Exact solution of a periodic-cluster Hubbard model with an electron-lattice interaction

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(Received 24 December 1987)

An exact solution of a modified Hubbard model for a tetrahedral cluster with periodic boundary conditions is presented. It includes a *static* electron-lattice interaction in which the intersite bond-hopping parameter is a function of the bond electron occupation. It is found that the intrasite Coulomb repulsion and the effective attractive electron-lattice interaction have, generally speaking, opposite (although not identical) effects. They cancel each other *exactly* along a line of singularities in parameter space. The state vectors are easily obtained analytically. A study is made of magnetic and superconducting static correlation functions as functions of the parameters. Various forms of anisotropic superconducting fluctuations are favored in the various regimes. There is an indication of possible states with coexisting nonuniform, nonisotropic superconductivity and antiferromagnetism caused by a "compromise" between the competing forces.

I. INTRODUCTION

The Hubbard model[1] has become, since its introduction in 1963, the most popular example of a system of fermions in a lattice with strong short-range interactions. It is an extremely useful model, but it is also a particularly complex quantum-mechanical many-body problem. It has been used to study a variety of effects in metals,[2–16] such as ferromagnetism and antiferromagnetism,[2] metal-insulator transitions,[3–6] spin- and charge-density waves[2,7] and—with the arrival recently of high-T_c oxide superconductors—superconductivity;[8–16] it has also served as a model to study[17] the normal phase of ^{3}He.

In this work a study is made of the effects of the nonlinear electron-lattice interaction in a particular version of the Hubbard model, that for the face-centered-cubic (fcc) lattice with an electron occupation of slightly less than one electron per site. A *static* electron-lattice interaction is incorporated into the model in the following way: Suppose a system of two identical nuclei with a given number of electrons; i.e., a homopolar molecule or molecular ion. The addition (or subtraction) of one electron changes the equilibrium separation of the two centers and, as a consequence, there is a change in the one-electron transfer integral or hopping probability between the centers. In other words, the one-electron integral between centers in each bond depends on the number of electrons in the bond. This is, from the point of view of the lattice, a *static* effect which exists over and above the *dynamic* electron-phonon interaction. It is to electron dynamics as the Debye-Waller effect is to x-ray scattering (whereas the dynamic electron-phonon interaction is, to the electron motion, analogous to phonon-mediated *inelastic* scattering of x rays.)

As far at the authors are aware, this effect has never been studied in connection with the Hubbard model, which is not naturally suited to incorporate an electron-lattice interaction. The motivation for this study is the various proposals,[8–16] recently put forward in connection with high-temperature superconductivity, which suggest that the Hubbard model in some limits or under specific conditions of interaction strength and electron density may provide, in addition to strong intrasite electron repulsion, an *attractive* electron-electron interaction at distances of the order of the nearest-neighbor separation. Such type of interaction may result in Cooper-pair formation and high-temperature superconductivity. The presence of an isotope effect in the high-T_c oxides[18] unequivocally indicates that the *dynamic* electron-phonon interaction must play a role in the superconducting properties, even if that role is a minor one. Although the dynamics of the lattice is not included in the present contribution, i.e., there is no phonon dynamic dependence and hence no isotope effect, the lattice-deformation effect considered here provides an effective *attractive* interaction between the electrons, and therefore favors superconductivity.

The approach used in this contribution is the exact diagonalization of a four-site tetrahedral cluster with periodic boundary conditions;[19] it can be shown[20] that this is equivalent to an infinite fcc lattice if the Brillouin-zone sampling is restricted to four reciprocal-lattice points, the zone center Γ and the three square-face-center points X. The method has been used before—for various lattices and several model or realistic Hamiltonians—to solve a variety of problems.[20–29] Section II describes the model and the method of calculation. Section III describes the results, particularly the nature and properties of the ground state as a function of the parameters. Section IV contains the conclusions and discussion.

II. MODEL AND METHOD OF CALCULATION

The model is defined by the following Hamiltonian[30]

$$H = H_1 + H_2 + H_3 + H_C \ , \tag{2.1}$$

where

$$H_1 = t \sum_{\langle i,j\rangle,\sigma} c_{i\sigma}^{\dagger} c_{j\sigma} (1-n_{i\bar{\sigma}})(1-n_{j\bar{\sigma}}) , \tag{2.2}$$

$$H_2 = (t+\delta) \sum_{\langle i,j\rangle,\sigma} c_{i\sigma}^{\dagger} c_{j\sigma} [\, n_{j\bar{\sigma}}(1-n_{i\bar{\sigma}}) + n_{i\bar{\sigma}}(1-n_{j\bar{\sigma}})] , \tag{2.3}$$

$$H_3 = (t+\gamma) \sum_{\langle i,j\rangle\sigma} c_{i\sigma}^{\dagger} c_{j\sigma} n_{i\bar{\sigma}} n_{j\bar{\sigma}} , \tag{2.4}$$

$$H_C = U \sum_i n_{i\uparrow} n_{i\downarrow} . \tag{2.5}$$

Here $c_{i\sigma}$ ($c_{i\sigma}^{\dagger}$) is the destruction (creation) operator for an electron in an s orbital, with spin σ, located at site i of a tetrahedral cluster ($i,j=0,1,2,3$), and

$$n_{i\sigma} = c_{i\sigma}^{\dagger} c_{i\sigma} \tag{2.6}$$

is the corresponding number operator. For the transfer integral there are three different values, depending on the number of electrons in the $\langle i,j\rangle$ bond: t if there is only one electron, $t+\delta$ if there are two electrons, and $t+\gamma$ if there are three electrons. This is schematically illustrated in Fig. 1. Finally, (2.5) is the intrasite two-particle term, where U is the single-site Coulomb repulsion parameter (only the case of a repulsive interaction, $U>0$, is considered here).

In the limit $\delta=\gamma=0$ the Hamiltonian reduces to

$$H = t \sum_{\langle i,j\rangle,\sigma} c_{i\sigma}^{\dagger} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} , \tag{2.7}$$

the standard Hubbard model. Note that the limit $U=0$ of (2.1) remains, because of the presence of the electron-lattice interaction, an interacting many-body problem.

Since there are four occupation probabilities per site and four sites, there are $4^4=256$ possible eigenstates of (2.1). Since the number of electrons n is conserved, and $0 \le n \le 8$, for a given n there are $8!/[(8-n)!n!]$ eigenstates. These eigenstates can be classified according to their spin and their spatial symmetries. Since the total spin of the cluster S is conserved by (2.1), the cluster states can be labeled as spin singlets, doublets, triplets, quartets, and quintets.

