

Model of a superconducting phase transition

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A model of a superconducting phase transition is studied in terms of two competing dynamical symmetry chains. It is shown that a sharp phase transition occurs in the limit of large-dimensional representations and that, for finite representations, the smoothed-out phase transitions can be understood clearly in analytical terms. It is also shown, both numerically and analytically, that the Mottelson approximation becomes exact for large-dimensional representations.

I. INTRODUCTION

An analysis of the detailed behavior of a system in the neighborhood of a phase transition poses interesting and challenging problems. A basic difficulty is that the system invariably undergoes a transition from one type of symmetry to another with the consequence that methods which work on one side of the transition point often break down at precisely the point of interest.

Many examples of phase transitions are to be found in both classical and quantal physics. Consider, for example, the small-amplitude normal-mode vibrations of a classical system about equilibrium and their behavior as some parameter in the Hamiltonian is varied. Situations arise where the frequency of one normal mode falls with increase in the value of the parameter and at some critical point vanishes. If the parameter is further increased one invariably finds that the normal-mode theory returns an imaginary, and hence unphysical, value for the frequency in question indicating that the assumed equilibrium configuration is no longer stable. Physically, one interprets the situation as corresponding to a decrease in the restoring force for small displacements in the associated normal mode until, at the critical point, the restoring force vanishes and the system moves to a new equilibrium configuration. Frequently the new equilibrium configuration has a different symmetry. If it has less symmetry, one can associate a *Goldstone boson* with the corresponding normal mode. Parallel situations are familiar in the quantum mechanics of many-body systems when the normal-modes are treated in the small-amplitude time-dependent Hartree-Fock approximation or, equivalently, in the *random-phase approximation*.

In this paper we examine a familiar model of a many-fermion system in which a phase transition from a normal to a superconducting state is induced by a change of the strength of a pairing interaction. We show exact numerically calculated results for this model in a form which reveals the particular features of the ground-state wave function that characterize the phase transition. We show, for example, that the essential ingredients of the phase transition are present in finite as well as infinite systems. A new approximation is introduced which admits simple analytical solutions to the model and enables one to predict all the results of the numerical calculations to a

high degree of accuracy. Comparisons of exact ground-state wave functions are also made with those obtained in the BCS approximation¹ and in the number-projection approximation of Mottelson.² The remarkable success of the latter is explained.

The analysis presented in this paper is directed specifically towards understanding pairing phenomena and the nature of superconductivity. It is also a preliminary exploration of the more general situation in which there are competing dynamical symmetries such that with a small change of some term in a Hamiltonian one can have a dramatic change in the character of the system. Changes in the Hamiltonian can be brought about in physical situations in many ways. For example, in looking at a sequence of nuclear isotopes or isobars, one often encounters sudden changes in their behavior over a small range. The changes at closed shells are familiar examples of this. Others are given by shape changes signaled by the onset of rotational bands. The competition between dynamical symmetries that reflect the dominance of pairing correlations, which favor spherical shapes, versus those characteristic of deformed rotational nuclei is an old and essentially unsolved problem. The analysis of this paper is thus a first study of some of the kinds of behaviors one can expect in the neighborhood of a phase transition.

II. THE MODEL

The model is a relatively realistic caricature of a situation that occurs in nuclear physics and other many-fermion systems in which, in the absence of residual interactions, one has an independent-particle Hamiltonian H_0 with a ground state described by a set of fully occupied single-particle levels below the Fermi surface and a set of empty single-particle levels above.

In this paper we consider, for simplicity, just two levels, one above and the other below the Fermi surface. The lower (occupied) level comprises a set of single-particle states labeled by an index m_1 spanning the range $m_1 = -j_1, \dots, +j_1$ in integer steps and the upper (unoccupied) level similarly comprises states with $m_2 = -j_2, \dots, +j_2$. The independent-particle Hamiltonian is then expressed

$$H_0 = \sum_{i=1}^2 \epsilon_i \sum_{m_i=-j_i}^{j_i} a_{j_i m_i}^\dagger a_{j_i m_i} \quad (1)$$

with $\epsilon_2 > \epsilon_1$. The ground state of the system is the state

$$|\phi_0\rangle = \prod_{m_1=-j_1}^{+j_1} a_{j_1 m_1}^\dagger |-\rangle, \quad (2)$$

where $|-\rangle$ is the bare particle vacuum state. Excited states are given by the states $a_{j_2 m_2}^\dagger a_{j_1 m_1} |\phi_0\rangle$ at excitation

energy $\epsilon_2 - \epsilon_1$, the states $a_{j_2 m_2}^\dagger a_{j_1 m_1} a_{j_2 m_2}^\dagger a_{j_1 m_1} |\phi_0\rangle$ at excitation energy $2(\epsilon_2 - \epsilon_1)$, etc.

One can interpret j_1 and j_2 as single-particle angular momenta or simply as labels each representing a set of angular-momentum states which, in the model, have been assigned common single-particle energies. For example, if level one comprises a set of single-particle states of angular momentum $j = \frac{3}{2}, \frac{5}{2},$ and $\frac{7}{2}$ then m would index $\sum(2j+1) = 18$ states and we would set $j_1 = \frac{17}{2}$. For simplicity we set $j_1 = j_2$ in the model.

The residual interaction is assumed to be of the pairing type

$$V = -G \sum_{\substack{k,l \\ m_k, m_l > 0}} a_{j_k m_k}^\dagger a_{j_k \bar{m}_k}^\dagger a_{j_l \bar{m}_l} a_{j_l m_l}, \quad (3)$$

where

$$a_{j \bar{m}}^\dagger = (-1)^{j+m} a_{j-m}^\dagger.$$

The eigenstates of the Hamiltonian

$$H = H_0 + V \quad (4)$$

are easily determined numerically and one finds that as the coupling constant G increases from zero, the ground state goes from the independent-particle (closed subshell) state to one in which both levels are equally occupied. The transition from one limit to the other is characterized by the ground-state pair correlation function

$$K = \left\langle \psi_0 \left| \sum_{\substack{k,l \\ m_k, m_l > 0}} a_{j_k m_k}^\dagger a_{j_k \bar{m}_k}^\dagger a_{j_l \bar{m}_l} a_{j_l m_l} \right| \psi_0 \right\rangle, \quad (5)$$

shown in units of $(2j+1)(2j+3)/4$ in Fig. 1 for two values of $j_1 = j_2 = j$ as a function of $\chi = G/G_{\text{crit}}$, where $G_{\text{crit}} = \epsilon/(2j+1)$. One notes that there is a rapid increase in the value of K with G in the neighborhood of G_{crit} and that the increase is much sharper for the larger value of j . The indications are that a sharp phase transition occurs at $G \approx G_{\text{crit}}$ in the limit $j \rightarrow \infty$. Our objective in this paper is to investigate the nature of this transition.

