Magnetism and pairing in a C$_{60}$ molecule: A variational Monte Carlo study

D. N. Sheng, Z. Y. Weng, and C. S. Ting

Texas Center for Superconductivity, University of Houston, Houston, Texas 77204-5506

J. M. Dong

Department of Physics, Nanjing University, Nanjing, China

(Received 4 December 1992; revised manuscript received 31 August 1993)

The ground-state properties of electrons in the C$_{60}$ geometry is studied based on the t-J-like Hamiltonian. By using a variational Monte Carlo method, it is found that the Gutzwiller projected Fermi-sea state and the pure RVB state have the lowest variational energies in the undoped case as compared to other spin singlet states. For a doped C$_{60}$ molecule, the electron pairing and itinerant ferromagnetism are discussed. A comparison with related works is also presented.

I. INTRODUCTION

The discovery of superconductivity in the alkali-doped C$_{60}$ system$^1$ naturally leads to the question of mechanism: whether the superconductivity is due to the conventional electron-phonon interaction or to the electron-electron correlations. It is still a controversial$^{2-7}$ subject, and one of the important issues is how the special band structure of C$_{60}$ plays a role in the renormalization of the Coulomb pseudopotential.$^{5,8,9}$

In the C$_{60}$ crystal, the band structure calculations$^{10}$ show that those energy levels which have considerable dispersion below and above the Fermi level mainly come from the π-bond states of a C$_{60}$ molecule. These π-electron states can be described by the tight-binding model$^{11}$ and form many narrow subbands with an overall bandwidth $\sim 10$ eV. With the presence of a moderate bare on-site Coulomb interaction (at $U \sim 6-12$ eV), the electron-electron correlations would become crucial if the system was a square lattice, like in the copper oxide materials. In the latter case, the low-energy physics in the weak- and intermediate-coupling regimes can be continuously scaled down to the strong-coupling regime, without encountering a Mott-insulator phase-transition point $U_c$ (at the half-filling). In the C$_{60}$ system, however, a finite $U_c$ could exist and if $U < U_c$, one expects that the usual screening retardation effect in determining the Coulomb pseudopotential is valid.$^{2,3}$ But when $U > U_c$, the on-site electron-electron correlations would become so predominant that their effect should be included before any screening effects are considered.

In this paper, instead of determining whether the realistic regime lies at $U > U_c$ or $U < U_c$, we will confine ourselves to a less ambitious goal by assuming $U > U_c$ and then asking what the possible ground state is in this strong-coupling case. Since the hopping inside the C$_{60}$ molecule is much stronger than between the molecules, we will consider the Hubbard model on a single C$_{60}$ molecule. This model has been previously discussed by Chakravarty, Gelfand, and Kivelson$^4$ in the weak-coupling regime. We will be interested in its large-$U$ version, which is similar to the well-known t-J model on the square lattice,

$$
\hat{H} = J_1 \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J_2 \sum_{\langle\langle ij \rangle\rangle} \mathbf{S}_i \cdot \mathbf{S}_j - t_1 \sum_{\langle ij \rangle} \rho_d \mathbf{C}_{\sigma} \mathbf{C}_{\sigma} \rho_d \mathbf{P}_d - t_2 \sum_{\langle\langle ij \rangle\rangle} \rho_d \mathbf{C}_{\sigma} \mathbf{C}_{\sigma} \rho_d + \text{H.c.},
$$

(1.1)

where the primed sum runs over all of the 30 interpentagon bonds and the double-primed sum runs over all of the 60 intrapentagon bonds on the surface of the C$_{60}$ molecule. In the undoped case only the first two terms, namely, the superexchange coupling, in (1.1) exist. $\mathbf{S}_i$ is the spin operator of the π electron. Spin exchange $J_1$ will usually be slightly larger than $J_2$ because the pentagon bonds are slightly longer. The remaining terms in (1.1) describe the hopping processes, with $\rho_d$ being the projection operators which impose the constraint of no vacant sites under the electron doping.

