

Electronic pair binding and Hund's rule violations in doped C₆₀Hong-Chen Jiang¹ and Steven Kivelson²¹*Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory and Stanford University, Menlo Park, California 94025, USA*²*Department of Physics, Stanford University, Stanford, California 94305, USA*

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We calculate the electronic properties of the t - J model on a C₆₀ molecule using the density-matrix renormalization group and show that Hund's first rule is violated and that for an average of three added electrons per molecule, an effective attraction (pair binding) arises for intermediate values of t/J . Specifically, it is energetically favorable to put four electrons on one C₆₀ and two on a second rather than putting three on each. Our results show that a dominantly electronic mechanism of superconductivity is possible in doped C₆₀.

DOI: [10.1103/PhysRevB.93.165406](https://doi.org/10.1103/PhysRevB.93.165406)**I. INTRODUCTION**

Interest in the superconductivity of the alkali-metal doped C₆₀ compounds (fullerides) [1–3] derives in part from their status as a new class of superconductors with large values of the superconducting critical temperatures T_c [4]. There has been a great effort over the last two decades to characterize and understand both the normal-state and the superconducting properties of fullerides. A source of renewed interest in these systems is the surprising indication of magnetism derived from strong electron-electron repulsions in crystals in which the C₆₀-C₆₀ distance is modestly expanded [5–9]. Several examples are now known where this kind of expansion first leads to superconductivity with a dome-shaped T_c , followed by a Mott insulating state. A superconducting dome proximate to an antiferromagnetic Mott insulating state is a hallmark of strong electron correlations in the high-temperature superconducting cuprates and organic charge-transfer salts; its appearance in alkali-metal doped C₆₀ suggests that electron correlations are crucial in understanding the superconductivity in these materials, as well.

Although most theoretical work has focused on phonon mechanisms, a dominantly electronic mechanism has also been considered. In particular, it was argued in Refs. [10,11] that the special geometry of the C₆₀ molecule (that of a truncated icosahedron—or more colloquially a soccer ball) permits subtle intramolecular electronic correlation effects that give rise to an effective attraction (i.e., positive pair binding energy) between doped electrons and violations of Hund's first rule. This conjecture was supported by extrapolating second-order perturbative calculations for the one-band Hubbard model on the C₆₀ structure to intermediate values of U/t (where, strictly speaking, low-order perturbation theory is not justified). These inferences were also supported [12] by exact diagonalization (ED) studies of smaller “Hubbard molecules”—especially the somewhat analogous 12-site truncated tetrahedron. However, various later numerical studies [13–21] of the C₆₀ problem gave inconclusive and conflicting results. Most significantly, the best existing quantum Monte Carlo (QMC) calculations [22] on the same system suggested significant failures of the extrapolated perturbation theory; in particular, the QMC results seemingly support the validity of Hund's rule and an absence of pair binding.

In order to resolve the issues of principle, we use density-matrix renormalization group (DMRG) [23–25] to investigate the ground-state properties of the t - J model on a single C₆₀ molecule, including the magnetic properties and electronic pair binding energy of doped electrons. The t - J model [see Eq. (1)] is a simplified model of doped C₆₀ which, in common with the Hubbard model, can plausibly be assumed to capture the most significant correlation effects of the system. Moreover, since the t - J model is defined on a significantly smaller Hilbert space, it is much less numerically demanding than the Hubbard model. Our most important conclusion is that electronic pair binding (an effective attractive interaction) arising from a purely electron-electron repulsion is a now established feature of the t - J model for a finite interval of the dimensionless parameter, t/J . In particular, it is energetically favorable to add four electrons to one C₆₀ molecule and two to a second rather than to add three electrons to each of two C₆₀ molecules—i.e., there is a positive pair binding energy. In addition, we find that Hund's first rule is violated; the ground state is the state of minimal total spin rather than maximal. For instance, we find that the ground states with two and four doped electrons has spin zero while the ground state with three doped electrons has spin 1/2.

