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Effects of electron correlation on superconductivity in the Hatsugai–Kohmoto model*

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Understanding how electrons form pairs in the presence of strong electron correlations demands going beyond the BCS paradigm. We study a correlated superconducting model where the correlation effects are accounted for by a U term local in momentum space. The electron correlation is treated exactly while the electron pairing is treated approximately using the mean-field theory. The self-consistent equation for the pair potential is derived and solved. Somewhat contrary to expectation, a weak attractive U comparable to the pair potential can destroy the superconductivity, whereas for weak to intermediate repulsive U, the pair potential can be enhanced. The fidelity of the mean-field ground state is calculated to describe the strength of the elelectron correlation. We show that the pair potential is not equal to the single-electron superconducting gap for the strongly correlated superconductors, in contrast to the uncorrelated BCS limit.

Keywords: strong correlated superconductivity, exactly solvable model, mean-field theory

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As one of the most important and challenging problems in condensed matter physics, electron correlations are responsible for a rich variety of properties of the many-body quantum systems. Among them, the correlated superconductivity is most extensively investigated in heavy-fermion materials, organic compounds, high-temperature cuprates[1] and nickelate,[2] as well as iron pnictides and chalcogenides.[3] Soon after, the early discovery of the high-T_c cuprates by Bednorz and Müller[4] in 1986, the single-band Hubbard model[5] was suggested by Anderson[6] to describe the unusual properties in both the normal and superconducting states. The Hubbard Hamiltonian includes an on-site repulsive U term to account for the strong electron correlation. After decades of intensive research, the highly nontrivial problem of solving the Hubbard model for general cases is still far from being settled.

Recently, a correlated electron model formulated by Hatsugai and Kohmoto (HK)[7] was revisited as a toy model whose metallic phases exhibit non-Fermi liquid character with a superconducting instability.[8] Similar to the Hubbard model, the HK model also possesses a U term reflecting the interaction between spin-up and spin-down electrons. However, the U term in the HK model is local in momentum space instead of real space. The locality of interaction in $\boldsymbol{k}$ makes the HK model exactly soluble.[9–12] Phillips *et al.*[8] demonstrated an analogous Cooper instability for the HK model of a doped Mott insulator. This intriguing observation motivates us to investigate the correlation effect on the superconductivity when a weak pairing interaction is present in the HK model.

To study how the electron pairing is influenced by U, we first elucidate some typical normal phases of the HK model. The Hamiltonian of the HK model is of the form

$$\hat{H}_0 = \sum_{\boldsymbol{k}} \hat{H}_{0,\boldsymbol{k}} = \sum_{\boldsymbol{k}} \left[\xi_{\boldsymbol{k}}(\hat{n}_{\boldsymbol{k}\uparrow} + \hat{n}_{\boldsymbol{k}\downarrow}) + U\hat{n}_{\boldsymbol{k}\uparrow}\hat{n}_{\boldsymbol{k}\downarrow}\right], \tag{1}$$

where $\xi_{\boldsymbol{k}} = \varepsilon_{\boldsymbol{k}} - \mu$ represents the single-particle energy dispersion relative to the chemical potential μ; and $\hat{n}_{\boldsymbol{k},\sigma} = c^{\dagger}_{\boldsymbol{k}\sigma}c_{\boldsymbol{k}\sigma}$ denotes the electron number operator. The HK Hamiltonian is exactly solvable since it can be decomposed into subsystems denoted by $\hat{H}_{0,\boldsymbol{k}}$. For each subsystem, there are four occupation states for each energy level $\xi_{\boldsymbol{k}}$, namely $|n_{\boldsymbol{k}\uparrow}, n_{\boldsymbol{k}\downarrow}\rangle = (c^{\dagger}_{\boldsymbol{k}\uparrow})^{n_{\boldsymbol{k}\uparrow}}(c^{\dagger}_{\boldsymbol{k}\downarrow})^{n_{\boldsymbol{k}\downarrow}}|0_{\boldsymbol{k}}\rangle$ with $n_{\boldsymbol{k}\sigma} = 0, 1$. For the occupation number $n_{\boldsymbol{k}} = n_{\boldsymbol{k}\uparrow} + n_{\boldsymbol{k}\downarrow}$ equal 0, 1, and 2, the corresponding eigenenergy $\eta_{n_{\boldsymbol{k}}}$ is, respectively,

$$\eta_0 = 0,\ \eta_1 = \xi_{\boldsymbol{k}},\ \eta_2 = 2\xi_{\boldsymbol{k}} + U. \tag{2}$$

Whether the lowest-lying state of each subsystem is empty, singly occupied or full relies on $\xi_{\boldsymbol{k}}$ and U as shown in Figs. 1(a) and 1(b). Consequently, the electron distribution in the energy band is changed due to the electron correlation, and the system undergoes metal–insulator transition with the variations in U and the band filling (or chemical potential).