III. BCS AND MOTTELSON APPROXIMATIONS

The conventional interpretation of a superconducting phase transition is given in terms of the BCS approximation. The BCS ground state is a quasiparticle vacuum state, $|\rangle$, defined³⁻⁵ by the equation

$$a_{j_i m_i} |\rangle = 0, \quad i = 1, 2 \quad (6)$$

where

$$a_{j_i m_i}^\dagger = u_i a_{j_i m_i}^\dagger - v_i a_{j_i \bar{m}_i}, \quad i = 1, 2 \quad (7)$$

with

$$u_i^2 + v_i^2 = 1. \quad (8)$$

The parameters u_i and v_i are chosen to minimize the free energy $\langle |H - \lambda \hat{N}| \rangle$ of the quasiparticle vacuum state where

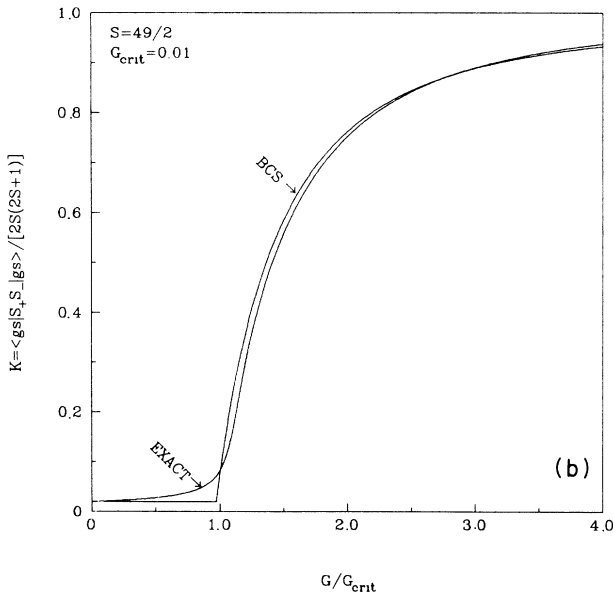
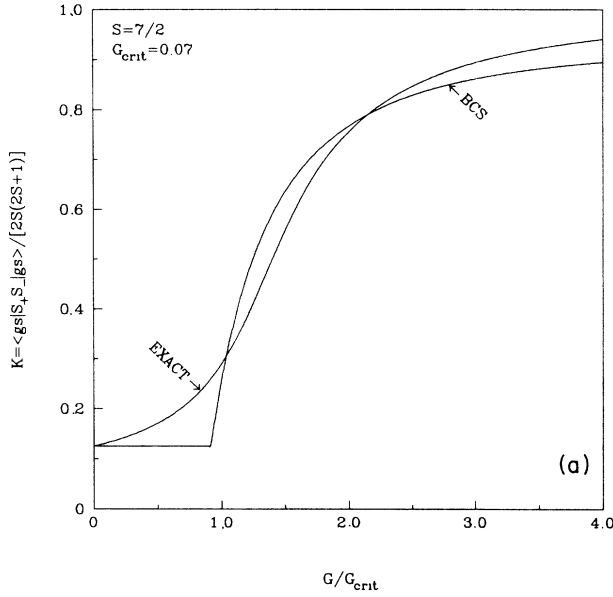


FIG. 1. The pair correlation function of Eq. (5) plotted as a function of G/G_{crit} for two values of $s = (2j+1)/4$ with $j_1 = j_2 = j$. The results for finite s are from exact numerical calculations and are seen to approach the BCS approximation as $s \rightarrow \infty$.

$$\hat{N} = \sum_{i, m_i} a_{j_i, m_i}^\dagger a_{j_i, m_i} \quad (9)$$

is the fermion number operator and λ , the chemical potential, is a Lagrange multiplier introduced to ensure that the mean fermion number

$$\langle |\hat{N}| \rangle = N \quad (10)$$

has the desired value (in our case $N = 2j + 1$).

The pair correlation functions for the BCS solutions are shown in comparison to those of the exact solutions in Fig. 1 and are seen to indicate sharp phase transitions for all (nonzero) values of j . The BCS predictions accurately reproduce the exact results for very large j . However, in the absence of exact results it would be hard to know if the phase transition predicted by the BCS approximation were genuine or an artifact of the variational constraint to quasiparticle vacuum states. Thus the BCS approximation is not very useful for explaining the nature of the rapid transition that takes place in finite systems. It also has the disconcerting property that it only conserves the fermion number of the system on average. Indeed, one easily shows that the quasiparticle vacuum (the BCS ground state) is given to within a normalization factor by

$$| \rangle = \exp \left[\sum_{i=1}^2 \frac{v_i}{u_i} \sum_{m_i} a_{j_i, m_i}^\dagger a_{j_i, \bar{m}_i} \right] | - \rangle \quad (11)$$

and has a distribution of fermion number values of width given by

$$\langle |(\hat{N} - N)^2| \rangle = 2 \sum_i (2j_i + 1) (u_i v_i)^2. \quad (12)$$

The component of the BCS ground state of particle number N is seen to be given by

$$|N\rangle = \frac{1}{(N/2)!} \left[\sum_{i=1}^2 \frac{v_i}{u_i} \sum_{m_i} a_{j_i, m_i}^\dagger a_{j_i, \bar{m}_i} \right]^{N/2} | - \rangle, \quad (13)$$

which is of the variational form of the approximate ground-state wave function proposed by Mottelson.² It is therefore of interest to compare the results of the best wave function of this form with those of exact calculations. The approximation (13) is known to be remarkably accurate even for more general situations. We find that the pair correlation function calculated for the best wave functions of the form (13) are indistinguishable from exact results on the scale of Fig. 1. Thus, in addition to understanding the nature of the phase transition at G_{crit} we would also like to understand why a wave function of the Mottelson type should be such a good approximation for the ground state.