In the noninteracting limit, the electronic structure of the C₆₀ molecule is well known [26], and the electronic states can be labeled according to the irreducible representations of the icosahedral group. The neutral C₆₀ molecule has a unique ground state and a substantial gap between the filled and empty orbitals. The lowest unoccupied molecular orbitals are the threefold-degenerate t_{1u} orbitals, whose degeneracy is an important property of the molecule. For many purposes, the C₆₀ molecule can be approximated as a sphere, and the t_{1u} orbitals can then be thought of as p orbitals with “angular momentum” $L = 1$. The electrons donated by the alkali-metal atoms to the C₆₀ molecule enter the threefold-degenerate t_{1u} orbitals. In the presence of orbital degeneracy and weak interactions, the Hund's rules can be derived perturbatively [10], where Hund's first rule is that the exchange energy is minimized when the molecular state has the highest possible total spin and the second rule is that it has the highest total orbital angular momentum compatible with the first rule. These rules, if they applied, would imply that the ground state has a total spin 1 and “angular momentum” 1 when doped with two

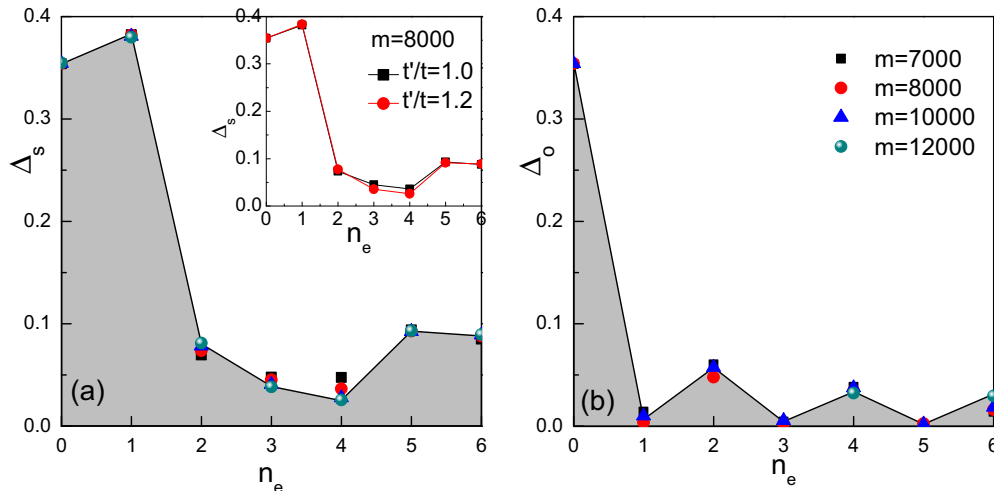


FIG. 1. (a) The “spin gap” Δ_s and (b) orbital gap Δ_o (defined in Sec. IV) as a function of number of added electrons n_e , for different number of DMRG states m . Here $t/J = 2$. The inset in (a) shows the “spin gap” Δ_s for $t'/t = 1.0$ and $t'/t = 1.2$.

or four electrons, and a total spin $3/2$ and “angular momentum” 0 when doped with three electrons.

II. VERIFYING CONVERGENCE

The steps we have taken to test that all our DMRG results for the t - J model on the C_{60} molecule have converged with high accuracy are described in detail in Appendix B. To get convincing results we have had to keep large numbers of DMRG states (e.g., up to $m = 12000$ states), and to iterate the DMRG a large number of times (e.g., up to 100 sweeps). However, by doing this we have been able to obtain results that we are confident have converged to the exact answer. The Hubbard model on a single C_{60} would, presumably, require keeping an even larger number of states; we have not currently succeeded in obtaining clearly converged results for this more difficult problem.

As a further test of the reliability of our simulation, we have benchmarked the DMRG method on the one-band Hubbard model on the C_{20} molecule. (See Appendix A for details.) We find that the DMRG results converge very rapidly to the exact diagonalization (ED) results, even with a relatively small number of DMRG states, and in particular gets values for both the ground-state energy and the pair binding energy that are more accurate than those obtained using QMC. (See Fig. 3 in Appendix A for details.)