The $U < 0$ case. As shown in Fig. 1(a), the double occupation with $n_{\boldsymbol{k}} = 2$ is favored for the energy level satisfying $\xi_{\boldsymbol{k}} < -U/2$, whereas the empty state with $n_{\boldsymbol{k}} = 0$ is preferred for $\xi_{\boldsymbol{k}} > -U/2$ as shown in Fig. 1(a). Accordingly, the ground state of $\hat{H}_0$ is $|\mathrm{gs}\rangle = \prod_{\xi_{\boldsymbol{k}}<-U/2} c^{\dagger}_{\boldsymbol{k}\uparrow}c^{\dagger}_{\boldsymbol{k}\downarrow}|0\rangle$, indicating that the energy levels of the electronic band are either empty or fully occupied reminiscent of the Fermi-sea ground state

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of free electrons in metals. However, by examining the single-electron or single-hole excitation state, i.e., $c^{\dagger}_{\boldsymbol{k}\sigma}|\mathrm{gs}\rangle$ or $c_{\boldsymbol{k}\sigma}|\mathrm{gs}\rangle$, one can see that the ground state has an energy gap $-U/2$. Therefore, the normal state for the $U<0$ case is a strange metal for any band filling $0<n<2$.

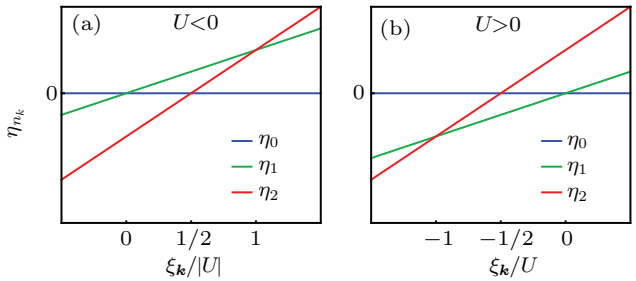


Fig. 1. The eigenenergies for empty (blue line), singly occupied (green line) and fully occupied (red line) states as functions of $\xi_{\boldsymbol{k}}$, for the cases of (a) $U<0$ and (b) $U>0$.

The $U>0$ case. As shown in Fig. 1(b), the doubly occupied state with $n_{\boldsymbol{k}}=2$ is favored for $\xi_{\boldsymbol{k}}<-U$, while the singly-occupied state with $n_{\boldsymbol{k}}=1$ is preferred for $-U<\xi_{\boldsymbol{k}}<0$. The ground state of $\hat{H}_0$ is, therefore, $|\mathrm{gs}\rangle=\prod_{-U<\xi_{\boldsymbol{k}}<0}c^{\dagger}_{\boldsymbol{k}\sigma}\prod_{\xi_{\boldsymbol{k}}<-U}c^{\dagger}_{\boldsymbol{k}\uparrow}c^{\dagger}_{\boldsymbol{k}\downarrow}|0\rangle$. Consequently, the normal phases of the $U>0$ case is richer than the $U<0$ one. Suppose that the electron band $\varepsilon_{\boldsymbol{k}}$ is within the energy range $\varepsilon_1\le\varepsilon_{\boldsymbol{k}}\le\varepsilon_2$ with bandwidth $W=\varepsilon_2-\varepsilon_1$. (i) For $U<W$ and $\varepsilon_1+U<\mu<\varepsilon_2$, the empty, singly and doubly occupied energy levels all exist in the ground state. The gapless single-electron excitations can be created by adding the electron into either the empty or the singly occupied energy levels. This normal phase is referred to as weakly correlated metal. (ii) For $\varepsilon_1<\mu<\min(\varepsilon_2,\varepsilon_1+U)$, the energy levels of the electronic band are either empty or singly occupied, and therefore the band filling $0<n<1$. The gapless single-electron excitations can only be created by adding an electron into the empty energy level. This normal phase is referred to as strongly correlated metal. (iii) $\max(\varepsilon_2,\varepsilon_1+U)<\mu<\varepsilon_2+U$. The energy levels of the electronic band are either singly or doubly occupied, and accordingly the band filling $1<n<2$. The gapless single-electron excitations can only be created by adding the electron into the singly occupied energy levels. The normal phase is also called strongly correlated metal and related to the phase (ii) by particle-hole transformation. (iv) For $U>W$ and $\varepsilon_2<\mu<\varepsilon_1+U$, the system is a Mott insulator at half filling since all energy levels are singly occupied but the single-particle excitations are gapped.

For the three correlated metallic phases, (i), (ii) and (iii), there are $\boldsymbol{k}$ segments on which the energy levels are singly occupied by either spin-up or spin-down electrons, which results in highly degenerate ground states of the correlated metallic phases. This high degeneracy leads to possible instability of the normal phase in the presence of other electron-electron interactions towards the formation of magnetic or superconducting orders. Indeed, the superconducting instability is unveiled[8] after studying the Cooper problem in the correlated metals.