For the undoped case, (1.1) has been studied recently by Coffey and Trugman$^{12}$ by using the classical spin (large-S) method with the zero-point spin fluctuations included in the second-order perturbation. In that calculation, they found the long-range spin order to survive quantum fluctuations on the C$_{60}$ sphere. However, the antiferromagnetic frustration within an elementary pentagon may make the C$_{60}$ molecule a proper candidate to have a spin singlet ($S=0$) ground state. In the present paper, various possible spin singlet states on the C$_{60}$ geometry will be systematically studied by the numerical variational Monte Carlo (VMC) method.$^{13,14}$ Furthermore, electron-doping effects, including pairing and itinerant ferromagnetism, will be discussed for a range of parameters. In Sec. II, we consider the undoped C$_{60}$ molecule described by (1.1). Various resonating-valence-bond (RVB) states are reexamined for the present spherical lattice system. In this system they exhibit the differ-
ent trends as compared to the square lattice case. In Sec. III, the electron-doped case is investigated and a rich variety of possible phases is found in the metallic regime. Finally, Sec. IV is devoted to the summary and a brief discussion.

II. UNDOPED C₆₀ MOLECULE

For a square lattice, various RVB states with short-range spin-spin correlations have been proposed as the possible ground states for the t-J model. In the undoped case, however, the long-range antiferromagnetic state turns out to have the lowest energy. Nevertheless, the RVB states are believed to become energetically competitive once some proper frustration is introduced. In the present C₆₀ geometry, the frustration of antiferromagnetic coupling is obvious: Unlike in the square lattice case, within a pentagon (cf. Fig. 1) there exists no spin configuration that would allow every bond to reach the maximum classical energy of −J₁/4. In the following, we will re-examine various RVB states in the C₆₀ molecule by using the variational Monte Carlo method.

For the undoped case, there is one electron per site, and only the superexchange coupling terms in (1.1) remain. The Hamiltonian (1.1) then reduces to the form

\[
H_J = \sum_{(ij)} \left( \sum_{\sigma} C_{i\sigma}^\dagger C_{j\sigma} \right) \frac{\sigma}{4} C_{j\sigma}^\dagger C_{j'\sigma'} \\
+ \frac{1}{2} \sum_{(ij)} \left( \sum_{\sigma} C_{i\sigma}^\dagger C_{j-\sigma}^\dagger C_{j'\sigma'} \right) P_d \\
+ J_2 \sum_{(ij)} \left( \sum_{\sigma} C_{i\sigma}^\dagger C_{i\sigma} \right) \left( \sum_{\sigma'} C_{j\sigma'}^\dagger C_{j\sigma'} \right) \\
+ \frac{1}{2} \sum_{(ij)} \left( \sum_{\sigma} C_{i\sigma}^\dagger C_{i-\sigma} C_{j\sigma}^\dagger C_{j\sigma} \right) P_d, \tag{2.1}
\]

after the spin operator \(S_i\) is expressed by the electron operators \(C_{i\sigma}\) as \(S_i = \frac{1}{2} \sum_{\sigma} C_{i\sigma}^\dagger (\sigma) C_{i\sigma}\). Here, \(\sigma\) is the Pauli matrix and the spin index \(\sigma (\sigma') = \pm 1\). The Hamiltonian (2.1) is then expressed as the sum of the mean-field Hamiltonian \(H_{MF}\) and the interaction part. For C₆₀, the Pauli spin matrices are expressed as

\[
H_{MF} = -\frac{3}{8} J_1 g_1^2 p_1 \sum_{(ij)} C_{i\sigma}^\dagger C_{j\sigma} - \frac{3}{8} J_2 g_2^2 p_2 \sum_{(ij)} C_{i\sigma}^\dagger C_{j\sigma} + H.c. \\
-\frac{3}{8} J_1 \Delta_1 \sum_{(ij)} C_{i\sigma}^\dagger C_{j-\sigma}^\dagger - \frac{3}{8} J_2 \Delta_2 \sum_{(ij)} C_{i\sigma}^\dagger C_{j-\sigma}^\dagger + H.c. - \mu \left( \sum_{\sigma} C_{i\sigma}^\dagger C_{i\sigma} - N_e \right), \tag{2.3}
\]