IV. THE DYNAMICAL SYMMETRY OF THE PAIRING HAMILTONIAN

Before proceeding, it is useful to express the Hamiltonian in terms of its spectrum generating algebra in order to explicitly expose the nature of the dynamical symmetries involved. Following Kerman, Lawson, and Macfarlane,⁶ the Hamiltonian (4) is expressed in terms of

an $\text{su}(2)_1 \times \text{su}(2)_2$ quasispin algebra by means of the identification

$$\begin{aligned} S'_+ &= \sum_{m_i > 0} a_{j_i, m_i}^\dagger a_{j_i, \bar{m}_i} \\ S'_- &= \sum_{m_i > 0} a_{j_i, \bar{m}_i} a_{j_i, m_i} \\ S'_0 &= \frac{1}{2} \sum_{m_i > 0} (a_{j_i, m_i}^\dagger a_{j_i, m_i} - a_{j_i, \bar{m}_i}^\dagger a_{j_i, \bar{m}_i}). \end{aligned} \quad (14)$$

With $\lambda = \frac{1}{2}(\varepsilon_2 + \varepsilon_1)$ and $\varepsilon = \varepsilon_2 - \varepsilon_1$, the Hamiltonian $H' = H - \lambda \hat{N}$ is then expressed

$$H' = \varepsilon (S_0^2 - S_0^1) - GS_+ S_- , \quad (15)$$

where

$$S_+ = S_+^1 + S_+^2$$

is a summed quasispin operator. Since the eigenvalues of S_0^1 and S_0^2 span the respective ranges $-(2j_1 + 1)/4, \dots, (2j_1 + 1)/4$ and $-(2j_2 + 1)/4, \dots, (2j_2 + 1)/4$, the relevant representation of the $\text{su}(2)_1 \times \text{su}(2)_2$ algebra for the calculation of the ground state is the one with $s_1 = (2j_1 + 1)/4$ and $s_2 = (2j_2 + 1)/4$. In this paper, we restrict consideration primarily to the states of this representation, all of which one notes have angular momentum $J = 0$. We refer to these states as states of maximum $\text{su}(2)_1 \times \text{su}(2)_2$ symmetry. Excited $J = 0$ states of maximal symmetry are sometimes referred to as *broken pair* states (cf. Ref. 7 and references therein). They are also described as *pairing vibrational* states.^{8,9}

In the $G = 0$ limit, the ground state of the system is the state $|s_1, m_1 = s_1; s_2, m_2 = -s_2\rangle$, where the quantum numbers are those of the subalgebra chain

$$\text{su}(2)_1 \times \text{su}(2)_2 \supset u(1)_{s_1} \times u(1)_{s_2} . \quad (16)$$

On the other hand, when $\varepsilon = 0$, the eigenstates have good coupled quasispin and reduce the subalgebra chain

$$\text{su}(2)_1 \times \text{su}(2)_2 \supset \text{su}(2) \supset u(1) , \quad (17)$$

where the intermediate $\text{su}(2)$ algebra is spanned by the sum quasiparticle operators

$$S_0 = S_0^1 + S_0^2, \quad S_\pm = S_\pm^1 + S_\pm^2 . \quad (18)$$

The ground state is then the state $|s_1, s_2; S = s_1 + s_2, M = s_1 - s_2\rangle$. Thus the system has two limiting dynamical symmetry chains reminiscent of the *LS* versus *jj* coupling symmetry limits of fermion wave functions which can be discussed in much the same language.

Now, as the ratio G/ε increases from zero to a large value, one would expect a transition to occur from a ground state of $u(1)_1 \times u(1)_2$ symmetry to one of $\text{su}(2) \supset u(1)$ symmetry. However, it is clear from Fig. 1 that, for finite $s_1 = s_2 = (2j + 1)/4$, the pair correlation function changes continuously, even if rapidly, in the neighborhood of $G \sim G_{\text{crit}}$. Thus the system does not jump discontinuously from one symmetry extreme to the other, even for large spin values. Our problem then is to

understand why the first derivative dK/dG of the pair correlation function

$$K = \langle \psi_0 | S_+ S_- | \psi_0 \rangle$$

becomes discontinuous at G_{crit} as $s = s_1 = s_2 \rightarrow \infty$.

V. NUMERICAL SOLUTION

To understand what is happening, we consider the diagonalization of the Hamiltonian H' in the uncoupled basis

$$|m\rangle = |s_1 = s, m_1 = m; s_2 = s, m_2 = -m\rangle,$$

$$m = -s, \dots, +s$$

for the subspace of states of maximal $\text{su}(2)_1 \times \text{su}(2)_2$ symmetry. The eigenvectors of H' are then expanded

$$|\psi\rangle = \sum_m C_m |m\rangle. \quad (19)$$

From the well-known matrix elements of the $\text{su}(2)$ algebra

$$\langle s_1 m_1 \pm 1 | S_{\pm}^1 | s_1 m_1 \rangle = \sqrt{(s_1 \mp m_1)(s_1 \pm m_1 + 1)},$$