III. t - J MODEL ON A C_{60} MOLECULE

We now investigate the ground-state properties of the t - J model on the single C_{60} molecule using DMRG. The t - J model Hamiltonian on the C_{60} molecule is

$$H = \sum_{\langle ij \rangle \sigma} t_{ij} (c_{i\sigma}^+ c_{j\sigma} + \text{H.c.}) + J \sum_{\langle ij \rangle} \left(\vec{S}_i \cdot \vec{S}_j - \frac{1}{4} n_i n_j \right), \quad (1)$$

where $\langle ij \rangle$ are nearest-neighbor (NN) sites, $c_{i\sigma}^+$ ($c_{i\sigma}$) is a fermionic creation (annihilation) operator with spin- σ on site i , \vec{S}_i is the spin, and $n_i = \sum_{\sigma} c_{i\sigma}^+ c_{i\sigma}$ is the number of holes on site i . The Hilbert space is constrained by the no-double

occupancy condition, $n_i \leq 1$. The sign of the hopping term in Eq. (1) is the opposite of the usual convention. We are interested in “electron-doped” C_{60} in which the total number of electrons is $N_e = 60 + n_e$, where $n_e = 0-6$ is the number of “doped” electrons added to the neutral C_{60} molecule. However, in deriving Eq. (1), we have made a particle-hole transformation, which results in this sign change, and correspondingly it is to be understood that $\sum_i n_i = 60 - n_e$. In the C_{60} molecule, there are two inequivalent sets of NN bonds—those bounding pentagonal plaquettes $t_{ij} = t$ and those connecting the pentagons $t_{ij} = t'$. The relation between them is believed to be $1.0 < t'/t < 1.3$ [10]. In our simulation, we consider two cases with different values of t'/t , i.e., $t'/t = 1$ and $t'/t = 1.2$. As shown in Figs. 1(a) and 2, both cases give qualitatively similar results. Thus, to

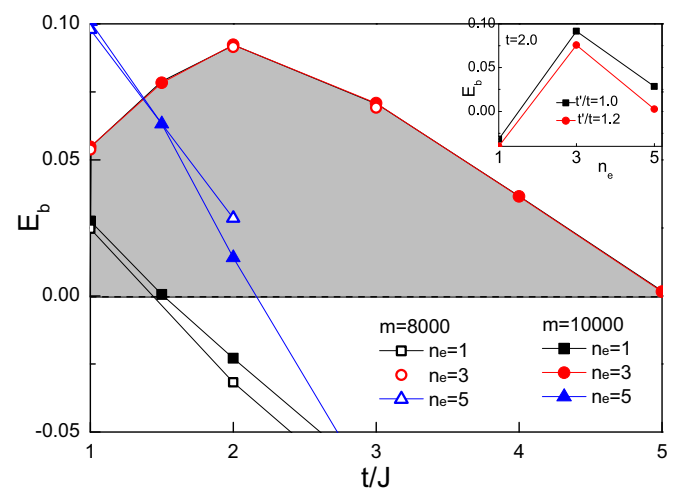


FIG. 2. Electronic pair binding energy $E_b(n_e)$ as a function of t/J with different n_e for both $m = 8000$ and $m = 10000$ number of DMRG states. The shaded region and lines connecting the data points are guides to the eye only. The inset is the electronic pair binding energy $E_b(n_e)$ as a function of n_e for both $t'/t = 1.0$ and $t'/t = 1.2$ with $t/J = 2$ and $m = 8000$.

simplify the discussion, unless otherwise specified we will set $t' = t$, and will consider the range of parameters $t/J = 1-5$, which approximately corresponds to the Hubbard model at $U/t \sim 4t/J = 4-20$. We will define the unit of energy such that $J = 1$ and employ the standard approach [24,25] to choose a suitable one-dimensional path over all sites of the C_{60} molecule. (See Appendix C for details.) We perform up to 100 sweeps and keep up to $m = 12\,000$ DMRG states with a typical truncation error $\sim 10^{-4}$. This led to excellent convergence for the results that we report here. Extrapolating to $m = \infty$ gives typical fractional errors in the total energy of about $\sim 10^{-3}$.

