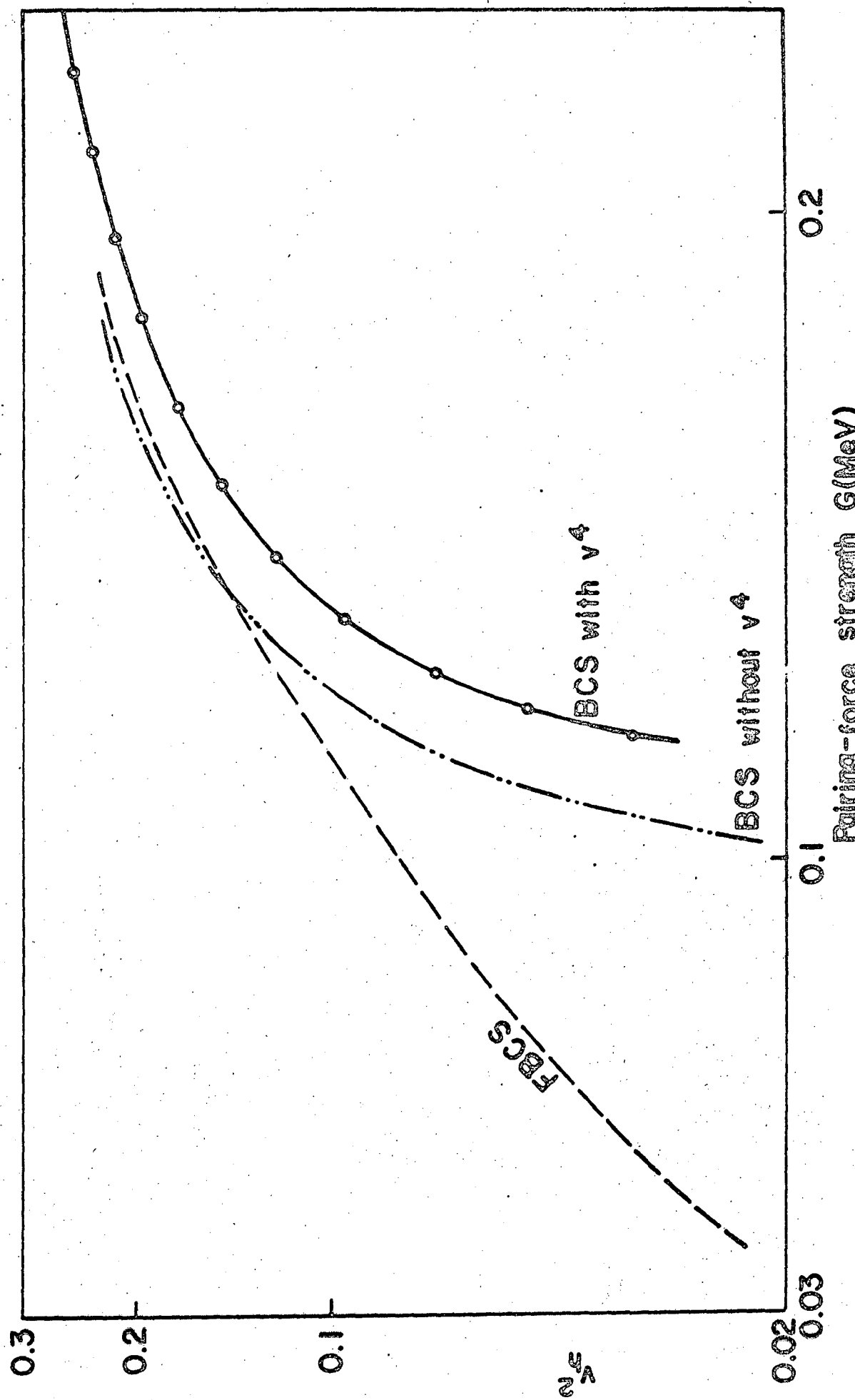
0.3
0.2
0.1
0.02
0.03
0.1
0.2
ν_Δ^2
Pairing-force strength G(MeV)
BCS with v^4
BCS without v^4
FBCS

FIGURE 2.