With the knowledge of the normal phases of the HK model, we then examine the electron pairing when an effective electron-electron attraction is present. The model Hamiltonian is written as

$$\hat{H}=\hat{H}_0+\hat{H}_1, \tag{3}$$

where $\hat{H}_1$ denotes an isotropic pairing interaction of the BCS type

$$\hat{H}_1=-V_0\sum_{\boldsymbol{k},\boldsymbol{k}'}c^{\dagger}_{\boldsymbol{k}\uparrow}c^{\dagger}_{-\boldsymbol{k}\downarrow}c_{-\boldsymbol{k}'\downarrow}c_{\boldsymbol{k}'\uparrow}. \tag{4}$$

Here $V_0>0$ denotes the matrix element of electron-pair scattering. The quartic terms of fermions in Eq. (4) is further decoupled into the quadratic form by applying the mean-field approximation, and we have

$$\hat{H}_1\approx\sum_{\boldsymbol{k}}\left[\left(-\Delta c^{\dagger}_{\boldsymbol{k}\uparrow}c^{\dagger}_{-\boldsymbol{k}\downarrow}+\mathrm{H.c.}\right)+\Delta\left\langle c^{\dagger}_{\boldsymbol{k}\uparrow}c^{\dagger}_{-\boldsymbol{k}\downarrow}\right\rangle\right]. \tag{5}$$

The pair potential[13] Δ in Eq. (5) is defined as follows:

$$\Delta=V_0\sum_{\boldsymbol{k}}\left\langle c_{\boldsymbol{k}\downarrow}c_{-\boldsymbol{k}\uparrow}\right\rangle. \tag{6}$$

Here we note that in the presence of U, the pair potential Δ is *not* necessarily the superconducting single-electron energy gap, contrarily to the case of the uncorrelated BCS superconductors. This will be addressed later in this paper.

According to Eqs. (1), (4) and (5), the system Hamiltonian (3) can be approximately described by the following mean-field Hamiltonian, which is written as

$$\hat{H}^{\mathrm{mf}}=\sum_{\boldsymbol{k}}{}'\hat{H}^{\mathrm{mf}}_{\boldsymbol{k}}, \tag{7}$$

where

$$\hat{H}^{\mathrm{mf}}_{\boldsymbol{k}}=\hat{H}_{0,\boldsymbol{k}}+\hat{H}_{0,-\boldsymbol{k}}-\left(\Delta c^{\dagger}_{\boldsymbol{k}\uparrow}c^{\dagger}_{-\boldsymbol{k}\downarrow}+\Delta c^{\dagger}_{-\boldsymbol{k}\uparrow}c^{\dagger}_{\boldsymbol{k}\downarrow}+\mathrm{H.c.}\right). \tag{8}$$

Equation (7) shows that the Hamiltonian is decomposed into subsystems identified by $\boldsymbol{k}$. Because the U term couples the $\boldsymbol{k}\uparrow$ and $\boldsymbol{k}\downarrow$ while the Δ term couples $\boldsymbol{k}\uparrow$ and $-\boldsymbol{k}\downarrow$ electrons, the four single-particle states $\boldsymbol{k}\uparrow$, $-\boldsymbol{k}\downarrow$, $-\boldsymbol{k}\uparrow$, $\boldsymbol{k}\downarrow$ are mixed together. Obviously, this sector of the four single-particle states is identical under the inversion $\boldsymbol{k}\to-\boldsymbol{k}$. Thus, the primed summation as shown in Eq. (7) is restricted on the folded momentum space. Because the subsystem Hamiltonian $\hat{H}^{\mathrm{mf}}_{\boldsymbol{k}}$ is commutative with each other, the eigenstates of $\hat{H}^{\mathrm{mf}}$ are the products of the eigenstate of each subsystem.

For each subsystem, $\hat{H}^{\mathrm{mf}}_{\boldsymbol{k}}$ lives in the Fock subspace $\mathcal{H}_{\boldsymbol{k}}$ spanned by all possible occupations of the four single-particle states. Therefore, the natural basis vectors are $|n_1n_2n_3n_4\rangle_{\boldsymbol{k}}=c^{\dagger n_1}_{\boldsymbol{k}\uparrow}c^{\dagger n_2}_{-\boldsymbol{k}\downarrow}c^{\dagger n_3}_{-\boldsymbol{k}\uparrow}c^{\dagger n_4}_{\boldsymbol{k}\downarrow}|0_{\boldsymbol{k}}\rangle$ with $n_i=0,1$, and the dimension of $\mathcal{H}_{\boldsymbol{k}}$

is 16. Since $H_{\boldsymbol{k}}^{\rm mf}$ conserves the fermion parity, $\mathcal{H}_{\boldsymbol{k}}$ can be further divided into even and odd sectors, each of which is in 8 dimensions.