IV. HUND'S RULE VIOLATION

One of our main observations is that Hund's first rule is violated for this range of parameters. The state with the minimal possible total spin has $s_{\min} = 1/2$ for n_e odd and $s_{\min} = 0$ for n_e even, i.e., $\vec{S} \cdot \vec{S} \geq s_{\min}(s_{\min} + 1)$ where $\vec{S} = \sum_i \vec{S}_i$ is the total spin operator. The ground state is generically an eigenstate of total spin, so in testing for violations of Hund's first rule, we measure the "excess spin," $\delta S^2 \equiv \langle \vec{S} \cdot \vec{S} \rangle - s_{\min}(s_{\min} + 1)$, which is zero in the minimal spin state, and satisfies the inequality $\delta S^2 \geq 2$ otherwise. We always find that, for a large enough number of kept states, $\delta S^2 = 0$ to high accuracy ($\delta S^2 < 1.2 \times 10^{-2}$); representative data for $t/J = 2$ for all values of n_e in the range 0-6 are shown in Fig. 4(a). (See Appendix B for details.) In addition, we define the "spin gap," $\Delta_s \equiv E_0(s_{\min} + 1) - E_0(s_{\min})$, where $E_0(S_z)$ is the ground-state energy for a given value of the z component of total spin S_z . In any state with more than the minimal spin, $\Delta_s = 0$, while, barring an accidental degeneracy, in a minimal spin state, $\Delta_s > 0$. The value of Δ_s as a function of n_e is shown in Fig. 1(a) for $t/J = 2$; the different colored points represent the results with different numbers of kept states m . [A more complete presentation of the convergence to the $m \rightarrow \infty$ limit is shown in Fig. 4(a).] It is clear that Δ_s is nonzero in all cases, which is independent confirmation of the conclusion that the ground state has the minimum possible spin. For $n_e = 2, 3$, and 4 this represents a violation of Hund's first rule.

In Fig. 1(b) we show the "orbital gap," $\Delta_o \equiv E_1(s_{\min}) - E_0(s_{\min})$, where $E_1(S_z)$ is the energy of the first excited for given S_z . If the ground state is an orbital singlet, $\Delta_o > 0$, while for any orbital multiplet (higher angular momentum) $\Delta_o = 0$. For n_e even, both Δ_s and Δ_o are nonzero, implying that the ground states are both orbital and spin singlets. For odd n_e , that $\Delta_s > 0$ and $\Delta_o = 0$ implies that the ground states have spin 1/2 and are orbital multiplets.

All these findings are consistent with an analysis [10] in which the ground states are adiabatically connected to appropriate (symmetry determined) combinations of the noninteracting ground states: The states with one or five electrons in a p orbital have total spin $s = 1/2$ and angular momentum $l = 1$ (i.e., an orbitally degenerate minimal spin state consistent with what we find). The states with two or four electrons can have $s = 1$ and $l = 1$ (the state favored by Hund's first rule), $s = 0$ and $l = 2$ (the state favored by Hund's second rule, if the first were to be ignored), or $s = 0$ and $l = 0$ (i.e., an orbitally nondegenerate minimal spin state consistent with what we find). The states with three electrons can have $s = 3/2$ and $l = 0$ (the state favored by Hund's first

rule), or $s = 1/2$ and $l = 2$ or $l = 1$ (either of which is an orbitally degenerate minimal spin state consistent with what we find). From the weak-coupling perspective, the fact that the ground state is an orbital and spin singlet when $n_e = 0$ or 6 appears obvious (corresponding to an empty or full t_{1u} orbital). However, the fact that the ground states of the t - J model have the same symmetries as the noninteracting ground states even in these cases is a nontrivial observation. In particular, for $n_e = 0$, this is a statement concerning the ground state of the spin-1/2 Heisenberg model on the C_{60} lattice, a problem which has many interesting features in its own right [27].

V. PAIR BINDING ENERGY

The electronic pair binding energy is defined as $E_b(n_e) = 2E_0(n_e) - E_0(n_e + 1) - E_0(n_e - 1)$, where $E_0(n_e)$ is the ground-state energy of the system with n_e doped electrons. If we consider a system with an average of n_e doped electrons per molecule, a positive pair binding energy can be interpreted as an effective attraction between electrons in the sense that it is then energetically favorable to add $n_e + 1$ electrons to half the molecules and $n_e - 1$ to the other half, rather than to place n_e electrons on every molecule. For n_e even, we always find that the pair binding energy is negative. However, for $n_e = 1, 3$, and 5, $E_b(n_e)$ is positive for a range of intermediate t/J . This is illustrated in Fig. 2, which shows $E_b(n_e)$ as a function of t/J for $n_e = 1, 3$, and 5. Importantly, for the whole t/J parameter region we have explored, $E_b(n_e = 3)$ is positive, although at our largest value of $t/J = 5$ it is close to zero and appears to be headed to negative values at still larger t/J . For $n_e = 1$ and $n_e = 5$, E_b is positive for small enough t/J , but crosses zero and is distinctly negative (corresponding to an effective repulsion between electrons) beyond a critical value of t/J .

