Test of the Bardeen-Cooper-Schrieffer and the resonant-valence-bond wave functions as solutions of the Hubbard model: A small-cluster calculation

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With the purpose of assessing the validity of commonly used approximations, best variational solutions are calculated for a four-site (tetrahedral-cluster) Hubbard model with periodic boundary conditions and compared with exact results. In particular, the optimum number-conserving Bardeen-Cooper-Schrieffer-type variational solution is obtained for two, four, and six electrons, and the optimal resonating-valence-bond state for four electrons. For an attractive interaction U, the exact ground state of the system is obtained in all four cases. If the interaction U is repulsive, the exact ground state is obtained only when the cluster contains two and six electrons. For four electrons the BCS approximation is only satisfactory for relatively small U. For any positive U the resonating-valence-bond state on the other hand, gives very good (albeit not exact) energies for the ground state.

I. INTRODUCTION

With the arrival of high-T_c superconductivity and the growing interest in systems of highly correlated electrons, many theories have been proposed where the dominant effects can be explained by assuming approximate solutions of the Hubbard model[1–7] in a variety of two- and three-dimensional periodic lattices. These approximate solutions are, in turn, variances of two basic models: the Bardeen-Cooper-Schrieffer (BCS) variational-type[8] state function and the resonating-valence-bond (RVB) model.[2,9] The object of this contribution is to test these proposals in a small system where both the ground-state energy and the optimization associated with the approximate solutions can be carried out exactly.

In the case of a four-site tetrahedral cluster with periodic boundary conditions the complete spectrum of eigenvalues and eigenvectors has been obtained analytically;[6] it can be shown[7] that this small cluster is equivalent to an infinite face-centered-cubic (fcc) lattice if the Brillouin-zone sampling is restricted to four points in reciprocal space: the zone center Γ and the center points X of the three square faces.

The Hubbard model in the infinite fcc lattice is defined by the Hamiltonian

$$H=-t\sum_{i\delta\sigma}c^{\dagger}_{i\sigma}c_{(i+\delta)\sigma}+U\sum_{i}c^{\dagger}_{i\uparrow}c_{i\uparrow}c^{\dagger}_{i\downarrow}c_{i\downarrow}$$
$$=\sum_{\mathbf{k}\sigma}\epsilon_{\mathbf{k}}\,a^{\dagger}_{\mathbf{k}\sigma}a_{\mathbf{k}\sigma}+(U/N)\sum_{\mathbf{k}\mathbf{k}'\mathbf{q}}a^{\dagger}_{\mathbf{k}+\mathbf{q}\uparrow}a^{\dagger}_{\mathbf{k}'\downarrow}a_{\mathbf{k}'+\mathbf{q}\downarrow}a_{\mathbf{k}\uparrow}\ , \tag{1}$$

where

$$\epsilon_{\mathbf{k}}=-t\sum_{\delta}e^{i\mathbf{k}\cdot\delta}\ . \tag{2}$$

In Eq. (1), $c_{i\sigma}$ ($c^{\dagger}_{i\sigma}$) is the annihilation (creation) operator for an electron in a fully symmetric orbital, with spin $\sigma=\uparrow,\downarrow$, located at site i in the lattice. The first term is a one-electron band energy, i.e., the "hopping" between site i and its 12 nearest neighbors ($i+\delta$). The second term is the intrasite two-particle term, where U is the on-site interaction parameter; both cases $U>0$ and $U<0$ are considered here. In addition $a_{\mathbf{k}\sigma}$ ($a^{\dagger}_{\mathbf{k}\sigma}$) is the annihilation (creation) operator for an electron in the Bloch $\mathbf{k}$ state, with spin σ, and N is the number of sites in the lattice ($N\to\infty$). The vectors $\boldsymbol{\delta}$ connect each lattice site to its 12 nearest neighbors.