where \(N_e = N_a\) at half-filling, with \(N_e\) being the total number of electrons and \(N_a = 60\) being the total number of sites per molecule. The order parameters \(p_1 (\Delta_1)\) and \(p_2 (\Delta_2)\) are defined by \(p_1 = \sum_{\sigma} (C_{i\sigma}^\dagger C_{j\sigma})\) \((\Delta_1 = \sum_{\sigma} (C_{j\sigma}^\dagger C_{i-\sigma})\) and \(p_2 = \sum_{\sigma} (C_{i\sigma}^\dagger C_{j\sigma})\) \((\Delta_2 = \sum_{\sigma} (C_{i\sigma}^\dagger C_{j-\sigma})\), corresponding to nonpentagon and pentagon bonds, respectively.

FIG. 1. Geometry of the molecule C₆₀. The pentagon bonds (solid lines) are slightly longer than the hexagon bonds (dashed lines).

The ground state is expected to be the ground state of the mean-field Hamiltonian (2.3) without

\[
\langle P_d S_i \cdot S_j \rangle = g_s \langle S_i \cdot S_j \rangle, \tag{2.4}
\]

where \(g_s = g_s^1\) for nonpentagon bond and \(g_s = g_s^2\) for pentagon bond. \(\langle \cdots \rangle_0\) is the expectation value under the ground state of the mean-field Hamiltonian (2.3) without

has been replaced in (2.3) by the so-called renormalization factor \(g_s^{1,2}\), in the following way:
imposing the no-double-occupancy constraint.

In the following, we will take $g^+_1 p_1 \rightarrow p_1$ and $g^+_2 p_2 \rightarrow p_2$ as two independent variational parameters and construct variational wave functions based on (2.3). We will minimize the energy expectation value of the original Hamiltonian (2.1) under these trial wave functions by performing VMC calculation to exactly implement the constraint (2.2).

A. Gutzwiller-projected Fermi-sea state

The simplest spin singlet state is the so-called projected Fermi-sea state with only the nearest-neighbor hopping order parameters $p_1$ and $p_2$ (putting $\Delta_1 = \Delta_2 = 0$). Diagonalizing (2.3) to get the ground-state wave function $|\Psi_0\rangle$, we obtain

$$|\Psi_0\rangle = \prod_{\{i\}} \gamma^+_{i\uparrow} \gamma^+_{i\downarrow} |0\rangle,$$

(2.5)

where $\gamma^+_{i\sigma}$ is the raising operator of an eigenstate of (2.3), $\gamma^+_{i\sigma} = \sqrt{N_c} \sum_a c_{i\sigma}^a$. The product in (2.5) runs over 30 eigenstates with the lowest energy. Thus the variational wave function, after projecting out double occupancy, is the product of two determinants:

$$|\Psi\rangle = P_d |\Psi_0\rangle = \sum_{\{i\} \{j\}} \det(a_{i\uparrow}) \det(a_{j\downarrow}) C_{i\uparrow}^\dagger C_{j\downarrow}^\dagger \cdots C_{i\downarrow}^\dagger |0\rangle,$$

(2.6)

Both $s_1$ and $s_2$ run over 30 occupied eigenstates. The sum includes only the configurations in which all the sites occupied by the spin-up electrons $\{i\}$ (30 sites) and the spin-down electrons $\{j\}$ (30 sites) have no overlap. Given the variational wave function (2.6), the energy expectation value of original Hamiltonian (2.1), i.e., $E(p_1/p_2) = \langle \Psi | H | \Psi \rangle$, can be evaluated by the Monte Carlo (MC) method.\textsuperscript{13,14}