For $t/J \lesssim 1$, it can be plausibly argued that the t - J model is unphysical, and in particular has, in effect, microscopically attractive interactions, so the results for $n_e = 1$ and 5 are of uncertain physical significance, as pair binding is only seen for $t/J \lesssim 1.5$ and $t/J \lesssim 2$, respectively. But the pair binding for $n_e = 3$ is manifestly robust in the regime $2 < t/J < 5$, where these concerns do not arise. [Note that the absence of pair binding as $t/J \rightarrow \infty$ is expected on general grounds. For $n_e = 1$, a rigorous proof exists [28] that $E_b \leq 0$ in this limit, as a corollary of a generalized version of Nagaoka's theorem. Under the assumption that the fully spin polarized (Nagaoka) state is the ground state for large enough t/J for $n_e = 3$ it follows that $E_b(3) = 0$ at large t/J .]

VI. CONCLUSIONS

In this paper, we have studied the t - J model on the C_{60} molecule through DMRG simulation. Several different quantities are calculated, including the ground-state energy, spin excitation gaps, and electronic pair binding energy, for $n_e = 0-6$ and $1 \leq t/J \leq 5$. In all cases, the ground state has the minimum possible spin, which for $n_e = 2, 3$, and 4 constitutes a violation of Hund's first rule. Correspondingly, for all n_e , there is a nonzero spin gap. The ground state is an orbital singlet for the even values of n_e and orbitally degenerate for the odd values. For $n_e = 3$ we find a positive

pair binding energy for the entire range of t/J ; thus, we establish that it is possible that an effective attraction of the sort necessary to mediate superconducting pairing, can arise from purely repulsive electron-electron interactions on a single C_{60} molecule. This establishes an important point of principle.

Naturally, our results do not address the issue of what differences arise in considering more realistic (nonzero range) microscopic electron interactions, some of which can be expected to enhance [20,21] and others to suppress [12,13,17–19] pair binding. It also leaves open the relevance of our findings to the physical problem of superconductivity in alkalimetal doped C_{60} where both intermolecular interactions and electron-phonon interactions [4] must be included in a complete analysis of the problem. In this context, it is important to note that the purely electronic model we have solved results in precisely the same inversion of Hund’s rule that elsewhere [29,30] has been attributed to the effect of Jahn-Teller phonons. The putative signatures of a dynamical Jahn-Teller effect—including the remarkable recent experimental observations reported in Ref. [31]—in most cases depend more on the emergent symmetries of the molecular ground states than on the details of the mechanism that produces these states. As there is no distinction in symmetry between the molecular ground states favored by the dynamical Jahn-Teller effect and those of the t - J model, unraveling the relative importance of the various contributions to the physics of real materials is likely to be more subtle than was previously believed.

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APPENDIX A: HUBBARD MODEL ON THE C_{20} MOLECULE

The one-band Hubbard model on the C_{20} molecule is given by the Hamiltonian

$$H = -t \sum_{\langle ij \rangle \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.}) + U \sum_i n_{i\uparrow} n_{i\downarrow}. \quad (\text{A1})$$

Here $c_{i\sigma}^\dagger$ is the electron creation operator with spin- σ on site i , and $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$ is the number of electrons with spin- σ on site i . t is the nearest-neighbor hopping constant and U is the on-site Coulomb interaction. Previous studies [32,33] using QMC and exact diagonalization methods have found a negative pair binding energy (repulsive interaction) on this molecule. Moreover, they found that Hund’s rule is obeyed for the corresponding range of parameters $U/t \leq 3$ where the ground state has the maximum values of total spin ranging from spin 1 for 20 electrons through spin 2 for 22 electrons, while Hund’s rule is violated for larger $U/t > 4.2$. However, due to the presence of the geometrical frustration, a systematic weakness of QMC simulation was also recognized, for both large U/t range where the sign problem becomes significantly worse and small U/t range where the ground state is a spin multiplet state.