The small-cluster approach considers only a finite, small number n of lattice sites ($n=4$ here) but conserves periodic boundary conditions and the correct number of nearest neighbors. Therefore (1) reduces to

$$H=-4\,t\sum_{\langle ij\rangle\sigma}c^{\dagger}_{i\sigma}c_{j\sigma}+U\sum_{i}c^{\dagger}_{i\uparrow}c_{i\uparrow}c^{\dagger}_{i\downarrow}c_{i\downarrow}$$
$$=\sum_{\mathbf{k}\sigma}\epsilon_{\mathbf{k}}\,a^{\dagger}_{\mathbf{k}\sigma}a_{\mathbf{k}\sigma}+(U/4)\sum_{\mathbf{k}\mathbf{k}'\mathbf{q}}a^{\dagger}_{\mathbf{k}+\mathbf{q}\uparrow}a^{\dagger}_{\mathbf{k}'\downarrow}a_{\mathbf{k}'+\mathbf{q}\downarrow}a_{\mathbf{k}\uparrow}\ . \tag{3}$$

where now the subscripts $i,j=0,1,2,3$ are restricted to the four lattice sites of the small cluster,

$$\mathbf{r}_0=0\ ,$$
$$\mathbf{r}_1=(a/2)(\hat{\mathbf{y}}+\hat{\mathbf{z}})\ ,$$
$$\mathbf{r}_2=(a/2)(\hat{\mathbf{z}}+\hat{\mathbf{x}})\ ,$$
$$\mathbf{r}_3=(a/2)(\hat{\mathbf{x}}+\hat{\mathbf{y}})\ , \tag{4}$$

the symbol $\langle i,j\rangle$ indicates summation over the 12 ordered, distinct pairs of nonidentical sites, and the vectors

$\mathbf{k}$, $\mathbf{k}'$, $\mathbf{q}$, $(\mathbf{k}+\mathbf{q})$, and $(\mathbf{k}'+\mathbf{q})$ are all restricted to the four following points of the Brillouin zone:

$$\begin{aligned} \Gamma &= 0 \ , \\ X_x &= (2\pi/a)\hat{\mathbf{x}} \ , \\ X_y &= (2\pi/a)\hat{\mathbf{y}} \ , \\ X_z &= (2\pi/a)\hat{\mathbf{z}} \ . \end{aligned} \tag{5}$$

The factor of 4 in the first term in (3) accounts for the fact that each site i has four identical nearest-neighbor sites of each of the other three types of sites j, a consequence of the periodic boundary conditions. The one-electron energies (2) are now restricted to two values

$$\epsilon_\Gamma = -12\ t \ , \ \epsilon_X = 4\ t \ , \tag{6}$$

which for positive (negative) t correspond to the bottom (top) and the top (bottom) of the band, respectively. Note that the fcc lattice, because of its triangular sets of nearest neighbors, exhibits an asymmetry between the bottom and top of the band. This asymmetry leads in turn to an asymmetry between electrons and holes.

II. BCS APPROXIMATION

In 1957, Bardeen, Cooper, and Schrieffer wrote their celebrated papers[8] describing the superconducting state with a trial number-nonconserving variational wave function

$$|\ \Psi_{\rm BCS}\rangle = \prod_{\text{all } \mathbf{k}} (1 + \ g_{\mathbf{k}}\ a^\dagger_{\mathbf{k}\uparrow} a^\dagger_{-\mathbf{k}\downarrow}) \ |\ 0\rangle \ , \tag{7}$$

where the coefficients $g_{\mathbf{k}}$ are variational parameters.

The violation in the conservation of the number of electrons was handled by BCS by working in the grand canonical ensemble and imposing the condition that *only* the average number of particles must be equal to the actual number in the system. The statistical fluctuations in particle number are then of the order $N^{1/2}$, which are negligible compared with N for macroscopic systems.

In a small-cluster calculation, however, these fluctuations are large compared with the number of particles. It is therefore necessary to conserve the number of particles *exactly*. This is attained by the use of a modified version of variational BCS-type function

$$|\ \Psi_\nu\rangle = P_\nu\ |\ \Psi_{\rm BCS}\rangle, \tag{8}$$

where P_ν is a projection operator[9–12] on the subspace of fixed particle number ν.