$$\langle s_1 m_1 | S_0^1 | s_1 m_1 \rangle = m_1,$$

one then easily determines that

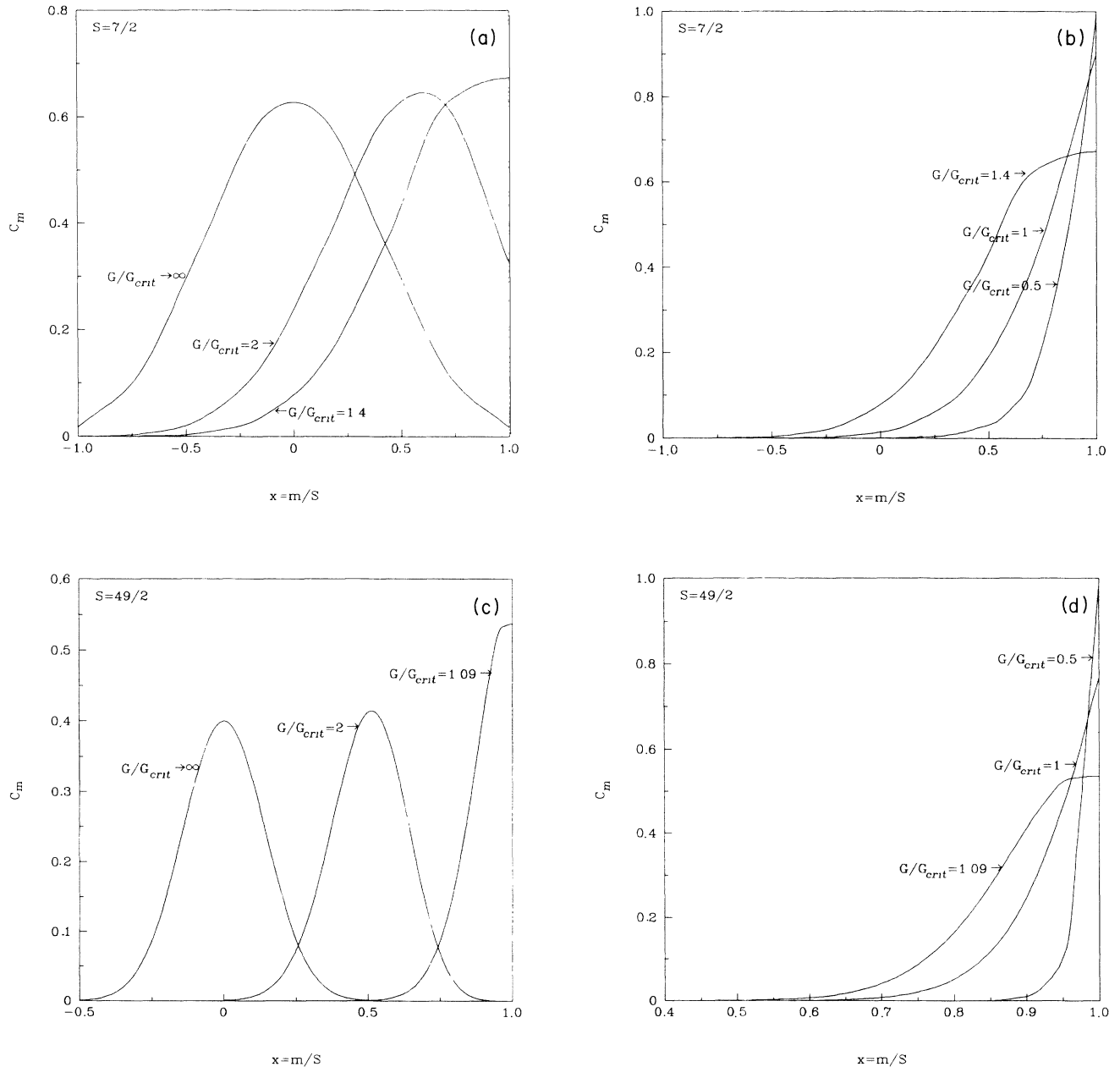


FIG. 2. The wave functions $\psi(x) = C_{m,x} = m/s$ for different $\chi = G/G_{\text{crit}}$ obtained by exact numerical calculations for $s = \frac{7}{2}$ and $s = \frac{49}{2}$. The results for $\chi \approx 1$ are shown on an enlarged scale.

$$\begin{aligned} \langle m | H' | \psi \rangle = & -[2\epsilon m + 2Gs(s+1) - 2Gm^2]C_m \\ & -G[s(s+1) - m(m-1)]C_{m-1} \\ & -G[s(s+1) - m(m+1)]C_{m+1}. \end{aligned} \quad (20)$$

The eigenvalue equations are therefore easily solved numerically.

The expansion coefficients C_m are shown for the ground state for different values of $\chi = G/G_{\text{crit}}$ and for two values of s in Fig. 2. However, in order that results for different values of s can be meaningfully compared, it is convenient to plot C_m as a function of $x = m/s$ and to define

$$\psi(x) = C_m. \quad (21)$$

Then x takes discrete values over the common range of points $-1 \leq x \leq +1$ which simply get closer together as s becomes larger.

A few features of the ground-state solutions are particularly noteworthy. The first is that for G/G_{crit} large, the wave function $\psi(x)$ closely resembles a Gaussian with a width that becomes narrow for large values of the quasi-spin s . The second feature is that for $G/G_{\text{crit}} \approx 1$ the peak of the wave function is at the $x = 1$ boundary so that only half of the Gaussian appears. Finally, in the $G/G_{\text{crit}} = 0$ limit, the wave function becomes a delta function at $x = 1$.

Thus it becomes clear what is going on. For $G < G_{\text{crit}}$ the dominant component of the ground state is the independent-particle $m = s$ ($x = 1$) state and the admixtures of the small $m < s$ components rapidly fall off with decreasing m . The character of the ground state for $G < G_{\text{crit}}$ is therefore that of an independent-particle state with pairing correlations. The magnitude of the pair correlation function increases slowly with G/G_{crit} until

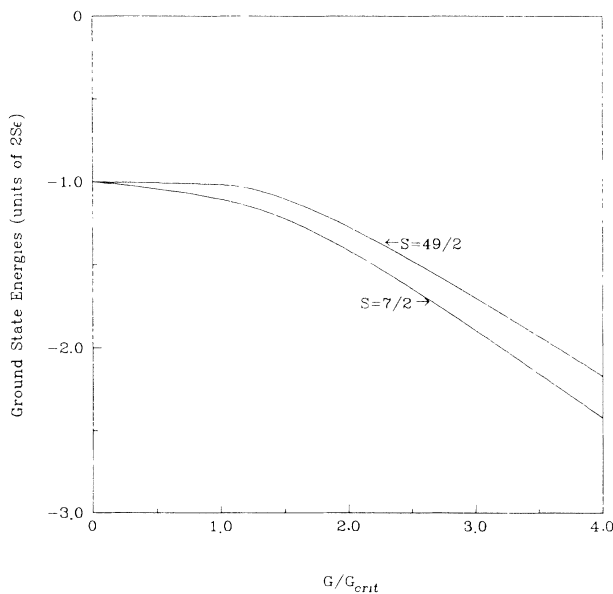


FIG. 3. The ground-state energy in units of $2s\epsilon$ for $s = \frac{7}{2}$ and $\frac{49}{2}$.

at $G/G_{\text{crit}} \approx 1$ the wave packet starts to break away from the $x = 1$ wall and a very rapid rate of increase sets in. For $G/G_{\text{crit}} \gg 1$ and sufficiently large s the wave function becomes detached from the wall and acquires a full Gaussian shape. As G/G_{crit} is further increased, its centroid simply moves to smaller values of x and approaches $x = 0$ in the $G/G_{\text{crit}} \rightarrow \infty$ limit. But, in the process, its shape remains essentially unchanged once it has broken free from the wall.