To demonstrate the reliability of the DMRG simulation, we have benchmarked the DMRG method on the one-band Hubbard model on the C_{20} molecule [see Eq. (A1)] by comparing the QMC and DMRG data. As we will see in Fig. 3, for both ranges of U/t , we find that the DMRG results

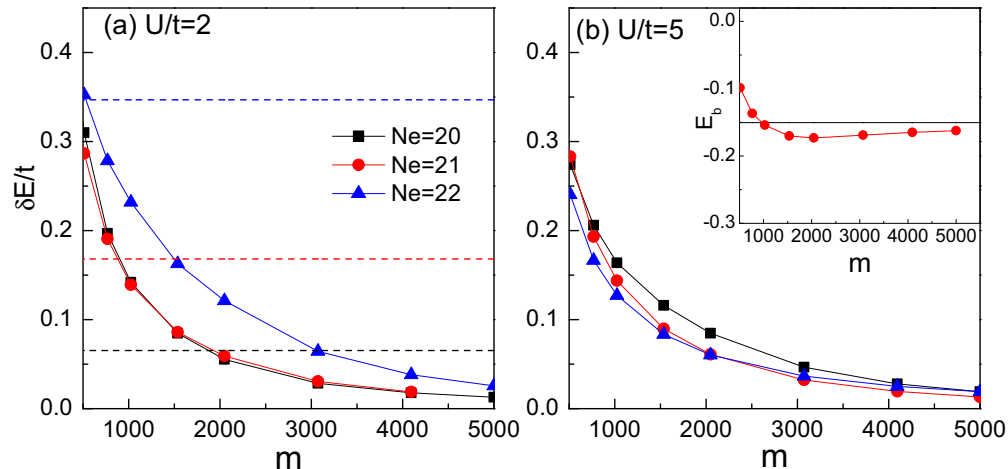


FIG. 3. Ground-state energy difference $\delta E = E_0(m) - E_0$ as a function of DMRG states m for the one-band Hubbard model [see Eq. (A1)] with N_e electrons on the C_{20} molecule at $U/t = 2$ in (a) and $U/t = 5$ in (b). Here E_0 is the ground-state energy obtained by exact diagonalization (see Refs. [32,33]), while $E_0(m)$ is the ground-state energy obtained by DMRG simulation with minimal value of z -component total spin $S_z = s_{\min}$, i.e., $s_{\min} = 0$ for $N_e = 20, 22$, and $s_{\min} = 1/2$ for $N_e = 21$. The dashed lines in (a) denote the ground-state energy difference between QMC and exact diagonalization with same N_e and S_z (see Table II in Ref. [33]), for comparison with the DMRG simulation labeled by the same color. The inset in (b) is the electronic pair binding energies $E_b = 2E_0(N_e = 21) - E_0(N_e = 22) - E_0(N_e = 20)$ from DMRG (red circle) and ED simulations (solid line). Note that here we use a different definition of the pair binding energy compared with Refs. [32,33], and a negative E_b means a repulsive interaction between doped electrons.