A. Two electrons

In the particular case $\nu = 2$, Eq. (8) becomes

$$|\ \Psi_2\rangle = \sum_{\mathbf{k}} g_{\mathbf{k}}\ a^\dagger_{\mathbf{k}\uparrow} a^\dagger_{-\mathbf{k}\downarrow}\ |\ 0\rangle \ ; \tag{9}$$

there are only four coefficients $g_{\mathbf{k}}$, denoted by

$$g_0 \equiv g_\Gamma \ , \ g_1 \equiv g_{X_x} \ , \ g_2 \equiv g_{X_y} \ , \ g_3 \equiv g_{X_z} \ . \tag{10}$$

With the use of the Fourier transform of the operators $a^\dagger_{\mathbf{k}\sigma}$, Eq. (9) can be rewritten as

$$|\ \Psi_2\rangle = \sum_{ij} G(\mathbf{r}_i - \mathbf{r}_j)\ c^\dagger_{i\uparrow} c^\dagger_{j\downarrow}\ |\ 0\rangle \ , \tag{11}$$

where

$$G(\mathbf{r}) = (1/4) \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} g_{\mathbf{k}} \ , \tag{12}$$

with $\mathbf{r}$ assuming the values (4) corresponding to the four lattice sites of the cluster.

Space-group symmetry analysis of the cluster indicates that it is possible to find four independent (orthogonal) solutions of Eqs. (9)–(12), corresponding to different arrangements of the pair of electrons in the cluster.

Two such solutions, which can be called s-like-symmetry solutions, have the complete cubic symmetry of the fcc lattice. They correspond to

$$G(\mathbf{r_0}) = \alpha \ , \ G(\mathbf{r_1}) = G(\mathbf{r_2}) = G(\mathbf{r_3}) = \beta \ , \tag{13}$$

which, with the use of (12), yield

$$\begin{aligned} g_0 &= \alpha + 3\beta \ , \\ g_1 &= g_2 = g_3 = \alpha - \beta \ . \end{aligned} \tag{14}$$

It is worth noting that this s-symmetry pairing corresponds to an arbitrary linear combination of same-site pairing ($\alpha \neq 0, \beta = 0$) with a symmetric combination of different-site pairing ($\alpha = 0, \beta \neq 0$). Clearly, the first arrangement is energetically very favorable when $U \to -\infty$, whereas the second becomes favorable when $U \to \infty$. Other linear combinations may be more suitable for general values of U.

The other two possible solutions are degenerate with each other. They correspond to states with d-like pairing characteristics. The first such state has $d_{x^2-y^2}$-like symmetry, and is defined by

$$G(\mathbf{r_0}) = G(\mathbf{r_3}) = 0 \ , \ G(\mathbf{r_1}) = -G(\mathbf{r_2}) = (1/2)\ \gamma \ , \tag{15}$$

which, according to (12), results in

$$\begin{aligned} g_0 &= g_3 = 0, \\ g_1 &= -g_2 = \gamma \ . \end{aligned} \tag{16}$$

The last symmetric combination is $d_{3z^2-r^2}$ like, and is defined by

$$G(\mathbf{r_0}) = 0 \ , \ G(\mathbf{r_1}) = G(\mathbf{r_2}) = -(1/2)\ G(\mathbf{r_3}) = (1/2)\ \delta \ , \tag{17}$$

and consequently yields

$$\begin{aligned} g_0 &= 0 \ , \\ g_1 &= g_2 = -(1/2)\ g_3 = \delta \ . \end{aligned} \tag{18}$$

Note that in both cases of d-like symmetry $G(\mathbf{r_0}) = 0$,

and consequently there is no contribution of the U interaction term to the pair energy in states with d-like BCS pairing.

It is now straightforward to calculate the expectation value of the Hamiltonian (3) with the trial BCS-like functions (8),

$$E_2(g_0,g_1,g_2,g_3)=\frac{\langle\Psi_2\mid H\mid\Psi_2\rangle}{\langle\Psi_2\mid\Psi_2\rangle}, \tag{19}$$

with g_0,g_1,g_2,g_3 given by (14), (16), or (18). This procedure results in the analytical expressions summarized in Table I. As expected from symmetry considerations, the two d-like trial functions produce identical (minimum) expectation values.