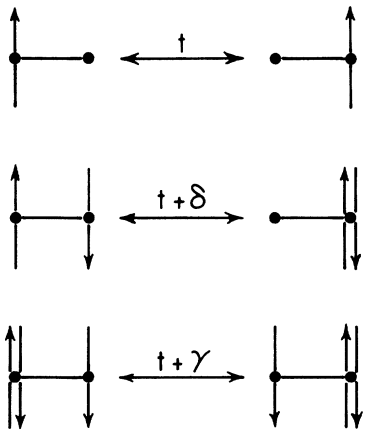

FIG. 1. Schematic representation of the *static* electron-lattice interaction. The hopping parameter between two neighboring centers takes different values, a function of the total occupation of that particular bond. Note that in order to take advantage of the energy enhancements, δ and/or γ, double-site occupation and two spins are necessary.

The symmetry of the spatial part of the Hamiltonian is defined by its space group, which in this case is the fcc lattice group[31] with only four translation operations and a total of $48\times4=192$ operators. This group has 20 irreducible representations (four one-dimensional, two two-dimensional, and four three-dimensional at Γ; eight three-dimensional and two six-dimensional at X). Because only s-like orbitals are involved in the present problem, only five representations survive: two one-dimensional, Γ_1 and Γ_2; one two-dimensional, Γ_{12}; and two three-dimensional, X_1 and X_2. In order to identify them it is sufficient to retain only the 24 point operations of the tetrahedral group T_d about the center of the tetrahedral point equidistant from the four sites in the lattice.[19]

Without the spatial symmetry, the electron number n and spin S symmetries reduce the original 256×256 secular problem to the diagonalization of matrices that range from 1×1 to 20×20 (the subspace $n=4$, $S=0$). The spatial symmetry makes the problem completely analytic, with at most a 3×3 secular equation to solve for any given energy level.[32]

Although the Hamiltonian (2.1) was diagonalized for all electron occupations ($0 \le n \le 8$), only results for the most interesting case ($n=3$, i.e., less than, but as close as possible, to one electron per site) are reported in the next section.

III. RESULTS

A. Ground state

In the subspace with $n=3$ electrons, there are 56 states; group-theoretical factorization and the calculation of the matrix elements of (2.1) in this subspace yield the six energy-eigenvalue equations[33] given in Table I.

The model given by Eq. (2.1) has four parameters: t, δ, γ, and U. If the energy is measured in units of the transfer integral t, the number of parameters is reduced by one: δ/t, γ/t, and U/t. There is, therefore, a three-dimensional parameter space.

The use of the equations in Table I yields the various ground states in this three-dimensional parameter space (it is assumed throughout that t, δ, and $\gamma \ge 0$). The results are shown in the plane $(U/t, \delta/t)$ for constant values of γ. Figure 2 corresponds to the case $\gamma=0$; Fig. 3 corresponds to $\gamma=0.6$. An examination of these figures elicits the following remarks.

(i) If $U=\delta=\gamma=0$ (origin in Fig. 2), 20 states, corresponding to the symmetries $^2\Gamma_{12}$, $^2X_1$, $^2X_2$, and $^4\Gamma_2$ are all degenerate, with energy $E=-3t$.

(ii) For $\delta=\gamma=0$ (a situation referred to as the absence of electron-lattice interaction), and $U>0$, the ground state is ferromagnetic, of symmetry $^4\Gamma_2$. This can be interpreted in the following way: with the chosen sign of t

TABLE I. Energy-eigenvalue equations.

$^2\Gamma_1$	$E-(t+U+\gamma)=0$
$^2\Gamma_{12}$	$E^2-E(U-2t-\gamma)-3(t+\delta)^2=0$
$^2X_1$	$E^3-E^2(3t+2U)+E(5tU-13t^2+U^2-3t\gamma-\gamma^2-22t\delta-11\delta^2)$ $+9t^2U+15t^3-2tU^2-t^2\gamma+2t\gamma^2+\delta(2t+\delta)(11U+7t-7\gamma)=0$
$^2X_2$	$E^2-E(U-2t+\gamma)-2t(U+\gamma)-3(t+\delta)^2=0$
$^4\Gamma_2$	$E+3t=0$
$^4X_2$	$E-t=0$

the lowest-energy ($\varepsilon=-t$) single-particle orbital is threefold degenerate and therefore can accommodate three particles with parallel spin. This would be the prediction of Hund's rules[19] for the ground state of an atom, and it is also the case in this small-cluster Hubbard system. The U-term Coulomb interaction makes no contribution to the energy of this spin-aligned state. For all other symmetries, all spin doublets, there is a contribution of the Coulomb term, linear in U for small U, caused by the finite probability of double-site occupation. For $U=\delta=\gamma=0$, the probability of a single-site double occupancy is 0.75 for the states of symmetries $^2\Gamma_{12}$ and $^2X_1$, 0.5 for the state of symmetry $^2X_2$, and 0 for the ferromagnetic $^4\Gamma_2$ state. For large enough U, as compared to δ and γ, the Coulomb interaction must dominate, and the ground state is the ferromagnetic $^4\Gamma_2$. This state, however, cannot take advantage of the electron-lattice interaction—all hopping processes involve bonds with only one electron (see Fig. 1)—and thus for δ and/or γ sufficiently large the other symmetries have an advantage and can therefore become the ground state of the system.

(iii) There is a surprising singular line, defined by the equation

$$U=2\gamma=4\delta+2\delta^2/t\ . \tag{3.1}$$

Along this line the effects of the Coulomb and of the electron-lattice interactions cancel *exactly*, and the 20 possible states of all four possible symmetries are degenerate, with energy $E=-3t$. This is precisely the ground-state energy for the noninteracting case $U=\delta=\gamma=0$. As seen in Fig. 3, infinitesimal changes of the parameters away from the singular line can produce ground states with any of the four possible symmetries.[34]

B. Magnetic correlation functions

The magnetic structure of the system can be examined by determining the following spin-spin correlation functions:

$$L_0=\tfrac{1}{16}\sum_i\langle(n_{i\uparrow}-n_{i\downarrow})^2\rangle \tag{3.2}$$

and

$$L_1=\tfrac{1}{16}\sum_{\langle i,j\rangle}\langle(n_{i\uparrow}-n_{i\downarrow})(n_{j\uparrow}-n_{j\downarrow})\rangle\ , \tag{3.3}$$

where $\langle\cdots\rangle$ indicates the expectation value of the various operators in the ground state.