One also sees clearly from the analysis why, for $G < G_{\text{crit}}$, a perturbative expansion of the ground state starting from the independent-particle ground state as unperturbed state will converge reasonably rapidly whereas for $G > G_{\text{crit}}$ it will not. Indeed, for large values

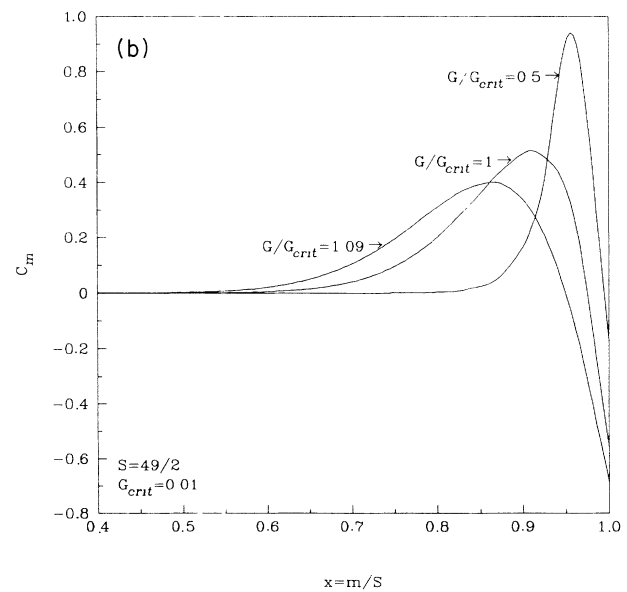
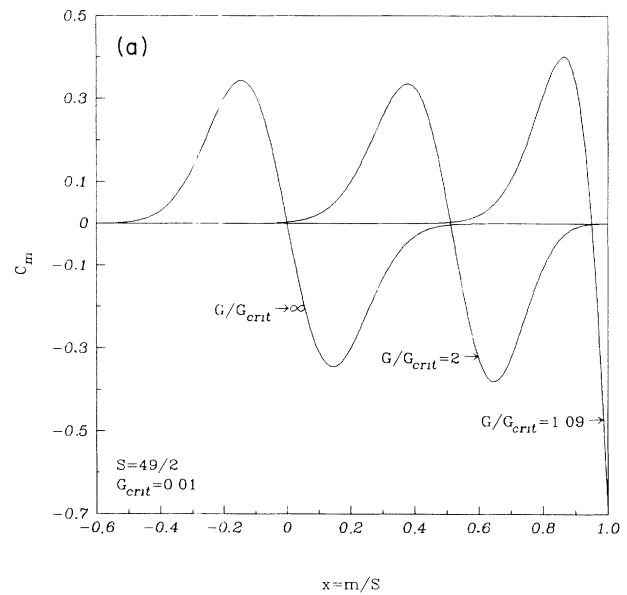


FIG. 4. Wave functions for the first excited state calculated numerically.

of s and $G \gg G_{\text{crit}}$, the independent-particle ground state is a negligibly small component of the correlated ground state. Interestingly enough, the results suggest that a perturbative expansion about an excited independent-particle state, with $|m\rangle$ given by the centroid of the Gaussian wave packet, might possibly converge.

The ground-state energy of the Hamiltonian H' is shown in units of $2s\varepsilon$ for two values of s in Fig. 3. One sees that as $s \rightarrow \infty$ the ground-state energy approaches a constant value of $-2s\varepsilon$ for $G < G_{\text{crit}}$ and that it asymptotically approaches the line $E_0 = -G/2G_{\text{crit}}$ as $G \rightarrow \infty$. For all values of s the ground-state energy E_0 and its derivative dE_0/dG are continuous. However, the second derivative d^2E_0/dG^2 becomes discontinuous at $G = G_{\text{crit}}$

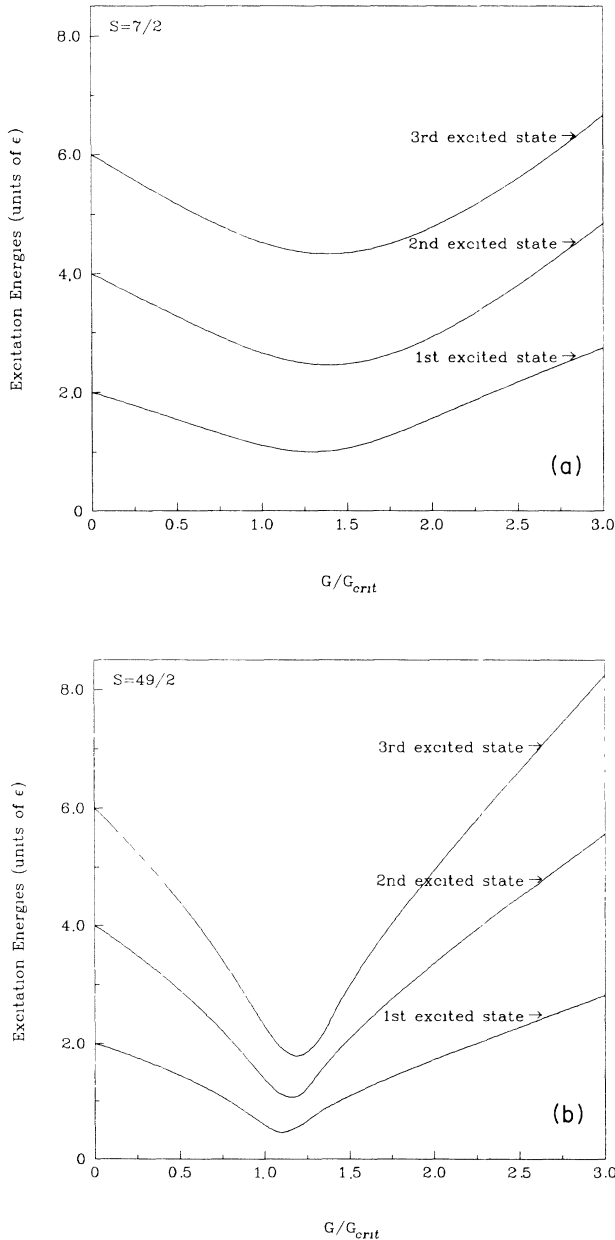


FIG. 5. Excited-state energies for $J=0$ (pairing-vibrational) states of maximal $\text{su}(2)_1 \times \text{su}(2)_2$ symmetry in units of ε .

at the $s \rightarrow \infty$ limit.

The wave functions of the first excited $J=0$ (pairing vibrational) states of maximal $\text{su}(2)_1 \times \text{su}(2)_2$ symmetry are shown for $s = \frac{49}{2}$ and several values of χ in Fig. 4. Like the ground-state wave functions the first excited-state wave functions closely resemble harmonic-oscillator wave functions for sufficiently large χ .

The excitation energies at the first few excited $J=0$ states of maximal symmetry are plotted in Fig. 5 in units of ε . One sees that the spectrum is harmonic with $\Delta E_v = v\Delta E_1$ and that $d\Delta E_v/dG$ becomes discontinuous at $G = G_{\text{crit}}$ in the $s \rightarrow \infty$ limit.