It is worth mentioning that in the case of the solutions with d-like symmetry [Eqs. (16) and (18)] the numerator and the denominator in (19) are homogeneous and of the same order in either γ or δ. The variational energies, therefore, become independent of the variational parameters, which become only normalization constants. The spatial symmetry of the problem completely determines the variational functions in these instances.

In the case of s-like symmetry there are two independent parameters α and β, and whereas one of them can be considered the normalization constant, the ratio between them is the only true variational parameter. If the quantity x is defined by

$$x\equiv\frac{\alpha+3\beta}{\alpha-\beta}\ , \tag{20}$$

then the minimization procedure yields

$$x_\pm=-1-\frac{64\,t}{U}\pm\left[4+\frac{128\,t}{U}+\frac{4096\,t^2}{U^2}\right]^{1/2}\ . \tag{21}$$

B. Six electrons

The case $\nu=6$ can be obtained easily by analogy to the $\nu=2$ case (two holes, as compared with two electrons). Here

$$\mid\Psi_6\rangle=\sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3} g_{\mathbf{k}_1}g_{\mathbf{k}_2}g_{\mathbf{k}_3} \times a^\dagger_{\mathbf{k}_1\uparrow}a^\dagger_{-\mathbf{k}_1\downarrow}a^\dagger_{\mathbf{k}_2\uparrow}a^\dagger_{-\mathbf{k}_2\downarrow}a^\dagger_{\mathbf{k}_3\uparrow}a^\dagger_{-\mathbf{k}_3\downarrow}\mid 0\rangle. \tag{22}$$

There are four independent terms in the summation in (22), exactly as in (9), and therefore, the s-like solutions are given by

$$\begin{aligned} &g_1g_2g_3=\alpha+3\beta\ ,\\ &g_0g_2g_3=g_0g_1g_3=g_0g_1g_2=\alpha-\beta\ , \end{aligned} \tag{23}$$

that is,

$$\begin{aligned} &g_0=(\alpha-\beta)/(\alpha+3\beta)^{2/3}\ ,\\ &g_1=g_2=g_3=(\alpha+3\beta)^{1/3}\ . \end{aligned} \tag{24}$$

Similarly, the d-like solutions are given by

$$\begin{aligned} &g_1g_2g_3=g_0g_1g_2=0\ ,\\ &g_0g_2g_3=-g_0g_1g_3=\gamma\ , \end{aligned} \tag{25}$$

i.e.,

$$\begin{aligned} &g_0=g_3=(\gamma/\epsilon)^{1/2}\ ,\\ &-g_1=g_2=\epsilon\ ,\\ &\epsilon\to 0\ , \end{aligned} \tag{26}$$

and

$$\begin{aligned} &g_1g_2g_3=0\ ,\\ &g_0g_2g_3=g_0g_1g_3=-(1/2)\ g_0g_1g_2=\delta\ , \end{aligned} \tag{27}$$

which results in

$$\begin{aligned} &g_0=-\delta/(2\epsilon^2)\ ,\\ &g_1=g_2=2\,\epsilon\ ,\\ &g_3=-\epsilon\ ,\\ &\epsilon\to 0\ . \end{aligned} \tag{28}$$

Minimization of

$$E_6(g_0,g_1,g_2,g_3)=\frac{\langle\Psi_6\mid H\mid\Psi_6\rangle}{\langle\Psi_6\mid\Psi_6\rangle} \tag{29}$$

yields, once again, the values given by (20) and (21), and the energies reported in Table I.