It should be noted that L_0, given by (3.2), is the average value in the cluster of the local magnetic moment. It

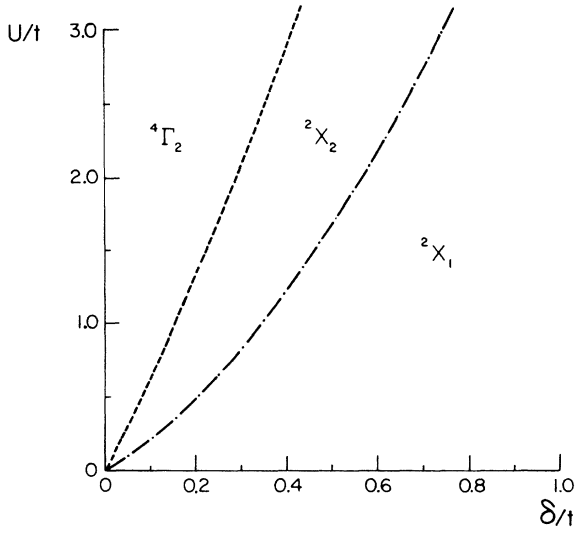

FIG. 2. The symmetry of the ground state as a function of the parameters δ/t and U/t for $\gamma=0$.

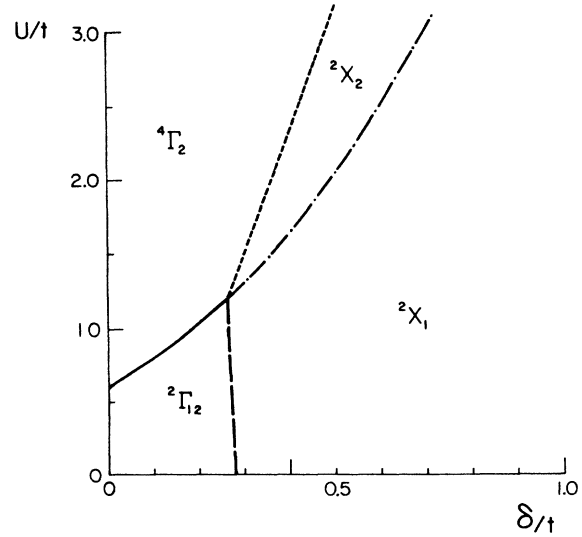

FIG. 3. The symmetry of the ground state as a function of the parameters δ/t and U/t for $\gamma=0.6$.

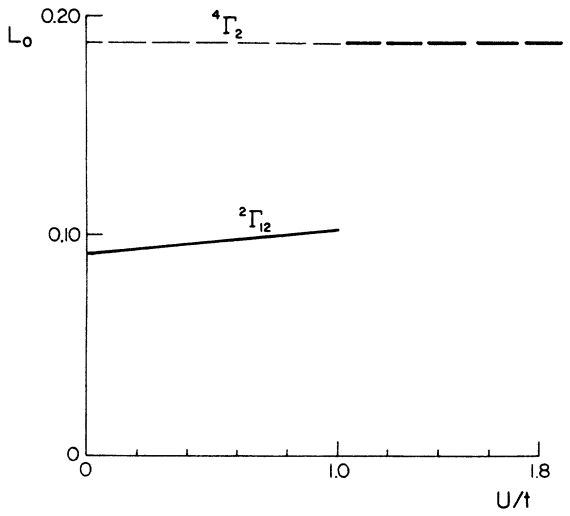

FIG. 4. The local-moment correlation function L_0 of the ground state as a function of U/t for $\delta/t=0.2$ and $\gamma/t=0.6$. The thin dashed line corresponds to the case $\delta=\gamma=0$, the ground state of symmetry $^4\Gamma_2$.

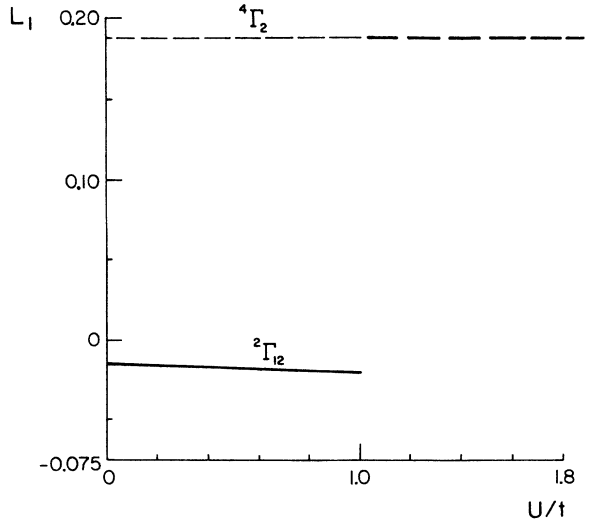

FIG. 6. The nearest-neighbor magnetic correlation function L_1 of the ground state as a function of U/t for $\delta/t=0.2$ and $\gamma/t=0.6$. The thin dashed line corresponds to the case $\delta=\gamma=0$, the ground state of symmetry $^4\Gamma_2$.

can be rewritten as

$$L_0=\tfrac{1}{4}\rho-\tfrac{1}{8}\sum_i\langle n_{i\uparrow}n_{i\downarrow}\rangle\ , \tag{3.4}$$

where $\rho=n/4$ is the number of electrons per site ($\rho=0.75$ for $n=3$ and four sites).

At the singular line L_0 takes the value $\frac{3}{16}$ for $^4\Gamma_2$, the value $\frac{5}{32}$ for $^2X_2$, and the value $\frac{3}{32}$ for $^2\Gamma_{12}$ and for $^2X_1$. Similarly, at the singular line L_1 takes the ferromagnetic (positive) value $\frac{3}{16}$ for $^4\Gamma_2$, the antiferromagnetic (negative) value $-\frac{3}{64}$ for $^2X_2$, and the small antiferromagnetic value $-\frac{1}{64}$ for $^2\Gamma_{12}$ and for $^2X_1$.

Figures 4 and 5 show L_0 as a function of U/t for ($\delta=0.2$, $\gamma=0.6$), and for ($\delta=0.3$, $\gamma=0.6$), respectively. With no electron-lattice interaction, the ground state is always the $^4\Gamma_2$ ferromagnetic state with no double-site occupancy; L_0 attains there its maximum value of $\frac{3}{16}$.