As proved in the appendix of this paper, for $\Delta \neq 0$, the mean-field ground state is in the 3D subspace of the even sector, which is spanned by the empty state $|0\rangle_{\boldsymbol{k}}$, the doubly occupied spin-singlet state $|s\rangle_{\boldsymbol{k}} = (|1100\rangle_{\boldsymbol{k}} + |0011\rangle_{\boldsymbol{k}})/\sqrt{2}$, and the fully occupied states $|f\rangle_{\boldsymbol{k}} = |1111\rangle_{\boldsymbol{k}}$. In this 3D subspace, $\hat{H}_{\boldsymbol{k}}^{\rm mf}$ can be expressed as

$$\begin{aligned}\hat{H}_{\boldsymbol{k}}^{\rm mf} &= 2\eta_1 |s\rangle_{\boldsymbol{k}\boldsymbol{k}}\langle s| + 2\eta_2 |f\rangle_{\boldsymbol{k}\boldsymbol{k}}\langle f| \\ &\quad -\sqrt{2}\Delta\left[|s\rangle_{\boldsymbol{k}\boldsymbol{k}}\langle 0| + |s\rangle_{\boldsymbol{k}\boldsymbol{k}}\langle f| + \text{H.c.}\right] \qquad (9)\\ &= \sum_{i=1}^{3} E_{\boldsymbol{k},i} |\phi_{\boldsymbol{k},i}\rangle\langle\phi_{\boldsymbol{k},i}|. \qquad (10)\end{aligned}$$

In Eq. (10), $E_{\boldsymbol{k},i}$ with $i = 1,2,3$ denote the three eigenenergies of $\hat{H}_{\boldsymbol{k}}^{\rm mf}$ and the corresponding eigenkets are

$$|\phi_{\boldsymbol{k},i}\rangle = x_{\boldsymbol{k},i}|0\rangle_{\boldsymbol{k}} + y_{\boldsymbol{k},i}|s\rangle_{\boldsymbol{k}} + z_{\boldsymbol{k},i}|f\rangle_{\boldsymbol{k}}. \qquad (11)$$

The eigenequation for the eigenvalues and eigenfunctions is

$$\begin{pmatrix} 0 & -\sqrt{2}\Delta & 0 \\ -\sqrt{2}\Delta & 2\eta_1 & -\sqrt{2}\Delta \\ 0 & -\sqrt{2}\Delta & 2\eta_2 \end{pmatrix} \begin{pmatrix} x_{\boldsymbol{k},i} \\ y_{\boldsymbol{k},i} \\ z_{\boldsymbol{k},i} \end{pmatrix} = E_{\boldsymbol{k},i} \begin{pmatrix} x_{\boldsymbol{k},i} \\ y_{\boldsymbol{k},i} \\ z_{\boldsymbol{k},i} \end{pmatrix}. \qquad (12)$$

For $\Delta \neq 0$ the three eigenvalues are nondegenerate and therefore can be arranged in strictly ascending order $E_{\boldsymbol{k},1} < E_{\boldsymbol{k},2} < E_{\boldsymbol{k},3}$ as shown in the appendix, and $|\phi_{\boldsymbol{k},1}\rangle$ is called ground-pair state, while $|\phi_{\boldsymbol{k},2(3)}\rangle$ excited-pair states. After diagonalization of the subsystem, the mean-field ground state of the whole system can be written as

$$|\text{gs}\rangle = \prod_{\boldsymbol{k}}{}' \left(x_{\boldsymbol{k},1}|0\rangle_{\boldsymbol{k}} + y_{\boldsymbol{k},1}|s\rangle_{\boldsymbol{k}} + z_{\boldsymbol{k},1}|f\rangle_{\boldsymbol{k}}\right), \qquad (13)$$

which indicates that all electrons are in the ground-pair states. The ground-state energy of $\hat{H}^{\rm mf}$ is then

$$\mathcal{E}_{\rm gs} = \sum_{\boldsymbol{k}}{}' E_{\boldsymbol{k},1}. \qquad (14)$$

Self-consistent equation for Δ. To study the effect of U on the superconductivity, the self-consistent equation of Δ should be established according to Eq. (6). The pairing amplitude $\langle c_{\boldsymbol{k}\downarrow}^{\dagger} c_{-\boldsymbol{k}\uparrow}^{\dagger}\rangle$ is related to the eigenket (13),

$$g(\xi_{\boldsymbol{k}},\Delta,U) = \langle c_{\boldsymbol{k}\downarrow}^{\dagger} c_{-\boldsymbol{k}\uparrow}^{\dagger}\rangle = (x_{\boldsymbol{k},1} + z_{\boldsymbol{k},1}) y_{\boldsymbol{k},1}/\sqrt{2}. \qquad (15)$$