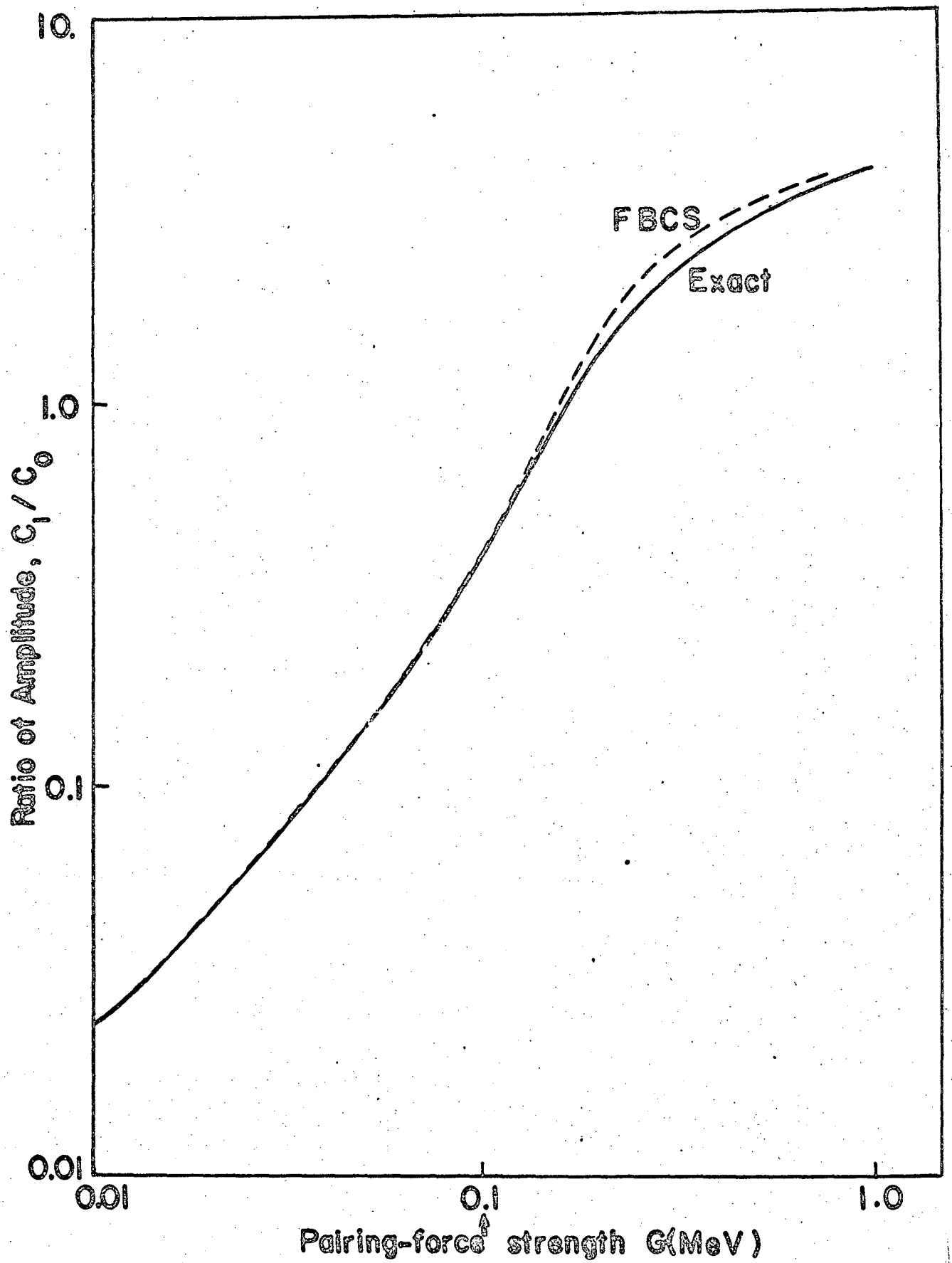
10.
1.0
0.1
0.01
0.01
0.1
1.0
Ratio of Amplitude, C_1 / C_0
FBCS
Exact
Pairing-force strength G(MeV)

FIGURE 3.