The general tendencies shown in Figs. 4 and 5 can be easily understood: (i) within each symmetry the local moment increases with increasing U; (ii) within each symmetry the local moment increases with decreasing δ and γ; (iii) both these features can be easily interpreted in terms of (3.4), based on the probability of double-site occupation; (iv) the states with symmetry $^2X_2$ have a fairly large magnetic moment—in fact, very close to the maximum value of $\frac{3}{16}$—and considerably larger than those of symmetry $^2\Gamma_{12}$ and $^2X_1$ (note that the states of symmetry $^2X_2$ become the ground state for values of U and/or δ *greater,* and/or values of γ *smaller* than those on the singular line, i.e., this ground state is a result of compet-

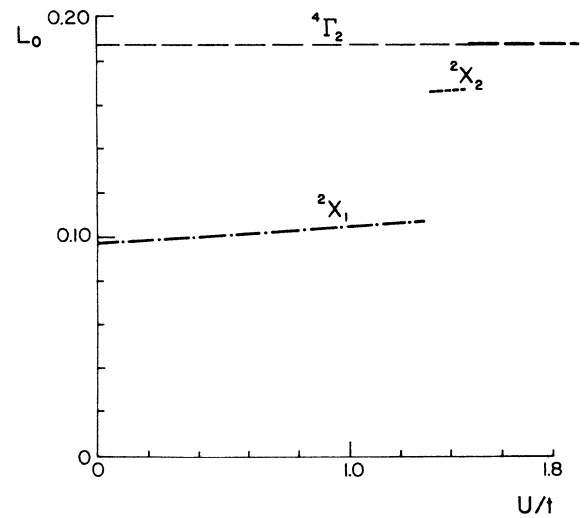

FIG. 5. The local-moment correlation function L_0 of the ground state as a function of U/t for $\delta/t=0.3$ and $\gamma/t=0.6$. The thin dashed line corresponds to the case $\delta=\gamma=0$, the ground state of symmetry $^4\Gamma_2$.

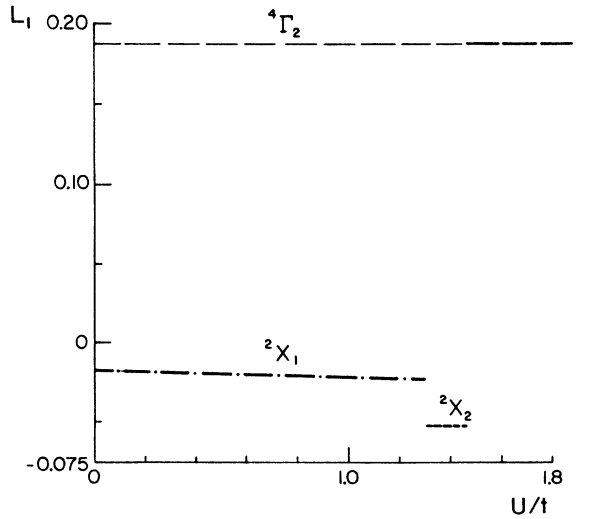

FIG. 7. The nearest-neighbor magnetic correlation function L_1 of the ground state as a function of U/t for $\delta/t=0.3$ and $\gamma/t=0.6$. The thin dashed line corresponds to the case $\delta=\gamma=0$, the ground state of symmetry $^4\Gamma_2$.

ing interactions).

Figures 6 and 7 show the nearest-neighbor spin-spin correlation function L_1 for the cases ($\delta=0.2$, $\gamma=0.6$) and ($\delta=0.3$, $\gamma=0.6$), respectively. In the ferromagnetic ${}^4\Gamma_2$ states L_1 reaches its maximum positive value of $\frac{3}{16}$. All other states are spin doublets and are *antiferromagnetically* correlated, i.e., L_1 takes negative values. It is interesting to notice that even though the ${}^2X_2$ state has a local moment L_0 close to the maximum value, its antiferromagnetic correlations are small. It is, however, not too far from $\frac{1}{16}$, which is the extreme value for the best three-spin antiferromagnetic arrangement in a frustrated triangular configuration compatible with the fcc lattice.

C. Superconducting correlation functions

The static superconducting correlation functions are defined by

$$S_\mu(\mathbf{r},\mathbf{q})=\langle \Delta_\mu^\dagger(\mathbf{r},\mathbf{q})\Delta_\mu(\mathbf{r},\mathbf{q})\rangle \ , \tag{3.5}$$

where $\Delta_\mu(\mathbf{r},\mathbf{q})$ are pairing operators[14–16] given by

$$\Delta_{\mathrm{SP}}(0,\mathbf{q})\equiv\Delta_{\mathrm{SP}}(\mathbf{q})=Z_{\mathrm{SP}}\sum_i e^{-i\mathbf{q}\cdot\mathbf{R}_i}c_{i\uparrow}c_{i\downarrow} \ , \tag{3.6a}$$

$$\Delta_{\mathrm{SPX}}(\mathbf{r},\mathbf{q})Z_{\mathrm{SPX}}\sum_i e^{-i\mathbf{q}\cdot\mathbf{R}_i}(c_{i+r\uparrow}c_{i\downarrow}-c_{i+r\downarrow}c_{i\uparrow}) \qquad \mathbf{r}\neq\mathbf{0} \ , \tag{3.6b}$$

$$\Delta_{\mathrm{TP}\sigma}(\mathbf{r},\mathbf{q})=Z_{\mathrm{TP}\sigma}\sum_i e^{-i\mathbf{q}\cdot\mathbf{R}_i}c_{i+r\sigma}c_{i\sigma} \ , \tag{3.6c}$$

$$\Delta_{\mathrm{TP0}}(\mathbf{r},\mathbf{q})=Z_{\mathrm{TP0}}\sum_i e^{-i\mathbf{q}\cdot\mathbf{R}_i}(c_{i+r\uparrow}c_{i\downarrow}+c_{i+r\downarrow}c_{i\uparrow}) \ . \tag{3.6d}$$

In these equations $\mathbf{r}$ is either the null vector zero, or one of the three vectors connecting an atom to the other three atoms in the cluster,

$$\begin{aligned}\mathbf{r}_1&=(a/2)(\hat{\mathbf{y}}+\hat{\mathbf{z}}) \ ,\\ \mathbf{r}_2&=(a/2)(\hat{\mathbf{z}}+\hat{\mathbf{x}}) \ ,\\ \mathbf{r}_3&=(a/2)(\hat{\mathbf{x}}+\hat{\mathbf{y}}) \ ,\end{aligned} \tag{3.7}$$

where a is the lattice constant of the cubic unit cell of the fcc lattice, and SP stands for singlet pairing, SPX for extended singlet pairing, and TP for triplet pairing; the latter takes values $\uparrow$, $\downarrow$, and 0, depending on the pair-spin orientation. The normalizing factors Z_μ are chosen so that the maximum eigenvalues of S_μ, calculated with the 56 three-electron states, are equal to 1.