The self-consistent equation for Δ then becomes

$$\Delta = V_0 \int N(\xi+\mu) g(\xi,\Delta,U)\,\mathrm{d}\xi, \qquad (16)$$

where $N(\varepsilon) = \sum_{\boldsymbol{k}} \delta(\varepsilon - \varepsilon_{\boldsymbol{k}})$ is the single-particle density of states. To concentrate on the effect of electron correlation on the superconductivity, we adopt a simple model of the electron band, in which the single-particle density of state is constant, i.e., $N(\varepsilon) = N_0$, within the energy window $\varepsilon \in [-W/2, W/2]$. Furthermore, in the following we consider the the usual weak-coupling superconducting case, i.e., $N_0 V_0 \ll 1$.

To solve the self-consistent equation for Δ, we calculate firstly the eigen-wavefunction $x_{\boldsymbol{k},1}$, $y_{\boldsymbol{k},1}$ and $z_{\boldsymbol{k},1}$ by diagonalizing the 3×3 eigenequation (12) exactly, then the pairing amplitude according to Eq. (15), and finally the integral of Eq. (16).

Figure 2 illustrates the U dependence of Δ at fixed band fillings $n = 1$ by setting the chemical potential $\mu = U/2$. As U varies, the normal phase of the system evolves from Mott insulator for negative U to correlated metal for $0 < U < W$ and finally back to Mott insulator when $U > W$. In Fig. 2, Δ_0 denotes the BCS value of the pair potential, i.e., Δ at $U = 0$. Near $U = 0$, Δ exhibits linear dependence on U. From Fig. 2 we find that Δ is suppressed by negative U and a rather weak negative U which exceeds $U_{\rm c} \approx -\Delta_0$ can destroy the superconductivity. On the contrary, Δ is enhanced by positive U provided that U is less than but not too close to W as shown in Fig. 2. For $U > W$ at half filling, the normal state is a Mott insulator which cannot accommodate superconductivity.

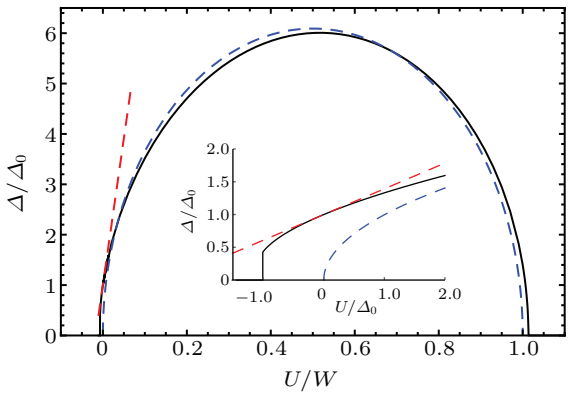


Fig. 2. Variation of the pair potential Δ as a function of U at half filling $n = 1$. Here $N_0V_0 = 0.2$, which gives rise to $\Delta_0/W \doteq 1/148$. The black solid line shows the exact numerical results. The red and blue dashed lines draw $\Delta(U)$ according to the approximate formulas Eqs. (27) and (35), respectively. The inset shows the U dependence of Δ in the vicinity of $U = 0$.

We then examine the U dependence of Δ at band fillings $n < 1$. As U varies, the normal phase of the system evolves from Mott insulator for negative U to weakly correlated metal for $0 < U < nW$ and to strongly correlated metal for $U > nW$. To fix the band filling when U increases, the variation of the chemical potential is $\mu = (U + n - 1)/2$ or $\mu = n - 1/2$ for the weakly or strongly correlated metallic phases, respectively. As shown in Fig. 3, when $U \lesssim nW$, $\Delta(U)$ is strengthened compared with Δ_0 for positive U in the $n < 1$ case, similar to the $n = 1$ case. On the other hand, when the system is strongly correlated, Δ is suppressed for $U \gtrsim nW$ and approaches to a finite non-zero value Δ_∞ when $U \to \infty$.

The suppression of Δ by negative U is attributed to the single-particle excitation gap of the Mott insulating phase,

which is proportional to $-U$. To have a better interpretation of the numerical results for positive U as shown in Figs. 2 and 3, in the following we will tackle the eigen problem of Eq. (12) approximately.

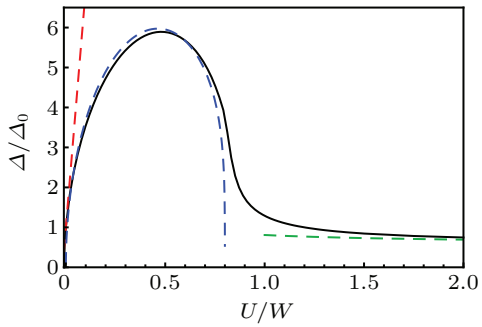


Fig. 3. Variation of the pair potential Δ as a function of U at band filling $n = 0.8$. Here $N_0V_0 = 0.2$, which gives rise to $\Delta_0/W \doteq 1/151$. The black solid line shows the exact numerical results. The red, blue and green dashed lines draw $\Delta(U)$ according to Eqs. (27), (35) and (36), respectively.