In Fig. 2 we plot the variational energy $E(p_1/p_2)$ as a function of $p_1/p_2$. The two curves correspond to $J_1/J_2 = 1.0$ and 1.1, respectively. The energy minimum appears around $p_1/p_2 \sim 0.9$, which is a very broad minimum, as shown in Fig. 2. At the minimal energy point, for $J_1 = J_2 = J$ case, $\langle S_i \cdot S_j \rangle = -0.34256 \pm 0.0001$ and the total energy is about $-30.83J$. This is much lower than the fully dimerized state ($p_1 = 1$ and $p_2 = 0$), and it compares very well with the energy of the Coffey-Trugman state with a long-range spin order (our energy is only 0.7\% higher).\textsuperscript{12} We have performed about 80 000 MC steps per site in order to gain high precision.

The spin-spin correlation $\langle \Psi | S_i \cdot S_j | \Psi \rangle$ as a function of the position of site $i$ relative to site 0 is also shown in Fig. 3. The sites 0 and $i$ for $i = 1, \ldots, 11$ have been defined in Fig. 1. The spin correlations are not sensitive to the exchange parameters $J_1$ and $J_2$. Figure 3 shows that the local spin structure is quite similar to the classical spin array obtained in Ref. 12. Considering this similarity and the closeness of the energies, one may find it amazing that these are, superficially, two quite different states: One is a spin singlet state while the other has a long-range spin order which survives the quantum fluctuation. Given such an extremely small energy difference (0.7\%) between the two states, it is hard to tell which of them is more stable. A possibility of a deep connection between these states needs further exploration.

B. Flux state and other RVB states

We have shown that the projected "Fermi-sea" state has a rather favorable energy. However, in the square lattice case, it is well known that there are two other kinds of spin liquid states which have even lower energy: i.e., the $\pi$-flux state and the $d$-wave RVB state. These two states are degenerate and actually related to each other by a SU(2) transformation at half-filling. We shall consider the generalization of these states in the $C_{60}$ case below.

In the flux state, it is an important fact that the particles' hopping amplitudes are always accompanied by phase factors. If one particle goes through a closed loop and returns to its original position, it can gain an extra phase which is proportional to the average number of particles enclosed in the loop. We will consider the $\pi$-flux state in which each electron contributes effectively a $\pi$ flux. For the geometry of the $C_{60}$ molecule, a di-
rect counting gives a $2\pi$ flux penetrating through each nonpentagon and a $3\pi/3$ flux going through each pentagon, respectively. The effective mean-field Hamiltonian (2.3) is then changed to the following form (with $\Delta_1 = \Delta_2 = 0$):

$$H_{MP} = -\frac{3}{8} J_1 p_1 \sum_{\langle ij \rangle} e^{i\Phi_{ij}} C^\dagger_{i\sigma} C_{j\sigma} - \frac{3}{8} J_2 p_2 \sum_{\langle ij \rangle} e^{i\Phi_{ij}} C^\dagger_{i\sigma} C_{j\sigma} + \text{H.c.}, \quad (2.7)$$

with the order parameters redefined as $p_1 = g_1^2 \langle \sum_{\sigma} e^{i\Phi_{ij}} C^\dagger_{i\sigma} C_{j\sigma} \rangle_1$ and $p_2 = g_2^2 \langle \sum_{\sigma} e^{i\Phi_{ij}} C^\dagger_{i\sigma} C_{j\sigma} \rangle_2$. $\Phi_{ij}$ is a phase factor connected to the fictitious magnetic field $A$ by $\Phi_{ij} = \int_{A} A \cdot dl$ with the aforementioned flux given by

$$\int A \cdot dl = \begin{cases} 2\pi & \text{for a hexagon,} \\ 5\pi/3 & \text{for a pentagon}. \end{cases} \quad (2.8)$$