Several remarks are now in order.

(i) Because the system is a finite cluster, there cannot be any phase transitions, superconductivity included. Fluctuations and susceptibilities can, however, always be calculated. The quantities S_μ should therefore be considered "superconducting static susceptibilities." States with large values of S_μ are those whose configuration space is favorable to the existence of μ-type superconducting fluctuations, and therefore those which on the thermodynamic limit are likely to lead to a superconducting ground state of type μ.

(ii) Because the sampling of the Brillouin zone is restricted to the Γ and X points, the $\mathbf{q}$ in Eqs. (3.5) and (3.6) can only take the following values:

$$\Gamma=0, \ X_x=(2\pi/a)\hat{\mathbf{x}}, \ X_y=(2\pi/a)\hat{\mathbf{y}}, \ X_z=(2\pi/a)\hat{\mathbf{z}} \ . \tag{3.8}$$

(iii) For the tetrahedral cluster, all eigenvalues and eigenvectors of $S_\mu(\mathbf{r},\mathbf{q})$ are calculated within the pertinent ground-state manifold. All eigenvalues are positive definite and, as mentioned above, normalized so that the maximum possible value is one.

Results for various $S_\mu(\mathbf{r},\mathbf{q})$ are presented in Tables II–IV and in Figs. 8–10. All values shown in the tables are those of the superconducting correlation functions along the singular line.

It is instructive to rewrite $S_{\mathrm{SP}}(0,\mathbf{q})$ in the form

$$S_{\mathrm{SP}}(0,\mathbf{q})=Z_{\mathrm{SP}}\sum_{i,j} e^{i\mathbf{q}\cdot(\mathbf{R}_i-\mathbf{R}_j)}\langle c_{i\downarrow}^\dagger c_{i\uparrow}^\dagger c_{j\uparrow}c_{j\downarrow}\rangle \ , \tag{3.9}$$

and, with the use of the Fourier transform

$$c_{i\sigma}=\frac{1}{\sqrt{N}}\sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{R}_i}c_{\mathbf{k}\sigma} \ , \tag{3.10}$$

obtain

$$S_{\mathrm{SP}}(0,\mathbf{q})=Z_{\mathrm{SP}}\sum_{\mathbf{k},\mathbf{k}'}\langle c_{-\mathbf{k}-\mathbf{q}\downarrow}^\dagger c_{\mathbf{k}\uparrow}^\dagger c_{\mathbf{k}'\uparrow}c_{-\mathbf{k}'-\mathbf{q}\downarrow}\rangle \ . \tag{3.11}$$

TABLE II. The singlet-pairing superconducting correlation functions at the singular line.

Symmetry	Eigenvalue	Γ	X_x
${}^2\Gamma_{12}$	First, second	0	$\frac{2}{3}$
${}^2\Gamma_{12}$	Third, fourth	0	0
${}^2X_1$	First through fourth	$\frac{2}{3}$	$\frac{1}{6}$
${}^2X_1$	Fifth, sixth	$\frac{2}{3}$	0
${}^2X_2$	First through fourth	0	$\frac{1}{6}$
${}^2X_2$	Fifth, sixth	0	0
${}^4\Gamma_2$	First through fourth	0	0

TABLE III. The extended-singlet-pairing superconducting correlation functions at the singular line.

Symmetry	Eigenvalue	Γ $\mathbf{r}$	X_x $\mathbf{r}_1$	X_x $\mathbf{r}_{2,3}$
${}^2\Gamma_{12}$	First, second	$\frac{2}{3}$	0	0
${}^2\Gamma_{12}$	Third, fourth	0	0	0
${}^2X_1$	First, second	$\frac{2}{3}$	$\frac{1}{6}$	0
${}^2X_1$	Third, fourth	0	$\frac{1}{6}$	0
${}^2X_1$	Fifth, sixth	0	0	0
${}^2X_2$	First through fourth	$\frac{1}{6}$	$\frac{2}{3}$	0
${}^2X_2$	Fifth, sixth	0	0	0
${}^4\Gamma_2$	First through fourth	0	0	0

TABLE IV. The triplet-pairing superconducting correlation functions at the singular line.

Symmetry	Eigenvalue	Γ r	X_x $\mathbf{r}_1$	X_x $\mathbf{r}_{2,3}$
$^2\Gamma_{12}$	First	0	0	$\frac{1}{3}$
$^2\Gamma_{12}$	Second through fourth	0	0	0
$^2X_1$	First, second	0	0	$\frac{1}{4}$
$^2X_1$	Third through sixth	0	0	0
$^2X_2$	First	0	0	$\frac{1}{4}$
$^2X_2$	Second, third	0	0	$\frac{1}{8}$
$^2X_2$	Fourth through sixth	0	0	0
$^4\Gamma_2$	First	0	0	1
$^4\Gamma_2$	Second	0	0	$\frac{1}{6}$
$^4\Gamma_2$	Third, fourth	0	0	0

From this last equation it is clear that $S_{SP}(\Gamma)$ is directly related to the traditional BCS-like $(\mathbf{k}\uparrow, -\mathbf{k}\downarrow)$ superconducting pairing.[35]

It can be seen from Table II and Fig. 8 that the symmetries $^2X_1$ (for $\mathbf{q}=\Gamma$), and $^2\Gamma_{12}$ (for $\mathbf{q}=X$) are the most favorable ones for SP superconductivity. For them $S_{SP}(\mathbf{q})$ could attain, among the 20 possible lowest band-energy states, the largest possible value of $\frac{2}{3}$. These symmetries constitute the ground state of the system only for small enough values of the Coulomb interaction parameter U. Which one is the ground state depends on the relative values of δ and γ. The type of favored pairing also depends on the symmetry: $^2X_1$ favors spatial uniform distribution of the order parameter, whereas $^2\Gamma_{12}$ gives large susceptibilities for order parameters that vary in space with any of the three X periodicities.