The weak-coupling case: $|U| \ll \Delta$. In the presence of a weak U, the superconductivity can be examined in the perturbed BCS framework by the first-order perturbation theory. The unperturbed system, i.e., Eq. (8) for $U = 0$, is a quadratic form whose eigen states can be obtained by Bogoliubov quasiparticle transformation[14] or by solving Eq. (12) exactly. The three eigenenergies are

$$E_{\boldsymbol{k},1} = 2\xi_{\boldsymbol{k}} - 2E(\xi_{\boldsymbol{k}},\Delta) \tag{17}$$

$$E_{\boldsymbol{k},2} = 2\xi_{\boldsymbol{k}}, \tag{18}$$

$$E_{\boldsymbol{k},3} = 2\xi_{\boldsymbol{k}} + 2E(\xi_{\boldsymbol{k}},\Delta), \tag{19}$$

where

$$E(\xi,\Delta) = \sqrt{\xi^2+\Delta^2} \tag{20}$$

is the energy of the Bogoliubov quasiparticle. The eigenkets are

$$|\phi^{(0)}_{\boldsymbol{k},1}\rangle = u^2_{\boldsymbol{k}}|0\rangle_{\boldsymbol{k}} + \sqrt{2}u_{\boldsymbol{k}}v_{\boldsymbol{k}}|s\rangle_{\boldsymbol{k}} + v^2_{\boldsymbol{k}}|f\rangle_{\boldsymbol{k}}, \tag{21}$$

$$|\phi^{(0)}_{\boldsymbol{k},2}\rangle = \sqrt{2}u_{\boldsymbol{k}}v_{\boldsymbol{k}}(|0\rangle_{\boldsymbol{k}} - |f\rangle_{\boldsymbol{k}}) - (u^2_{\boldsymbol{k}} - v^2_{\boldsymbol{k}})|s\rangle_{\boldsymbol{k}}, \tag{22}$$

$$|\phi^{(0)}_{\boldsymbol{k},3}\rangle = v^2_{\boldsymbol{k}}|0\rangle_{\boldsymbol{k}} - \sqrt{2}u_{\boldsymbol{k}}v_{\boldsymbol{k}}|s\rangle_{\boldsymbol{k}} + u^2_{\boldsymbol{k}}|f\rangle_{\boldsymbol{k}}, \tag{23}$$

where

$$u(v)_{\boldsymbol{k}} = \sqrt{[1+(-)\xi_{\boldsymbol{k}}/E(\xi_{\boldsymbol{k}},\Delta)]/2} \tag{24}$$

is the electron (hole) component of the Bogoliubov quasiparticle. According to the perturbation theory, the first-order correction to the ground state is

$$|\phi^{(1)}_{\boldsymbol{k},1}\rangle = \frac{U}{2E_{\boldsymbol{k}}}v^2_{\boldsymbol{k}}\left(2\sqrt{2}u_{\boldsymbol{k}}v_{\boldsymbol{k}}|\phi^{(0)}_{\boldsymbol{k},2}\rangle - u^2_{\boldsymbol{k}}|\phi^{(0)}_{\boldsymbol{k},3}\rangle\right). \tag{25}$$

Substituting Eqs. (21) and (25) into Eq. (15), the pairing amplitude is written as

$$g(\xi,\Delta,U) = \frac{\Delta}{2E(\xi,\Delta)} + \frac{U}{4}\left[\frac{\xi^2\Delta}{E(\xi,\Delta)^4} - \frac{\xi\Delta}{E(\xi,\Delta)^3}\right]. \tag{26}$$

The U-independent term on the right side of Eq. (26) is just the usual pairing amplitude of the BCS theory. Substituting Eq. (26) into Eq. (16), we have the first-order approximation of Δ,

$$\Delta = \Delta_0 + \frac{\pi}{8}U, \tag{27}$$

where $\Delta_0 = We^{-\frac{1}{N_0V_0}}$ denotes the pair potential for $U = 0$ at half filling. The linear behavior of $\Delta(U)$ given by Eq. (27) is in good agreement with the numerical results shown in Figs. 2 and 3.