C. Four electrons

The case $\nu=4$ is completely different from the other two. Here,

$$\mid\Psi_4\rangle=\sum_{\mathbf{k}_1,\mathbf{k}_2} C_{\mathbf{k}_1\mathbf{k}_2}\ a^\dagger_{\mathbf{k}_1\uparrow}a^\dagger_{-\mathbf{k}_1\downarrow}a^\dagger_{\mathbf{k}_2\uparrow}a^\dagger_{-\mathbf{k}_2\downarrow}\mid 0\rangle\ , \tag{30}$$

TABLE I. Variational expectation value of the energy for the BCS-like trial functions.

	s-like symmetry	d-like symmetry
E_2	$[U-16\,t-(U^2+32\,tU+1024\,t^2)^{1/2}]/2$	$8\,t$
E_4	$[3\,U-(U^2+1024\,t^2)^{1/2}]/2$	$-16\,t+\frac{3}{4}\,U$
E_6	$[5\,U+16\,t-(U^2-32\,tU+1024\,t^2)^{1/2}]/2$	$-8\,t+2\,U$

where

$$C_{\mathbf{k}_1\mathbf{k}_2} = g_{\mathbf{k}_1} g_{\mathbf{k}_2} \ . \tag{31}$$

The problem can be considered as a minimization of six coefficients C_{ij} subject to the constraints

$$C_{01}C_{23} = C_{02}C_{31} = C_{03}C_{12} \ . \tag{32}$$

If the constraints (32) are ignored and minimization of

$$E_4(C_{ij}) = \frac{\langle \Psi_4 \mid H \mid \Psi_4 \rangle}{\langle \Psi_4 \mid \Psi_4 \rangle} \tag{33}$$

is carried out, a problem in linear algebra, the six solutions E_4'— two nondegenerate and two pairs of doubly degenerate solutions — are given in Table II. The energies are

$$E_4'(S_\pm) = (3/2)\ U \pm (1/2)\ \left(U^2 + 1024\ t^2\right)^{1/2} \ , \tag{34}$$

$$E_4'(D_\pm) = (3/4)\ U \pm \left[(U^2/16) + 256\ t^2\right]^{1/2} \ . \tag{35}$$

The coefficients that appear in Table II are

$$y_\pm = \frac{32\ t}{U} \pm \left[1 + \frac{1024\ t^2}{U^2}\right]^{1/2} \tag{36}$$

and

$$z_\pm = \frac{64\ t}{U} \pm \left[1 + \frac{4096\ t^2}{U^2}\right]^{1/2} \ . \tag{37}$$

Examination of the coefficients in Table II clearly shows that the $S_\pm$ solutions satisfy the constraints (32) and are therefore extrema of the number-conserving BCS trial functions, with energies given by (34). The $D_\pm$ solutions, extrema of the linear problem, do not satisfy (32). When the constraints are reimposed the final solution to the problem is obtained with suitable linear combinations of the D solutions, corresponding either to

$$g_0 = \epsilon^{-1} \ , \ g_1 = \gamma\epsilon \ , \ g_2 = \delta\epsilon \ , \ g_3 = -(\gamma+\delta)\epsilon \ , \quad \epsilon \to 0 \ , \tag{38}$$

or to

$$g_0 = 0 \ , \ g_1 = i\left[(\gamma+\delta)\delta/\gamma\right]^{1/2} \ ,$$
$$g_2 = i\left[(\gamma+\delta)\gamma/\delta\right]^{1/2} \ , \ g_3 = -i\left[\gamma\delta/(\gamma+\delta)\right]^{1/2} , \tag{39}$$

with γ and δ as arbitrary constants (degenerate solutions) and the energy given in Table I.

The BCS solutions are always exact for negative U and $\nu = 2$, 4 and 6. In these cases the symmetry is s like. For positive U and $\nu = 2$ and 6 the BCS solutions are also exact, but their symmetry is either s like ($\nu = 2$, $t > 0$ and $\nu = 6$, $t < 0$) or d like ($\nu = 2$, $t < 0$ and $\nu = 6$, $t > 0$). For $\nu = 4$ and $U > 0$ the best BCS solution is d like, but a poor approximation to the exact solution which asymptotically has zero energy as $U \to \infty$; the BCS approximation diverges as $0.75\ U$.