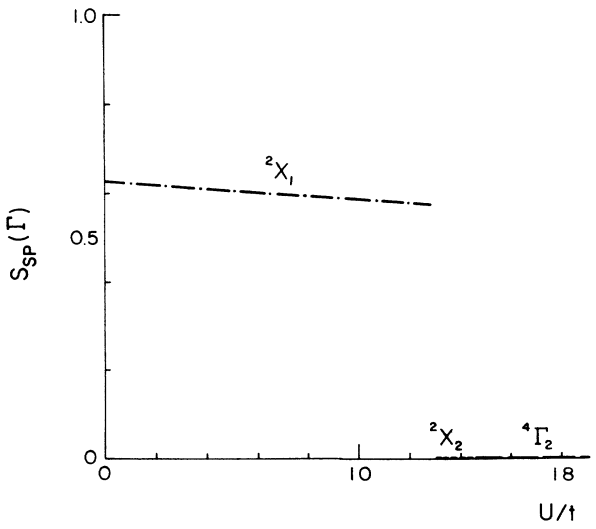

FIG. 8. The singlet-pairing superconducting correlation function of the ground state at the Γ point as a function of U/t for $\delta/t=0.3$ and $\gamma/t=0.6$. For the case $\delta=\gamma=0$, the ground state of symmetry $^4\Gamma_2$, the correlation function is zero.

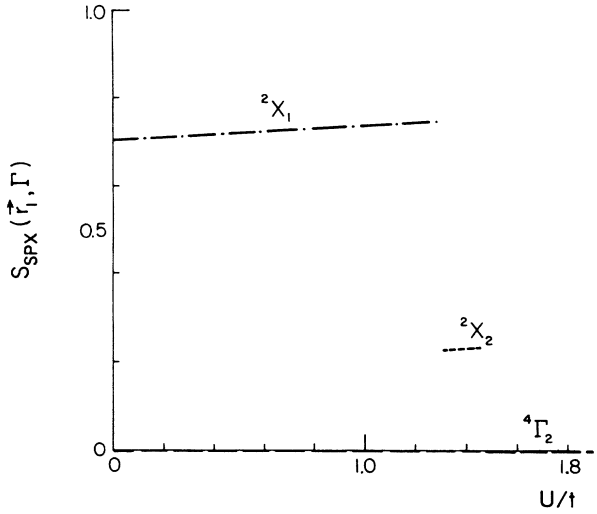

FIG. 9. The extended singlet-pairing superconducting correlation function of the ground state at the Γ point as a function of U/t for $\delta/t=0.3$ and $\gamma/t=0.6$. For the case $\delta=\gamma=0$, the ground state of symmetry $^4\Gamma_2$, the correlation function is zero.

As seen in Fig. 8, where the case $\delta=0.3$ and $\gamma=0.6$ is presented, for $U=0$ the ground state is of symmetry $^2X_1$; in that case $S_{SP}(\Gamma)$ takes values close to $\frac{2}{3}$. With increasing values of U, because of the admixing of higher-band-energy states, $S_{SP}(\Gamma)$ is a monotonically decreasing function. With the change of symmetry of the ground state, first to $^2X_2$ and subsequently to $^4\Gamma_2$, $S_{SP}(\Gamma)$ becomes identically zero. This behavior is easily understood: since the SP operator pairs electrons on the same site, and the repulsive Coulomb interaction in the Hubbard model is only effective for electrons also on the same site, increasing values of U should depress the SP susceptibility, and eventually change the ground-state symmetry to

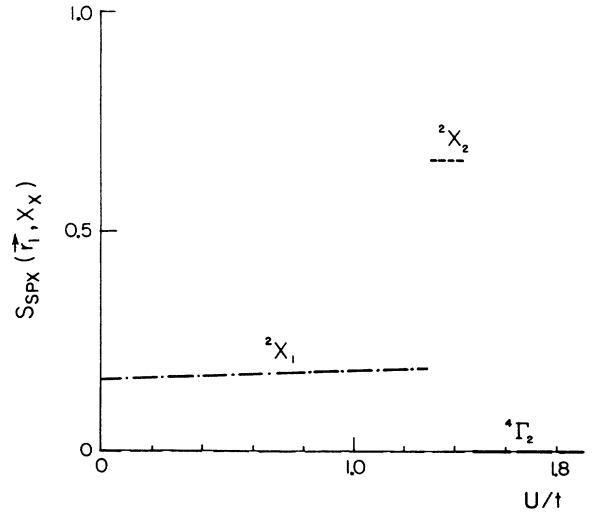

FIG. 10. The extended singlet-pairing superconducting correlation function of the ground state at the X_X point as a function of U/t for $\delta/t=0.3$ and $\gamma/t=0.6$. For the case $\delta=\gamma=0$, the ground state of symmetry $^4\Gamma_2$, the correlation function is zero.

states where same-site pairing is not allowed.

The SPX and TP superconducting correlation functions provide a different kind of information. It is useful to analyze some general properties of the corresponding order parameters. A change of variable $\mathbf{r}$ into $-\mathbf{r}$ in (3.6b)–(3.6d), and a substitution $\mathbf{R}_j=\mathbf{R}_i-\mathbf{r}$, yield

$$\Delta_{\mathrm{SPX}}(-\mathbf{r},\mathbf{q})=+e^{-i\mathbf{q}\cdot\mathbf{r}}\Delta_{\mathrm{SPX}}(\mathbf{r},\mathbf{q}) , \tag{3.12}$$

$$\Delta_{\mathrm{TP}}(-\mathbf{r},\mathbf{q})=-e^{-i\mathbf{q}\cdot\mathbf{r}}\Delta_{\mathrm{TP}}(\mathbf{r},\mathbf{q}) . \tag{3.13}$$

For $\mathbf{q}=\mathbf{0}$, Eqs. (3.12) and (3.13) simply state that for singlet (triplet) pairing the order parameter must be an even (odd) function of the relative coordinate $\mathbf{r}$.