The intermediate-coupling case: $\Delta \ll U \ll W$. The electron pairing is intimately related to the low-energy excitations of the normal state. As shown in Fig. 1(b), for $\xi_{\boldsymbol{k}} \approx 0$ the energies of the empty and spin-singlet states, $2\eta_0$ and $2\eta_1$, are close to each other, whereas the energy of the fully occupied state $|f\rangle_{\boldsymbol{k}}$ is around $2U$ and far above. Therefore, the electron pairing is effectively formed between $|0\rangle_{\boldsymbol{k}}$ and $|s\rangle_{\boldsymbol{k}}$. To the leading order, the eigenvalue equation (12) reduces to

$$\begin{pmatrix} 0 & -\sqrt{2}\Delta \\ -\sqrt{2}\Delta & 2\xi_{\boldsymbol{k}} \end{pmatrix}\begin{pmatrix} x_{\boldsymbol{k},1} \\ y_{\boldsymbol{k},1} \end{pmatrix} = E_{\boldsymbol{k},1}\begin{pmatrix} x_{\boldsymbol{k},1} \\ y_{\boldsymbol{k},1} \end{pmatrix}, \tag{28}$$

from which we obtain the approximate lowest-lying eigenenergy

$$E_{\boldsymbol{k},1} = \xi_{\boldsymbol{k}} - E(\xi_{\boldsymbol{k}},\sqrt{2}\Delta), \tag{29}$$

together with eigenfunctions

$$x_{\boldsymbol{k},1} = u_{\boldsymbol{k}}, \;\; y_{\boldsymbol{k},1} = v_{\boldsymbol{k}}, \;\; z_{\boldsymbol{k},1} = 0, \tag{30}$$

where $u(v)_{\boldsymbol{k}} = [(1+(-)\xi_{\boldsymbol{k}}/E(\xi_{\boldsymbol{k}},\sqrt{2}\Delta))/2]^{1/2}$. The forms of the lowest-lying eigenenergy and wavefunction according to Eqs. (29) and (30) for $U \gg \Delta$ in comparison to the BCS results as shown in Eqs. (17) and (21) for $U = 0$, together with the emergent $\sqrt{2}$ in Eq. (29), manifest the correlation effect on the electron pairing. Furthermore, despite of their similarity to the BCS coherent factors, u and v do not correspond to the quasiparticle since the Bogoliubov quasiparticles are not well-defined due to the electron correlation.

Analogically, for $\xi_{\boldsymbol{k}}$ in the vicinity of $-U$, $|s\rangle_{\boldsymbol{k}}$ and $|f\rangle_{\boldsymbol{k}}$ are close in energy, while $|0\rangle_{\boldsymbol{k}}$ is far above as illustrated in Fig. 1(b). As a result, the eigenvalue equation (12) is effectively reduced to

$$\begin{pmatrix} 2\xi_{\boldsymbol{k}} & -\sqrt{2}\Delta \\ -\sqrt{2}\Delta & 4\xi_{\boldsymbol{k}}+2U \end{pmatrix}\begin{pmatrix} y_{\boldsymbol{k},1} \\ z_{\boldsymbol{k},1} \end{pmatrix} = E_{\boldsymbol{k},1}\begin{pmatrix} y_{\boldsymbol{k},1} \\ z_{\boldsymbol{k},1} \end{pmatrix}. \tag{31}$$

After diagonalizing the above equation, we obtain

$$E_{\boldsymbol{k},1} = 3\xi_{\boldsymbol{k}} + U - E(\xi_{\boldsymbol{k}}+U,\sqrt{2}\Delta), \tag{32}$$

$$x_{\boldsymbol{k},1} = 0, \;\; y_{\boldsymbol{k},1} = u_{\boldsymbol{k}}, \;\; z_{\boldsymbol{k},1} = v_{\boldsymbol{k}}, \tag{33}$$

where $u(v)_{\boldsymbol{k}} = [(1+(-)(\xi_{\boldsymbol{k}}+U)/E(\xi_{\boldsymbol{k}}+U,\sqrt{2}\Delta))/2]^{1/2}$.

Substituting Eqs. (30) and (33) into Eq. (15) separately and combining the two results, we obtain an approximate formula for the pairing amplitude

$$g(\xi,\Delta,U) = \frac{\theta(\xi+U)\Delta}{2E(\xi,\sqrt{2}\Delta)} + \frac{[1-\theta(\xi)]\Delta}{2E(\xi+U,\sqrt{2}\Delta)}, \tag{34}$$

where $\theta(x)$ denotes the Heaviside step function. Figure 4 shows that the approximate formula as shown in Eq. (34) is in good agreement with the exact one for $U \gg \Delta$. Substituting the approximate equation of pairing amplitude into the equation for Δ, we obtain

$$\Delta = U^{\frac{1}{2}}\left[(nW-U)(2W-nW-U)\right]^{\frac{1}{4}} \mathrm{e}^{-\frac{1}{2N_0V_0}}. \tag{35}$$

The above approximate formula exhibiting the U dependence of Δ fits quite well to the exact results as shown in Figs. 2 and 3. For $U \ll W$, although the normal state is weakly correlated, the appearance of U as well as a factor of 2 in the exponential function as shown in the formula of Δ (35) indicates that the superconducting ground state is strongly correlated provided that $U \gg \Delta$. Furthermore, the enhancement of Δ by U is associated with the double-peak structure as shown in Fig. 4 in comparison with the single peak for the BCS case.