Treating $p_1/p_2$ as the variational parameter, we put a phase $\Phi_{ij}$ satisfying the constraint (2.8) on each bond and then diagonalize Hamiltonian (2.7). The variational energy of (2.1) under such a trial wave function is calculated as a function of $p_1/p_2$, and is shown in Fig. 4. At the energy minimum, $(S_i \cdot S_j) = -0.339$ for $J_1 = J_2$ case, which is about 1% higher than the projected "Fermi-sea" state. For $J_1 > J_2$, the energy minimum is always a little bit higher than the projected "Fermi-sea" state. We have also checked other flux states (each particle carrying a flux other than $\pi$), and found them to always give higher energies.

Next we consider the RVB state with nonzero order parameter $\Delta \propto (C_{ij} + C_{ji})$. Now we need to vary five variational parameters $p_1, p_2, \Delta_1, \Delta_2$, and the chemical potential $\mu$ in (2.3) and try to find the energy minimum of Hamiltonian (2.1). We may always rescale one of these parameters to unity (for example, set $p_2 = 1$) so that we have only four parameters left.

Basically two regions containing local energy minima have been found. One corresponds to $p_1 \sim p_2 \neq 0$ but with $\Delta_1 = \Delta_2 = 0$ which is just the Gutzwiller projected Fermi-sea state discussed in Sec. II A. There is an another minimum at $\Delta_1/\Delta_2 = 0.90$ but the hopping amplitude $p_1 = p_2 = 0$. This is the pure "RVB" state which resembles the $s$-wave RVB in the square lattice case. We note that the $s$-wave RVB state is equivalent to the projected Fermi-sea state through a SU(2) transformation on a square lattice. In the present pure "RVB" state, $(S_i \cdot S_j) = 0.34256 \pm 0.00016$ which is almost identical to that of the projected "Fermi-sea" state, even though we have no analytical proof for their equivalency here. We have performed around $6 \times 10^3 - 10 \times 10^3$ MC steps per site. The error bar is about $\pm 0.00016$. No other minimum is found in the region where $p_1, p_2$ as well as $\Delta_1$ and $\Delta_2$ are all finite.

In summary, we have carried out the VMC calculations for three kinds of states: the projected "Fermi-sea" state, the flux state, and the RVB states with the order parameter $(C_{ij} + C_{ji})$. The results are quite different from those of a square lattice case. The "Fermi-sea" state and the pure "RVB" (no hopping order parameters) are found to have the lowest energy among these states.

### III. ELECTRON-DOPED C$_{60}$ MOLECULE

In the previous section, we have discussed the possible ground states for the undoped C$_{60}$ molecule in the large-$U$ limit. Of them, the most energetically favorable are found to be the projected "Fermi-sea" state and the pure "RVB" state. In the present section, we shall study the doping effect after some additional electrons are added into the C$_{60}$ molecule.

In the doped case, the electron hopping terms will emerge, as in the Hamiltonian (1.1). Each site is either singly occupied or doubly occupied due to the doped electrons. The corresponding mean-field Hamiltonian is the same as (2.3) with $N_e = N_a + N_d$ and $N_d$ being the total number of the doped electrons on the molecule. The mean fields $p_1$ and $p_2$ now include both the electron hopping and the spin superexchange effects. The procedure for solving this variational problem is the same as in the undoped case.

For the case of two added electrons, we plot the energy difference $E_{1+} - E_{1+}$ (i.e., the difference between the total energies of one molecule with two doped electrons carrying opposite spins and parallel spins, respectively) in Fig. 5 as a function of $t/J$. For simplicity, we have
chosen \( t_1 = t_2 = t \) and \( J_1 = J_2 = J \), neglecting the small dimerization effect in the real system. Around \( t \sim 2J \) there is a transition as shown in Fig. 5. For smaller \( t/J, \ E_{\uparrow \downarrow} - E_{\uparrow \uparrow} < 0 \), the spin superexchange interaction is dominant and the doped electrons prefer to be in the singlet state. On the other hand, for a larger \( t/J, \ E_{\uparrow \downarrow} - E_{\uparrow \uparrow} > 0 \), the hopping term will be dominant and two doped electrons prefer to have parallel spins. Contrary to the undoped case, the nonzero order parameters \( \Delta_1 \) and \( \Delta_2 \) will always slightly lower the energy of the projected “Fermi-sea” state as \( t/J < 2 \) and thus a RVB state with both hopping and pairing parameters becomes stabilized upon doping.