However, in a fcc tetrahedral cluster with periodic boundary conditions the nearest-neighbor positions satisfy the condition $\mathbf{r}=-\mathbf{r}$. As a consequence there are the extra constraints

$$\Delta_{\mathrm{SPX\,(TP)}}(-\mathbf{r},\mathbf{q})=\Delta_{\mathrm{SPX\,(TP)}}(\mathbf{r},\mathbf{q}) , \tag{3.14}$$

which when replaced in (3.12) and (3.13), yield a set of conditions on $\mathbf{q}$ necessary to obtain nonvanishing values of Δ_μ. In particular, it is necessary to have $\mathbf{q}\cdot\mathbf{r}=0$ for Δ_{SPX} to be nonzero, and $\mathbf{q}\cdot\mathbf{r}=\pm\pi$ for a nonzero Δ_{TP}. In other words, for $\mathbf{q}=\Gamma$ it follows that for any $\mathbf{r}$

$$\Delta_{\mathrm{TP}}(\mathbf{r},\Gamma)=0 , \tag{3.15}$$

and for $\mathbf{q}=X_x$ the result implies

$$\begin{aligned}\Delta_{\mathrm{TP}}(0,X_x)&=\Delta_{\mathrm{TP}}(\mathbf{r}_1,X_x)\\&=\Delta_{\mathrm{SPX}}(\mathbf{r}_2,X_x)=\Delta_{\mathrm{SPX}}(\mathbf{r}_3,X_x)=0 ,\end{aligned} \tag{3.16}$$

with equivalent equations for X_y and X_z.

Table III and Figs. 9 and 10 show the SPX superconducting correlation functions for $\mathbf{k}=\Gamma$ and $\mathbf{k}=X_x$. It is found, in general, that strong superconducting susceptibilities exist for those symmetries, $^2X_1$ and $^2\Gamma_{12}$, favored by the presence of the electron-lattice interaction. The ferromagnetic state $^4\Gamma_2$, as expected, shows zero susceptibility for singlet pairing of any sort.

A very interesting case is the compromise antiferromagnetic states, $^2X_2$, stable for intermediate values of all parameters. These are the states with the strongest $S_{\mathrm{SPX}}(\mathbf{r}_1,X_x)$, $S_{\mathrm{SPX}}(\mathbf{r}_2,X_y)$, and $S_{\mathrm{SPX}}(\mathbf{r}_3,X_z)$. If, for *dynamical* reasons arising from the phonon structure and coupling, that particular form of superconductivity turns out to be the favored one, it will probably exist only for a finite range of intermediate values of the Coulomb interaction strength, assuming that the parameters δ and γ are also sizable.

For the $\mathbf{k}=\Gamma$ point of the Brillouin zone and SPX coupling, it is useful and interesting to make a completely different analysis of these superconducting susceptibilities. Three linear combinations of the three operators $\Delta_{\mathrm{SPX}}(\mathbf{r},\Gamma)$ can be defined

$$\Delta_s=\Delta_{\mathrm{SPX}}(\mathbf{r}_1,\Gamma)+\Delta_{\mathrm{SPX}}(\mathbf{r}_2,\Gamma)+\Delta_{\mathrm{SPX}}(\mathbf{r}_3,\Gamma) , \tag{3.17a}$$

$$\Delta_{d1}=\Delta_{\mathrm{SPX}}(\mathbf{r}_2,\Gamma)-\Delta_{\mathrm{SPX}}(\mathbf{r}_3,\Gamma) , \tag{3.17b}$$

$$\Delta_{d2}=2\Delta_{\mathrm{SPX}}(\mathbf{r}_1,\Gamma)-\Delta_{\mathrm{SPX}}(\mathbf{r}_2,\Gamma)-\Delta_{\mathrm{SPX}}(\mathbf{r}_3,\Gamma) . \tag{3.17c}$$

These three operators can be easily interpreted as the uniform ($\mathbf{k}=\Gamma$), extended-s-wave and d-wave superconducting order parameters.

Inversion of (3.17), and replacement of $\Delta_{\mathrm{SPX}}(\mathbf{r},\Gamma)$ into (3.5), yield

$$S_{\mathrm{SPX}}(\mathbf{r}_1,\Gamma)=\tfrac{1}{9}\langle(\Delta_s^\dagger+\Delta_{d2}^\dagger)(\Delta_s+\Delta_{d2})\rangle , \tag{3.18a}$$

$$\begin{aligned}S_{\mathrm{SPX}}(\mathbf{r}_2,\Gamma)=\tfrac{1}{4}\langle[\,&\tfrac{1}{9}(2\Delta_s^\dagger-\Delta_{d2}^\dagger)(2\Delta_s-\Delta_{d2})\\&+\tfrac{1}{3}(2\Delta_s^\dagger-\Delta_{d2}^\dagger)\Delta_{d1}\\&+\tfrac{1}{3}\Delta_{d1}^\dagger(2\Delta_s-\Delta_{d2})+\Delta_{d1}^\dagger\Delta_{d1}]\rangle ,\end{aligned} \tag{3.18b}$$

$$\begin{aligned}S_{\mathrm{SPX}}(\mathbf{r}_3,\Gamma)=\tfrac{1}{4}\langle[\,&\tfrac{1}{9}(2\Delta_s^\dagger-\Delta_{d2}^\dagger)(2\Delta_s-\Delta_{d2})\\&-\tfrac{1}{3}(2\Delta_s^\dagger-\Delta_{d2}^\dagger)\Delta_{d1}\\&-\tfrac{1}{3}\Delta_{d1}^\dagger(2\Delta_s-\Delta_{d2})+\Delta_{d1}^\dagger\Delta_{d1}]\rangle .\end{aligned} \tag{3.18c}$$

If these correlation functions are calculated for one of the two states of symmetry $^2X_1$ which are eigenstates of $S_{\mathrm{SPX}}(\mathbf{r}_1,\Gamma)$ with eigenvalue $\frac{2}{3}$ (see Table III), the results are

$$S_{\mathrm{SPX}}(\mathbf{r}_1,\Gamma)=\tfrac{2}{3},\quad S_{\mathrm{SPX}}(\mathbf{r}_2,\Gamma)=0,\quad S_{\mathrm{SPX}}(\mathbf{r}_3,\Gamma)=0 ; \tag{3.19}$$

in this case the relevant state is also an eigenstate of $S_{\mathrm{SPX}}(\mathbf{r}_2,\Gamma)$ and $S_{\mathrm{SPX}}(\mathbf{r}_3,\Gamma)$, but with eigenvalue 0. Similarly, a calculation for one of the two states of symmetry $^2\Gamma_{12}$ which are eigenstates of $S_{\mathrm{SPX}}(\mathbf{r}_1,\Gamma)$ with eigenvalue $\frac{2}{3}$ (Table III) yields