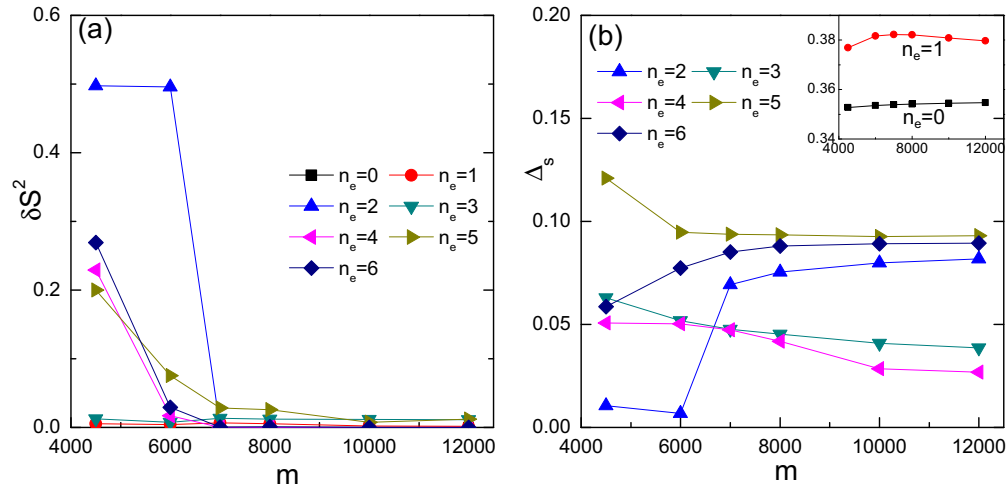


FIG. 4. (a) “Excess spin” $\delta S^2 = \vec{S} \cdot \vec{S} - s_{\min}(s_{\min} + 1)$ where $\vec{S} = \sum_i \vec{S}_i$ and (b) spin gap $\Delta_s = E_0(s_{\min} + 1) - E_0(s_{\min})$ as a function of number of DMRG states m , for $t/J = 2$ and different numbers of added electrons n_e . Here $E_0(S_z)$ is the ground-state energy for given value of spin S_z . Inset in (b): spin gap Δ_s as a function of m for $n_e = 0$ and 1.

converges very rapidly to the ED results with a relatively small number of DMRG states m . In particular, we can get values for both the ground-state energy and the pair binding energy E_b that are more accurate than those obtained using QMC [32,33]. For instance, with the same N_e and S_z , DMRG can easily produce a better ground-state energy than QMC with only a moderately number of DMRG states m , say $m \sim 1800$ for $N_e = 20$ while a much smaller value $m \sim 500$ is produced for $N_e = 22$. Compared with $U/t = 2$, where QMC already has a sign problem for the nonbipartite dodecahedral molecular geometry, a larger $U/t = 5$ introduce significantly more sources of negative probability weight, lowering the average value of the sign, thus making that a reliable QMC simulation is not applicable [32,33]. On the contrary, DMRG is immune to such a problem and still provides us with reliable results, including the ground-state energy and electronic pair binding energy $E_b(N_e = 21)$ as shown in Fig. 3(b). Especially, a relatively small number of state $m \sim 1000$ has given us a reliable E_b which is very close to the ED results. Therefore, the DMRG method works well for the Hubbard model on the C_{20} molecule.

APPENDIX B: t - J MODEL ON THE C_{60} MOLECULE

In the main text, we have introduced the t - J model on the C_{60} molecule and summarized the main DMRG results, including spin excitation gap and electronic pair binding energy. Now, we will show more details of the DMRG simulation about the convergence of the DMRG results. For this purpose, we first consider $t/J = 2$ as an example and the results are given in Fig. 4. As seen in the figure, “excess spin” $\delta S^2 > 0$ (see main text for details) when m is small, indicating that the DMRG simulation may get stuck in a metastable spin multiplet state. This is because the states with smaller values of $|S_z|$ may mix with higher-lying states that have the same value of $|S_z|$ but different total spin. However, such a state is not the true ground state, instead the true ground state is obtained when ≥ 7000 , where $S_T = 0$ for $n_e = 0-6$ cases. Therefore,

the ground state is a spin singlet state, which violates Hund’s rule.

In addition to “excess spin” δS^2 , we have also calculated the spin gap Δ_s (see main text for details). Figure 4(b) shows the spin gap Δ_s as a function of DMRG states m . Similar with δS^2 , Δ_s starts to converge and saturate to finite values when $m \geq 7000$, for $n_e = 0-6$. On the contrary, for the metastable state when $m \leq 6000$, Δ_s vanishes for $n_e = 2$, indicating that the metastable state is a spin multiplet state. Consistent with the minimal spin state, a finite spin gap Δ_s again indicates that the ground state is a minimal spin state. For $n_e = 2-4$, this indicates that Hund’s rule is violated, which is in contraction to the QMC results [22].

Until now, we have demonstrated that the ground state of the t - J model on the C_{60} molecule is a minimal spin state. To provide more information of the ground state, we have also computed the “orbital gap” $\Delta_o = E_1(s_{\min}) - E_0(s_{\min})$,

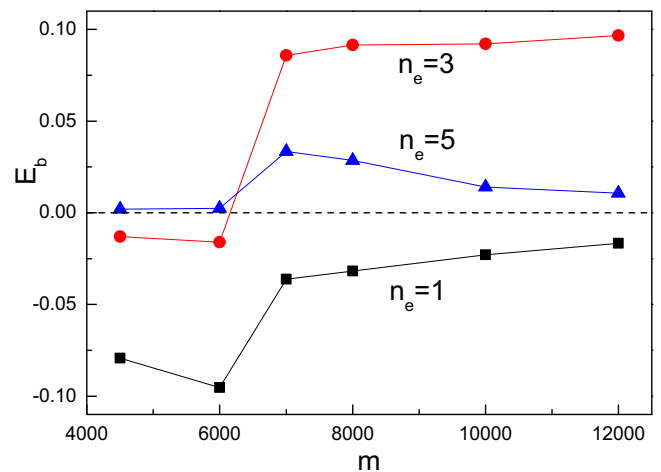


FIG. 5. Electronic pair binding energy $E_b(n_e)$ for $t/J = 2$ as a function of DMRG states m with different number of added electrons n_e . The dashed line indicates the zero. The lines connecting the data points are guides to the eye only.