A similar situation is found for the case of three and four doped electrons. In the case of three doped electrons, \( E_{\uparrow \uparrow \downarrow} - E_{\uparrow \uparrow \uparrow} \) is plotted in Fig. 6. A transition between the parallel and antiparallel spin states happens around \( t/J \sim 3 \). For the four electron case, we have three different situations: four spins parallel to each other, one flipped spin, and two flipped spins. Their corresponding energies are denoted by \( E_{\uparrow \uparrow \uparrow \downarrow} \), \( E_{\uparrow \uparrow \downarrow \downarrow} \), and \( E_{\uparrow \uparrow \uparrow \uparrow} \), respectively. Before doping, the lowest unoccupied eigenstates are threefold degenerate before the single-occupancy projection. One expects \( E_{\uparrow \uparrow \uparrow \uparrow} \) to be much higher than the other states because one doped electron has to occupy a higher-energy eigenstate. It turns out to be true even after the projection. In Fig. 7 we plot both \( E_{\uparrow \uparrow \downarrow \downarrow} - E_{\uparrow \uparrow \uparrow \uparrow} \) and \( E_{\uparrow \uparrow \uparrow \uparrow} - E_{\uparrow \uparrow \uparrow \uparrow} \) as functions of the parameter \( t/J \). The former energy difference is quite large and has a magnitude around \( (0.1-0.2)J \), which could be considered as the gap between the lowest unoccupied miniband and the second-lowest unoccupied miniband (before doping). As for \( E_{\uparrow \uparrow \uparrow \downarrow} - E_{\uparrow \uparrow \uparrow \uparrow} \), it is about several times smaller and there is also a transition around \( t/J \sim 2 \). For smaller \( t/J \) a spin singlet is preferred while for larger \( t/J \) a triplet is favored.

The above results suggest that for smaller \( t/J \), the spin singlet state, while for larger \( t/J \) \( (\geq 2) \), the spin triplet state is favorable which may lead to the itinerant ferromagnetism in the doped \( C_{60} \) crystal. In the latter case, the energy gap between the triplet state and the excited singlet state is quite small \( (\sim 0.013J) \) which suggests a low transition temperature ferromagnetism, in agreement with the experiment.\(^6\)

\[
\text{FIG. 6. The energy difference between two three-electron-doped states with different spins.}
\]

\[
\text{FIG. 7. The energy differences for the four-electron-doped cases.}
\]

In the doped \( C_{60} \) crystal \( [n \text{-electron doped molecule}] \) is denoted by \( C_{60}(n) \), the electrons may actually redistribute themselves to form, say, a mixture of \( C_{60}(n-1) \) and \( C_{60}(n+1) \) molecules, etc. Therefore, it is needed to check the stability of the molecule \( C_{60}(n) \) by calculating the binding energy defined as \( \Delta E_n = 2E_n - (E_{n+1} + E_{n-1}) \) where \( E_n \) is the lowest variational energy for a single \( C_{60}(n) \) molecule. If \( \Delta E_n < 0 \), one can say \( C_{60}(n) \) is locally stable, but when \( \Delta E_n > 0 \), electrons are likely to redistribute to form \( C_{60}(n-1) \) and \( C_{60}(n+1) \) molecules. \( \Delta E_n \) versus \( t/J \) for \( n = 1, 2, \) and 3 is shown in Fig. 8. For \( n = 1 \) and 3, the curves are similar. In smaller \( t/J \) region \( (\leq 2 \sim -4) \), \( \Delta E_n > 0 \) for \( n = 1 \) and 3, and thus the electrons prefer to redistribute themselves so that each molecule contains an even number of electrons. On the other hand, when \( t \) is sufficiently larger than \( J \), \( \Delta E_n < 0 \) for \( n = 1, 3 \) and the electrons will be distributed uniformly. As for the \( n = 2 \) case, the molecule is stable (i.e., \( \Delta E_2 < 0 \)) for most values of \( t/J \) as shown in Fig. 8. Only in an intermediate regime of \( t/J \sim 0.7-2.5 \), the charged molecule \( C_{60}(2) \) may not be stable due to \( \Delta E_2 > 0 \), but the absolute value of \( \Delta E_2 \) is very close to the error bar \( (\sim 0.013t) \) there.