$$S_{\mathrm{SPX}}(\mathbf{r}_1,\Gamma)=\tfrac{2}{3},\quad S_{\mathrm{SPX}}(\mathbf{r}_2,\Gamma)=\tfrac{1}{6},\quad S_{\mathrm{SPX}}(\mathbf{r}_3,\Gamma)=\tfrac{1}{6} ; \tag{3.20}$$

this state is not an eigenstate of either $S_{\mathrm{SPX}}(\mathbf{r}_2,\Gamma)$ or $S_{\mathrm{SPX}}(\mathbf{r}_3,\Gamma)$. Examination of these cases shows a lack of symmetry among the various $\mathbf{r}$, a clear indication of a contribution of d-type superconductivity, since pure s-wave pairing requires

$$S_{\mathrm{SPX}}(\mathbf{r}_1,\Gamma)=S_{\mathrm{SPX}}(\mathbf{r}_2,\Gamma)=S_{\mathrm{SPX}}(\mathbf{r}_3,\Gamma) . \tag{3.21}$$

A more detailed analysis shows that whereas (3.20) is compatible with pure d-wave superconducting pairing, (3.19) can only arise from a mixing of s- and d-wave pairing.

Contrary to the behavior of S_{SP} shown in Fig. 8, Figs. 9 and 10 show that the various S_{SPX}, within each ground-state symmetry, *increase* with increasing values of U.

Finally Table IV shows the values for S_{TP}, the triplet-pairing superconductivity. The selection rules discussed above give vanishing susceptibilities for all $\mathbf{k}=\Gamma$, as well as for $(\mathbf{r}_1,X_x)$, $(\mathbf{r}_2,X_y)$, and $(\mathbf{r}_3,X_z)$. It is not surprising to find out that the maximum triplet-pairing susceptibility appears in the ferromagnetic $^4\Gamma_2$ manifold, where it reaches its maximum possible value of 1.

IV. CONCLUSIONS AND DISCUSSION

The following conclusions can be drawn from the calculation and results presented above.

(i) The *static* electron-lattice interaction introduced in the Hamiltonian (2.1), in which the electron hopping matrix elements depend on the pertinent-bond occupation, constitutes an effective *attractive* electron-electron interaction as long as the bonds with higher occupation have a *larger absolute value* of the hopping elements than bonds with fewer elements.

(ii) The most interesting case, and the only one discussed in this paper, is for an occupation of $\rho=\frac{3}{4}$ electrons per site for a band structure in which the three one-electron orbitals at $\mathbf{k}=X$ have a lower energy than the single orbital at $\mathbf{k}=\Gamma$.

(iii) Although the electron-lattice interaction contains four- and six-fermion-operator terms (2.2)–(2.4), and has not only a different sign but also a different form from the intrasite Coulomb repulsion term (2.5), the attractive and repulsive effects cancel each other *exactly* at a singular line (3.1) in parameter space. Along the singular line there is an extra accidental degeneracy in the ground-state manifold (identical to the noninteracting case).

(iv) All possible symmetries of the noninteracting case can become the ground-state symmetry, depending on how the interaction parameters change away from the singular line (Figs. 2 and 3).

(v) As expected from simple physical considerations, larger values of the Coulomb-repulsion parameter U favor states with larger local moments (Figs. 4 and 5). The electron-lattice interaction, on the other hand, favors low-spin states with electrons paired locally.

(vi) The dominant state for extreme values of the Coulomb-repulsion parameter, $U\rightarrow\infty$, is the perfectly aligned, saturated ferromagnet ${}^4\Gamma_2$, with perfect nearest-neighbor ferromagnetic correlations (Figs. 6 and 7). The other three symmetries are antiferromagnetically correlated. In particular the ${}^2X_2$ states, which are the lowest-energy states only for values of the parameters in which the various interactions compete, is a well-developed, frustrated (because of crystal structure) antiferromagnet.

(vii) States with large ordinary singlet-pairing superconducting fluctuations are favored, as expected, by the electron-lattice interaction and hindered by the presence of a large Coulomb repulsion.

(viii) Triplet-pairing superconducting fluctuations can only exist in the ferromagnetic states ${}^4\Gamma_2$ in this model.

(ix) Competition between (and perhaps coexistence of) superconductivity and antiferromagnetism seems to be the dominant feature of the ${}^2X_2$ states; these are compromise states, stable over a fairly narrow "wedge" of parameter space (comparable values of U and δ, and considerably smaller values of γ). If superconductivity gets established for this ground-state symmetry, it must be anisotropic, either of pure d-wave character, or a mixture of extended-s- and d-wave type.

The calculations presented here are extremely instructive. They have all the advantages and drawbacks of the small-cluster approach.[16–26] They clearly show the competing effects of the Coulomb repulsion and the "phonon" lattice polarization. And although they cannot prove, or disprove, the assertion that the Hubbard-like models can sustain intermediate-range attractive interactions,[9–16] they exhibit the reaccommodation of the electrons in configuration space caused by the various interactions in the Hamiltonian, and the resulting availability of occupied and empty orbitals necessary to produce various types of fluctuations, superconductivity in particular.

ACKNOWLEDGMENTS

The authors would like to thank Ariel Reich for many stimulating discussions. The hospitality of the Nordisk Institut for Teoretisk Atomfysik (Copenhagen, Denmark) and the H. C. Ørsted Institute during the authors' stay in Copenhagen is acknowledged with thanks. One of the authors (C.R.P.) would like to acknowledge the financial support of the Consejo Nacional de Investigaciones Científicas y Técnicas (Argentina). This research was supported in part at the Lawrence Berkeley Laboratory by the Director, Office of Energy Research, Materials Science Division, U.S. Department of Energy, under Contract No. DE-AC03-76SF00098.

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[33]These equations are identical to those of Ref. 24 (Table V, $N=3$), with $\delta=\gamma=0$, and the substitutions $t\rightarrow -t$, $\Gamma_{12}\rightarrow\Gamma_3$, $X_1\rightarrow\Gamma_4$, and $X_2\rightarrow\Gamma_5$.

[34]It can be mentioned in passing that the attractive-interaction regime, $U<0$, favors the ${}^2\Gamma_2$ symmetry if $\delta=\gamma=0$, but changes in values of δ and γ with respect to U can lead to the other three symmetries. The singular line (3.1) extends to the region of negative U.

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