where E_0 is the ground-state energy and E_1 is the first excited state state, both in the same spin $S_z = s_{\min}$ sector. The results are given in Fig. 1(b). Similar with Δ_s , Δ_o is also finite for $n_e = 0, 2$, and 4, indicating a unique ground state without orbital degeneracy. Interestingly, for other n_e cases, $\Delta_o \sim 0$, indicating that the ground state is an orbital multiplet, which is consistent with [10].

Figure 5 shows the results of the electronic pair binding energy $E_b(n_e)$ (see main text for details) for $t/J = 2$ with $n_e = 1, 3$, and 5, as a function of the number of DMRG states m . Similar to δS^2 and spin gap Δ_s , E_b is also affected by the convergent problem for the numerical simulation when $m \leq 6000$, where E_b is either vanishingly small or negative (repulsive interaction between doped electrons). Interestingly, when $m \geq 7000$, our DMRG simulation is well converged, and we find a big and positive $E_b(n_e = 3) \sim 0.1J$. This suggests that it is energetically favorable to put four electrons on one C_{60} and two on the other (positive pair binding) that putting three electrons on each of the C_{60} molecules (negative pair binding). On the contrary, for both $n_e = 1$ and $n_e = 5$ cases, $E_b(n_e)$ is either zero or slightly negative, indicating that there is no attractive interaction between doped electrons.

APPENDIX C: MAPPING C_{60} MOLECULE TO ONE-DIMENSIONAL CHAIN FOR DMRG TREATMENT

As DMRG is a one-dimensional method, the two-dimensional lattice on cylinder and torus, such as square lattice, has to be mapped to a one-dimensional chain with long-ranged interactions. This is known as the multichain approach [24,25], which defines a suitable one-dimensional path over all sites of the two-dimensional lattice. Similarly, the spirit of the multichain approach can be naturally applied

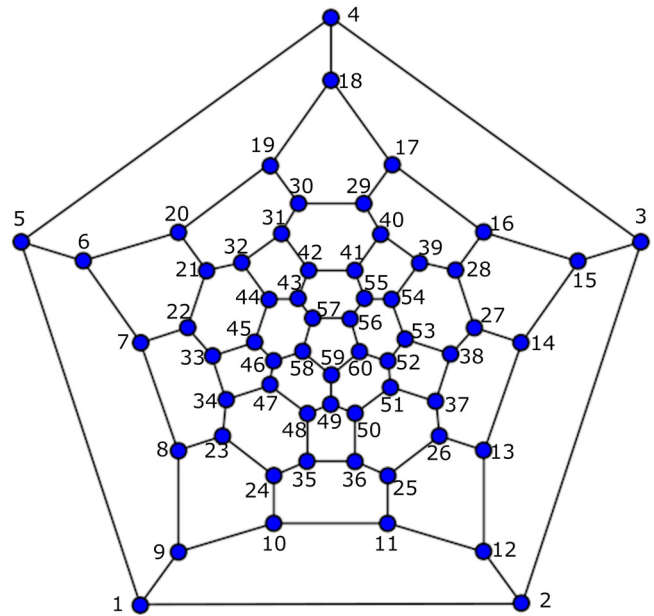


FIG. 6. We map the C_{60} molecule to a one-dimensional chain shown in the figure, where the sequence of sites is represented by the numbers.

to any system, including the C_{60} molecule that we study in this paper. Figure 6 shows the mapping of a C_{60} molecule to a one-dimensional path, where the numbers represent the sequence of site of the one-dimensional chain. Approximately, the numerical cost after this mapping is similar to the t - J model on the square lattice with system size $N = 10 \times 6$ on a cylinder, where 10 is the width and 6 is the length of the cylinder.

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