III. RVB STATE

Another approximation, much in vogue in the last five years, is the RVB state.[2,9] It postulates as a trial function for the ground state a linear combination of bonds; each bond contains two electrons shared by a pair of sites and perfectly correlated within that pair. In the Hubbard model discussed here a bond (ij) is described by the two-electron creation operator

$$P_{ij}^\dagger = \alpha\ (c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger + c_{j\uparrow}^\dagger c_{i\downarrow}^\dagger) + \beta\ (c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger + c_{j\uparrow}^\dagger c_{j\downarrow}^\dagger) \ , \tag{40}$$

where α and β are properly normalized coefficients which describe the "neutral" and "polar" parts of the bond, respectively. For the tetrahedral cluster under consideration here, and for $\nu = 4$ (the only non-trivial case), the RVB trial function is defined by

$$\mid \Psi_{\rm RVB}; \alpha, \beta, \Omega_1, \Omega_2 \rangle$$
$$\equiv \left\{ P_{01}^\dagger P_{23}^\dagger + \Omega_1 P_{02}^\dagger P_{13}^\dagger + \Omega_2 P_{03}^\dagger P_{12}^\dagger \right\} \mid 0 \rangle \ , \tag{41}$$

where Ω_1 and Ω_2 are two arbitrary phase factors. The variational solution is obtained by minimizing

$$E_{\rm RVB} = \frac{\langle \Psi_{\rm RVB} \mid H \mid \Psi_{\rm RVB} \rangle}{\langle \Psi_{\rm RVB} \mid \Psi_{\rm RVB} \rangle} \tag{42}$$

with respect to the four parameters α, β, Ω_1, and Ω_2.

Symmetry analysis yields extrema of two symmetries: nondegenerate solutions of ${}^1\Gamma_1$ symmetry for

$$\Omega_1 = \Omega_2 = 1 \tag{43}$$

TABLE II. Solutions for $\nu = 4$ ignoring the constraints (32). Energies are given by (34) and (35) in the text, and the parameters $y_\pm$ and $z_\pm$ in (36) and (37).

	$S_\pm$	$D_{\pm A}$	$D_{\pm B}$
C_{01}	$y_\pm$	$z_\pm$	$z_\pm$
C_{02}	$y_\pm$	$z_\pm$	$-z_\pm$
C_{03}	$y_\pm$	$-2\ z_\pm$	0
C_{23}	1	1	1
C_{31}	1	1	-1
C_{12}	1	-2	0

TABLE III. Comparison of the exact and approximate RVB solutions of symmetry ${}^1\Gamma_{12}$, for $\nu = 4$ and $U > 0$.

$(U/\mid t \mid)$	Exact energy (units of $\mid t \mid$)	Error of the RVB solution (units of $\mid t \mid$)
0	-16.0000	0
0.1	-15.9253	0.0000
0.3	-15.7773	0.0001
1	-15.2747	0.0013
3	-13.9600	0.0090
10	-10.4589	0.0363
30	-5.5529	0.0220
100	-1.8903	0.0014
300	-0.6389	0.0001

TABLE IV. Secular equations and symmetries for the exact solution of the Hubbard model in a tetrahedral cluster.

ν	t	U	Symmetry	Secular equation
2	positive	any		
	negative	negative	$^1\Gamma_1$	$E^2+(16\,t-U)E-(192\,t^2+16\,tU)=0$
2	negative	positive	$^1\Gamma_{12}\oplus{}^3X_2$	$E-8\,t=0$
4	any	positive	$^1\Gamma_{12}$	$E^3-3\,UE^2-(256\,t^2-2\,U^2)E+384\,t^2U=0$
4	any	negative	$^1\Gamma_1$	$E^2-3\,UE-(256\,t^2-2\,U^2)=0$
6	negative	any		
	positive	negative	$^1\Gamma_1$	$E^2-(16\,t+5\,U)E-(192\,t^2-48\,tU-6\,U^2)=0$
6	positive	positive	$^1\Gamma_1\oplus{}^3X_2$	$E+8\,t-2\,U=0$