VI. ANALYTICAL SOLUTION

The eigenvectors of H' are easily determined when $\varepsilon=0$. In particular, the ground state is then the state of maximum coupled quasi-spin $S=2s$ with S_0 component $M_s=0$. The corresponding eigenvalue of $-GS_+S_-$ has value $-2Gs(2s+1)$ and the coefficients of the wave function are the Clebsch-Gordan coefficients

$$C_m = (sm, s-m | 2s0) = \frac{1}{\sqrt{(4s)!}} \frac{(2s)!(2s)!}{(s+m)!(s-m)!}. \quad (22)$$

These coefficients can also be obtained by solving the eigenvector equation for H' as a recursion relation for C_m . As shown below, cf. Eq. (32), the Clebsch-Gordan coefficient (22) has the asymptotic form of a Gaussian, i.e., $C_m \sim Ce^{-m^2/s}$ as $s \rightarrow \infty$, consistent with the numerically computed result for $\psi(x=m/s) = C_m$ for $\chi \rightarrow \infty$ shown in Fig. 2.

When $\varepsilon \neq 0$, $\psi(x)$ is an eigenfunction of the Hamiltonian

$$H' = -GS_+S_- - 2sx\varepsilon$$

and one sees that the second term is simply a constraining field that has the effect of displacing the wave function in the positive x direction. Thus one is not surprised to see numerically computed wave functions that for sufficiently large s and small ε are given to a good approximation by

$$\psi'(x) \approx \psi(x-a)$$

for some suitable value of a .

To understand better the numerically calculated results, it is helpful to express the eigenvalue equation as a differential equation by defining

$$\mathcal{H}\psi(x) = \langle m | H' | \psi \rangle = \langle sx | H' | \psi \rangle.$$

Expanding

$$C_{m\pm 1} = \psi \left[x + \frac{1}{s} \right] = \psi(x) \pm \frac{1}{s} \frac{d\psi}{dx} + \frac{1}{2s^2} \frac{d^2\psi}{dx^2} + \dots,$$

we immediately get

$$\mathcal{H} = -2sx\varepsilon - 4Gs(s+1)$$

$$+ G \left[4s^2x^2 + 2x \frac{d}{dx} - \frac{s+1}{s} \frac{d^2}{dx^2} + x^2 \frac{d^2}{dx^2} \right] + \dots \quad (23)$$

Making the substitution

$$x = \frac{1}{2\sqrt{s}}(b + b^\dagger),$$

$$\frac{d}{dx} = \sqrt{s}(b - b^\dagger),$$

we obtain

$$\begin{aligned} \mathcal{H} = & -4Gs(s+1) - \sqrt{s}\varepsilon(b + b^\dagger) + 2Gs(b^\dagger b + bb^\dagger) \\ & + G[(b + b^\dagger)(b - b^\dagger) + (b - b^\dagger)(b + b^\dagger) \\ & + \frac{1}{4}(b + b^\dagger)^2(b - b^\dagger)^2] + \dots \end{aligned}$$

Then, for large s , we may neglect the higher-order terms in the $1/s$ expansion and keep only

$$\mathcal{H} = -4Gs(s+1) - \sqrt{s}\varepsilon(b + b^\dagger) + 2Gs(b^\dagger b + bb^\dagger). \quad (24)$$

The ground-state wave function for this Hamiltonian is given to within a normalization factor by

$$\psi_0(x) = \exp[-s(x-a)^2] \quad (25)$$

with $a = \varepsilon/4Gs$. We conclude that, for large s , the wave packet should be a Gaussian of width $1/\sqrt{2s}$ with centroid at $x = a$. Recall, however, that x is restricted to the domain $-1 \leq x \leq +1$. Moreover, the full wave packet (25) lies within this domain provided $s(1-a^2) \gg 1$. This condition is clearly satisfied for large s when $G \gg G_{\text{crit}}$, where

$$G_{\text{crit}} = \frac{\varepsilon}{4s}. \quad (26)$$

But, when G approaches G_{crit} from above, we see that the centroid of the wave packet approaches the $x = 1$ boundary. The wave function has a sharp cutoff at $x = 1$ and it is not surprising, therefore, that its properties should undergo a rapid change as $G \rightarrow G_{\text{crit}}$.

For $G > G_{\text{crit}}$ and large s , we can use the above wave packet to obtain the ground-state pair correlation function

$$K = \frac{\langle \psi_0 | S_+ S_- | \psi_0 \rangle}{2s(2s+1)} = 1 - \frac{2s}{2s+1} \left[\frac{G_{\text{crit}}}{G} \right]^2. \quad (27)$$

However, we note that because of the cutoff of the wave function for $x > 1$, K is bounded from below by $K_{\text{min}} = 1/(2s+1)$. Therefore, in the $s \rightarrow \infty$ limit, we predict

$$K = \begin{cases} 1 - (G_{\text{crit}}/G)^2 & \text{for } G > G_{\text{crit}} \\ 0 & \text{for } G < G_{\text{crit}} \end{cases} \quad (28)$$

in full accord with the numerically computed results shown in Fig. 1.

We also obtain from the analysis a prediction of excited-state wave functions given by (displaced) harmonic-oscillator wave functions and having excitation energies of $4Gs\nu$ where ν is a positive integer. These predictions are in good qualitative accord with the exact numerically computed results, shown Figs. 4 and 5, when s is large and $G \gg G_{\text{crit}}$.

VII. THE MOTTELSON GROUND-STATE WAVE FUNCTION

We now consider why a wave function of the Mottelson form (13) should be such a good approximation for the ground state. This wave function can be expressed, to within a normalization factor,

$$(S_+^1 + \beta S_+^2)^{2s} | - \rangle = k \left[1 + \beta \frac{S_+^2}{S_+^1} \right]^{2s} |s\rangle,$$

where $|s\rangle$ is the independent-particle closed-shell state

$$k|s\rangle = (S_+^1)^{2s} | - \rangle.$$

The utility of this expression is seen by writing

$$\begin{aligned} |m\rangle &= \frac{1}{\sqrt{(s-m+1)(s+m)}} \\ &\times S_+^1 |s_1=s, m_1=m-1; s_2=s, m_2=-m\rangle, \end{aligned}$$

whence one determines that

$$\frac{S_+^2}{S_+^1} |m\rangle = |m-1\rangle \quad \text{for } m > -s.$$

One then immediately finds that

$$(S_+^1 + \beta S_+^2)^{2s} | - \rangle = \sum_m \frac{(2s)!}{(s+m)!(s-m)!} \beta^{s-m} |m\rangle. \quad (29)$$