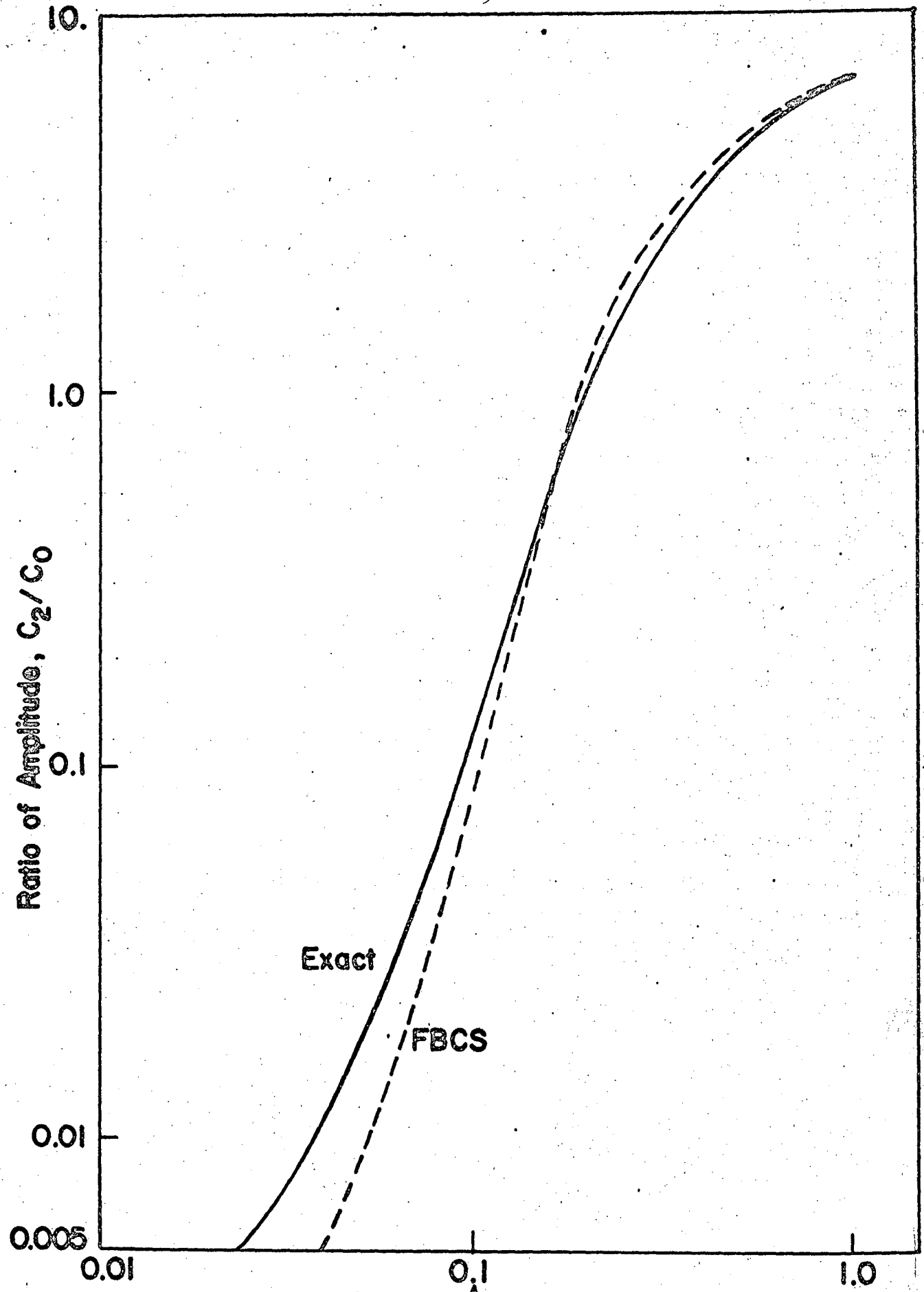
10.
1.0
0.1
0.01
0.005
0.01
0.1
1.0
Ratio of Amplitude, C_2/C_0
Exact
FBCS
Pairing-force strength G(MeV)

FIGURE 4.