and doubly degenerate solutions of $^1\Gamma_{12}$ symmetry for

$$\Omega_1=\Omega_2^*=(-1\pm i\sqrt{3})/2\ . \tag{44}$$

The first choice yields for the RVB state

$$E_{\rm RVB}(^1\Gamma_1)=(3/2)\,U-(1/2)\left[U^2+1024\,t^2\right]^{1/2}\ , \tag{45}$$

which is identical to the BCS approximation $E_4(S_-)$ and to the exact ground state for $U<0$. The second choice yields

$$E_{\rm RVB}(^1\Gamma_{12})=\lambda\ , \tag{46}$$

where λ is obtained as the minimum value of

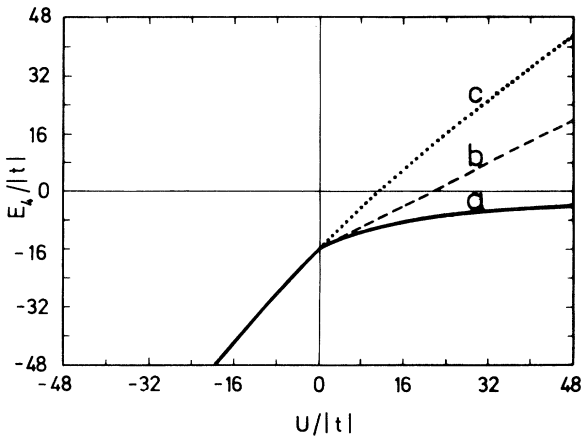

FIG. 1. $\nu=4$ case. The solid line (curve a) gives the energy of the exact ground state as a function of $(U/\mid t\mid)$. The BCS approximation with s-like symmetry coincides with the exact result for $U<0$, but diverges as U for $U>0$ (dotted line, curve c). For $U>0$ the best BCS result, which is poor in any case, has d-like symmetry (dashed line, curve b). The RVB result is exact for $U<0$ and an extremely good approximation for $U>0$; in fact it cannot be distinguished from the exact result in the scale of this drawing.

$$2\,U\,(1-\alpha^4)(1+2\alpha^2)^{-1}-32\mid t\mid\alpha(1-\alpha^2)^{1/2} \tag{47}$$

when varied with respect to α. This solution is a very good approximation to the ground state for $U>0$, as seen in Table III.

IV. DISCUSSION

The Hubbard model in a tetrahedral cluster with periodic boundary conditions has been solved exactly.[6,7] The ground-state energies and space-group symmetries[13,14] are given by the lowest roots of the equations given in Table IV.

Comparison of the entries in Table IV and the results of Secs. II and III yields the following conclusions (see Fig. 1).

(1) Both the BCS and the RVB approximations give the exact energies, symmetries, and wave functions for $\nu=2$ and $\nu=6$, regardless of the values of the parameters t and U.

(2) For $\nu=4$ (half-filled band), once again the BCS and RVB state functions describe the exact state for attractive interactions, $U<0$.

(3) For $\nu=4$, $U>0$, the BCS state is a very poor approximation and, whereas the exact solution behaves asymptotically as $(-t^2/U)$— a number always less than zero— the BCS energy increases without bound as $0.75U$.

(4) The RVB state function with $^1\Gamma_{12}$ symmetry— which is the correct one— yields an extremely accurate value of the energy for $\nu=4$ and $U>0$. As seen in Table III the error is always smaller than four parts in a thousand, and is largest for values of $U/\mid t\mid\approx$10–30. The RVB solution is exact in both limits, $U\to0$ and $U\to\infty$, and expansions about either limit yield agreement in the first two terms in either U or U^{-1} between the exact state and approximation. The source of the discrepancy can be understood if one realizes that there are three roots of the $^1\Gamma_{12}$ secular equations (see Table IV), and only two extrema in the RVB equations (46) and (47). The "missing" state of the trio, however, only contributes to the ground state (and in proportionally very small amounts) for intermediate values of $(U/\mid t\mid)$.

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