Now, in the $G \rightarrow \infty$ limit, this wave function approaches the exact $\beta = 1$ state

$$(S_+)^{2s} | - \rangle = \sum_m \frac{(2s)!}{(s+m)!(s-m)!} |m\rangle.$$

Comparison with the analytical solution (25) for $a = 0$, which is also exact for $G \rightarrow \infty$ and $s \rightarrow \infty$, then gives the large s asymptotic expression

$$\frac{(2s)!}{(s+m)!(s-m)!} \sim e^s e^{-m^2/s}. \quad (30)$$

It follows that

$$(S_+^1 + \beta S_+^2)^{2s} | - \rangle \sim \sum_m e^s e^{-m^2/s} \beta^{s-m} |m\rangle.$$

Therefore, setting $\beta = e^{-2a}$, we obtain

$$\begin{aligned} (S_+^1 + \beta S_+^2)^{2s} | - \rangle &\sim \exp[s(1-a)^2] \\ &\times \sum_m \exp[-(m-sa)^2/s] |m\rangle \end{aligned} \quad (31)$$

which, to within a normalization factor, is precisely the analytical solution (25) for large s . It follows that the Mottelson approximation is exact for the two-level problem in the large s limit. One also knows that it is exact, for arbitrary s , in the two limits when $G/\varepsilon = 0$ and $G/\varepsilon \rightarrow \infty$, for which it corresponds to the two exact dynamical symmetry chains (16) and (17). Thus, one understands why it should give such excellent results in general and provide a smooth interpolation between the various limiting cases.

As an aside, we note that Eq. (30) implies the interesting and possibly useful asymptotic expression for the

SU(2) Clebsch-Gordan coefficients (22),

$$(sm, s-m|2s0) \sim \frac{(2s)!}{\sqrt{(4s)!}} \exp[(s^2 - m^2)/s] \quad (32)$$

for large s .

Since the Mottelson wave function in this example is a function of a single variational parameter β and since it gives results that accurately approximate exact numerically computed results, it is of interest to plot the ground-state energy as a function of β . The Mottelson and, for comparison, the BCS ground-state energies $E_0(\beta)$ are plotted for $s = \frac{49}{2}$ in Fig. 6, where, in the BCS approximation, $\beta = \beta_2/\beta_1$ and $\beta_i = v_i/u_i$. On the small-

scale plot, the two energy functions are barely distinguishable. However, important differences can be seen for small values of β in the enlarged figure. In the Mottelson approximation, the derivative $dE_0(\beta)/d\beta$ vanishes at $\beta=0$ when $G=0$ and is negative whenever $G > 0$. Consequently, for finite s , the Mottelson energy function $E_0(\beta)$ always has a minimum at some positive value of β for any $G > 0$. The energy minima are marked with crosses in Fig. 6. Conversely, in the BCS approximation, $dE_0(\beta)/d\beta$ is positive at $\beta=0$ for all $G < G_{\text{crit}}$ and vanishes for $G = G_{\text{crit}}$. Consequently, in the BCS approximation, $E_0(\beta)$ always has a minimum at $\beta=0$ for $G \leq G_{\text{crit}}$ and at $\beta > 0$ for $G > G_{\text{crit}}$.

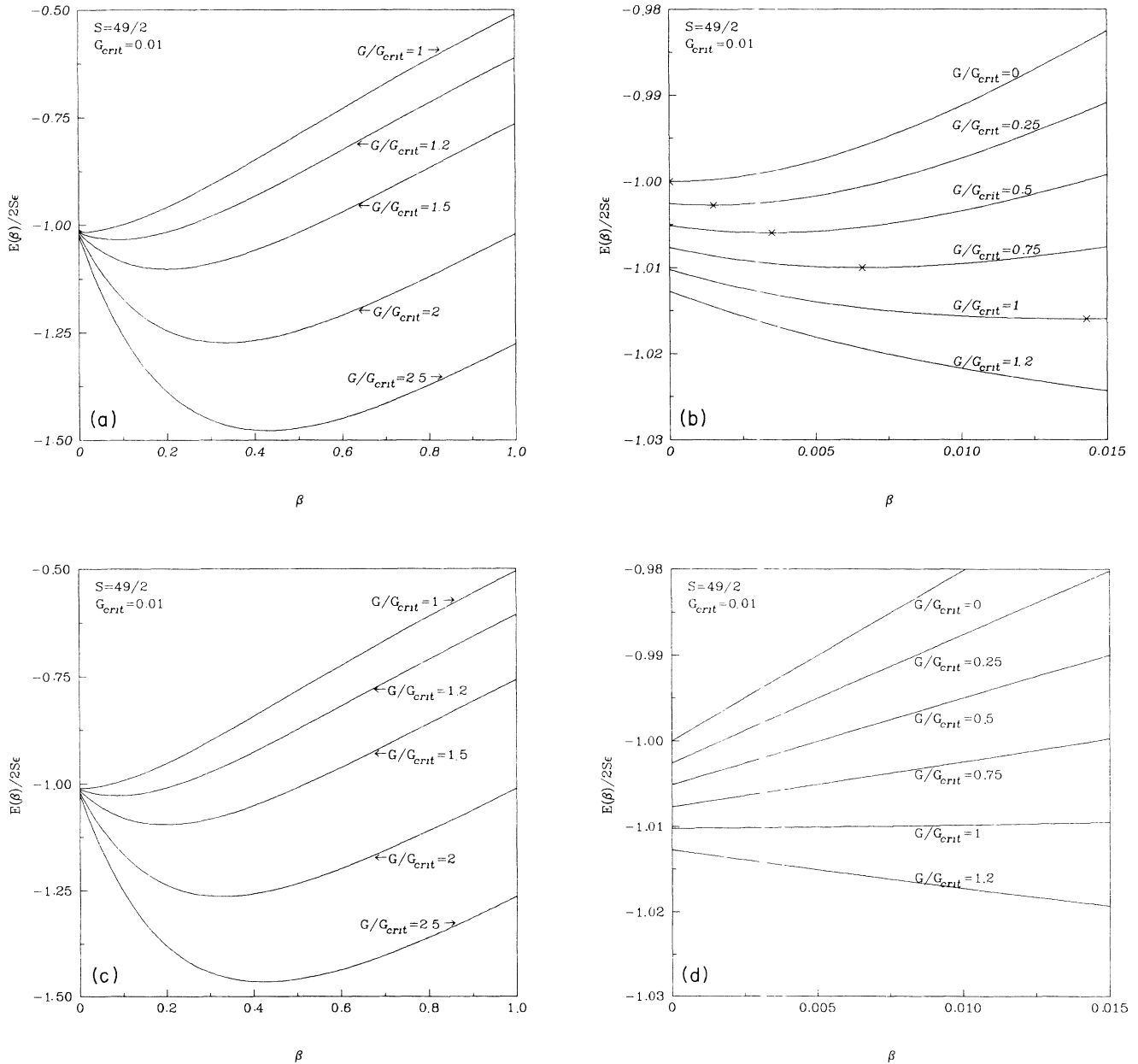


FIG. 6. The ground-state energy as a function of β for different values of G/G_{crit} . (a) and (b) are for Mottelson wave functions and (c) and (d) are for BCS variational wave functions. (b) and (d), respectively, contain the same information as (a) and (c) for small values of β but in more detail.