\[
\text{FIG. 8. The binding energy } \Delta E_n = 2E_n - (E_{n+1} + E_{n-1}) \text{ versus } t/J \text{ for } n = 1, 2, \text{ and } 3.
\]
IV. SUMMARY AND DISCUSSION

We have studied the Hubbard type model for the C$_{60}$ molecule proposed in Ref. 4 in the limit of large on-site Coulomb interaction. On the C$_{60}$ geometry, the frustration of the antiferromagnetic coupling naturally occurs so that the short-range singlet spin states become energetically favorable. We have investigated the variational energies of these states on the C$_{60}$ geometry by using the VMC numerical method.

In the undoped C$_{60}$ molecule, the Gutzwiller-projected “Fermi-sea” state and the pure “RVB” state have been shown to have the lowest variational energies among the various spin singlet states. In the square lattice case, the projected “Fermi-sea” state and the pure “RVB” state are actually equivalent due to the SU(2) invariance. For C$_{60}$ geometry, they are also found to be degenerate within the error bar of our numerical computation, even though an analytic proof is absent. In contrast to the square lattice, however, the counterparts of the flux state and the $d$-wave RVB state in C$_{60}$ have relatively higher energies than the projected “Fermi-sea” state. This is due to the antiferromagnetic frustration on the C$_{60}$ sphere. The local spin-spin correlations have shown a very similar structure to that given by the approach base on the classical spins.\textsuperscript{12} This fact may make it possible to construct a path-integral theory by defining a local spin reference axis, which would be useful for studying the breakdown point $U_c$ of the present large-$U$ approach.\textsuperscript{17}

When two electrons are added to the C$_{60}$ molecule, it is found that both the hopping amplitude and the RVB order parameters, $\Delta_1$ and $\Delta_2$, become nonzero when $t/J < 2$ and the doped electrons are in singlet pairing. If $t/J > 2$, the triplet state is more stable where $\Delta_1 = \Delta_2 = 0$ in most regime. For one-electron, three-electron, or four-electron doped cases, $\Delta_1$ and $\Delta_2$ seem too small to be determined in our work.

For different doped cases, it has been found that the larger spin state will be favored once $t/J$ is large enough. This leads to the possibility of the existence of itinerant ferromagnetism in the C$_{60}$ system.\textsuperscript{16} Chakravarty, Gelfand, and Kivelson\textsuperscript{4} have first discussed such an electron-electron interaction mechanism for itinerant ferromagnetism by using a second-order perturbation theory for $U$. Nevertheless, our phase diagram does not seem to be a simple extrapolation of what was obtained in the weak-coupling regime. Whether the present strong-coupling approach can be continuously extended down to the realistic region for C$_{60}$ system, without encountering a phase boundary, still needs further investigation.

V. ACKNOWLEDGMENTS

The authors would like to thank G. Baskaran, B. Friedman, and J. Yang for the helpful discussions. The critical reading of the manuscript by D. Frenkel is gratefully acknowledged. The present work is supported by a grant from Robert A. Welch Foundation and the Texas Center for Superconductivity at the University of Houston.

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