VIII. CONCLUDING REMARKS

In the above analysis, we have concentrated on the properties of the $J=0$ states belonging to the representation of the $su(2)_1 \times su(2)_2$ dynamical symmetry algebra having the maximal values $s_1=(2j+1)/4$ and $s_2=(2j-1)/4$ of the quasispin. This is appropriate because, as one can easily ascertain, the ground state belongs to this representation. Excited $J=0$ states of maximal symmetry are sometimes referred to as *broken pair states* (cf. Ref. 7 and references therein). These states are pairing-vibrational excitations in the terminology of Bohr⁸ and Bes and Broglia.⁹ Pairing-vibrational excitations of this kind were first considered, to our knowledge, by Högaasen-Feldman.¹⁰

Other representations obviously feature in the spectrum and are of essential importance for the consideration of excited states. In particular, the lowest $J \neq 0$ excited states belong to the representation with quasispins $s_1=(2j-1)/4$ and $s_2=(2j-1)/4$. An exact solution of the pairing Hamiltonian for these and other states in the multiple quasi-spin formalism presents no problems and has been studied on previous occasions in a variety of approximations.¹¹ The energies of the first excited $J=0$ pairing-vibrational state and $J \neq 0$ states are shown as functions of χ for $s = \frac{7}{2}$ and $\frac{49}{2}$ in Fig. 7.

Two features of the figure are noteworthy. First, observe that the excitation energy of the lowest $J \neq 0$ states increases slowly for $G < G_{\text{crit}}$ and rapidly for $G > G_{\text{crit}}$. These states are described as two quasiparticle states in the BCS theory and the rapid increase in their excitation energies with G for $G > G_{\text{crit}}$ is associated with a rapidly increasing gap parameter. Second, observe that the energy of the $J=0$ pairing-vibrational excitation falls rapidly with energy and approaches zero excitation energy in the $s \rightarrow \infty$ limit. After the phase transition its character changes and it increases rapidly. In the language of the random-phase approximation (RPA) and quasiparticle RPA one says that the ground state becomes unstable against pairing vibrations with increasing G and becomes superconducting at $G = G_{\text{crit}}$. For $G > G_{\text{crit}}$ the excited $J=0$ state starts to behave like a two-quasiparticle state. An analysis of excited states within the framework of the RPA has been given by Heiss *et al.*¹¹

In conclusion, we recall that one of our primary motivations in this analysis was to study a prototype of a phase transition in a system with competing dynamical symmetry chains. Unfortunately, it remains unclear to us what aspects of the model we have investigated will be shared with other models. To find out, it would be instructive to make similar analyses of other models. In particular, it would be interesting to determine if such systems, presumably in the limit of large-dimensional representations, generally feature sharp phase transitions in proceeding from one symmetry chain to another. This is a very fundamental question to which we are unaware that the answer is presently known.

Several models with competing dynamical subalgebra chains are known. For example, the interacting boson model¹² with its $u(6)$ dynamical symmetry algebra and three subalgebra chains

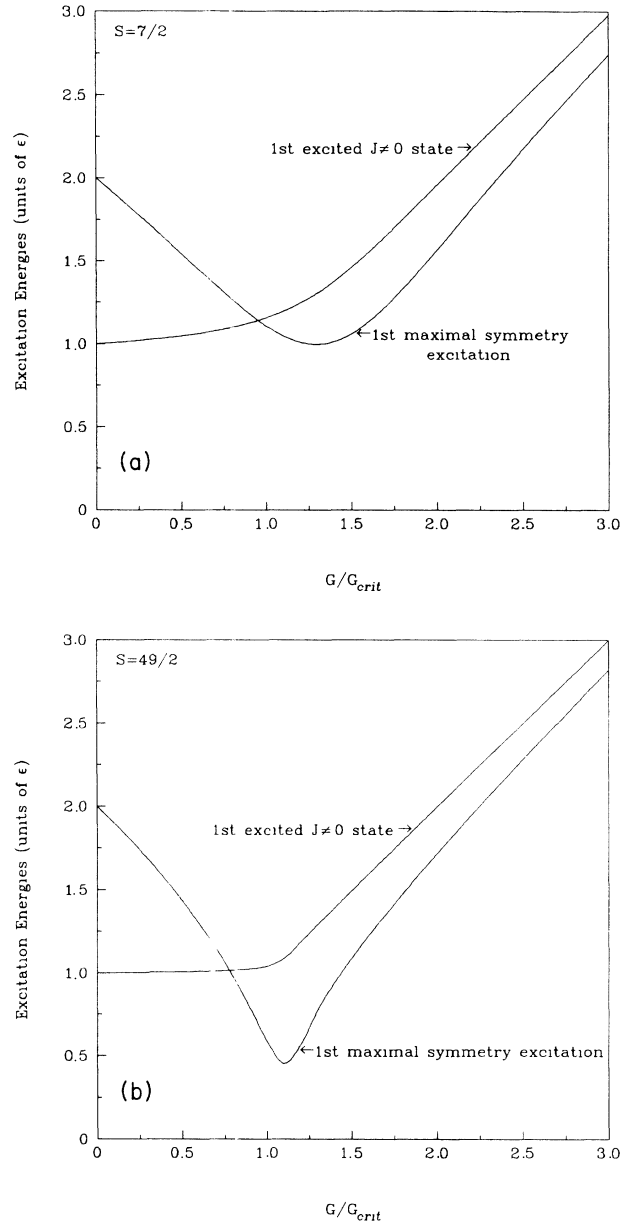


FIG. 7. The energies of the first excited $J=0$ and $J \neq 0$ states for $s = \frac{7}{2}$ and $\frac{49}{2}$ as a function of G/G_{crit} .

$$u(6) \supset su(3) \supset so(3),$$

$$u(6) \subset u(5) \subset so(3),$$

$$u(6) \supset o(6) \supset so(3),$$

provides a range of possibilities. Another example is provided by the competing $su(3)$ (Ref. 13) versus quasispin⁶ subalgebra chains of the harmonic-oscillator shell model. Such a study could be important for understanding the competition between quadrupole and pairing correlations and the corresponding phase transitions between deformed (rotational) and superconducting nuclei.

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