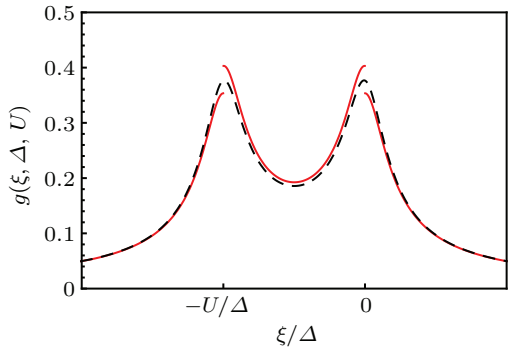


Fig. 4. The approximate and exact pairing amplitude $g(\xi,\Delta,U)$ as functions of ξ for $U/\Delta = 10$. Red solid line: approximate results calculated according to Eq. (34). Black dashed line: exact results calculated according to Eq. (15) utilizing the wavefunction obtained by exact diagonalization of Eq. (12).

The strong-coupling case: $U \gg W$. At half filling, the pair potential Δ vanishes trivially for $U > W$ as shown in Fig. 2 since the normal phase is Mott insulating. Thus, it is interesting to examine the case of doped Mott insulators, i.e., $n \neq 1$. Here, since the electron- and hole-doped cases are linked via electron-hole transformation, we only show the result for the $n < 1$ case. Distinct from the intermediate-coupling case, $|f\rangle_{\boldsymbol{k}}$ is excluded from electron pairing for *all* energy level $\xi_{\boldsymbol{k}}$. Employing the perturbation theory, we have the following expression for the pairing amplitude up to the first order of $1/U$,

$$g(\xi,\Delta,U) = \frac{\Delta}{2E(\xi,\sqrt{2}\Delta)} + \frac{\Delta}{4U}\left[1 - \frac{\xi(\xi^2+\Delta^2)}{E(\xi,\sqrt{2}\Delta)^3}\right],$$

from which the asymptotic behavior of $\Delta(U)$ is obtained as follows:

$$\Delta = \Delta_\infty\left(1+\frac{nW}{2U}\right) \tag{36}$$

with $\Delta_\infty = W\sqrt{2n(1-n)}\mathrm{e}^{-\frac{1}{N_0V_0}}$. This approximate result exhibits the correct asymptotic behavior for U much greater than the bandwidth as shown in Fig. 3.

The fidelity Considering that the ground state as shown in Eq. (13) of the correlated superconducting system has the similar structure to that of the uncorrelated BCS case, the effects of electron interaction can also be described by the fidelity, i.e., the overlap of these two quantum states,

$$f(U) = \left|\langle \mathrm{bcs}||\mathrm{gs}\rangle\right|^2 = \prod_{\boldsymbol{k}}{}' \left|\langle \phi^{U=0}_{\boldsymbol{k},1}|\phi^{U}_{\boldsymbol{k},1}\rangle\right|^2, \tag{37}$$

where $|\mathrm{gs}\rangle$ as shown in Eq. (13) denotes the ground state for arbitrary U while $|bcs\rangle$ denotes that of the BCS case. The second equality is derived using the product form of the ground state as shown in Eq. (13). Here $|\phi^U_{\boldsymbol{k},1}\rangle$ denotes the ground state of the $\boldsymbol{k}$ sector for arbitrary U as shown in Eq. (11), whose three components are calculated by solving Eq. (12). The three components of $|\phi^{U=0}_{\boldsymbol{k},1}\rangle$ for the BCS case are given by Eq. (21). The overlap as a function of U is shown in Fig. , which measures the closeness of the correlated superconducting state to the BCS ground state. As shown in the figure, at and below half filling the fidelity decreases with the magnitude of U for both positive and negative U, indicating that the ground-state wavefunction deviates from the BCS structure with the enhancement of electron correlation. The overlap diminishes for $U \gtrsim nW$ when the underlying normal states become Mott insulating ($n = 1$) or strongly correlated metallic ($n < 1$) phases.

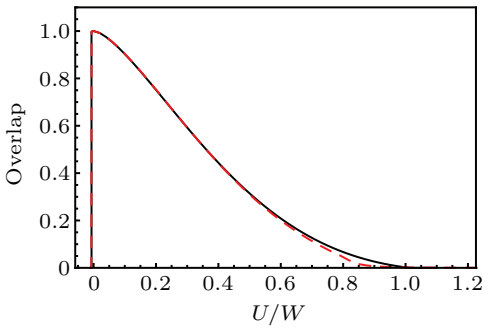


Fig. 5. The U dependence of the overlap of the correlated and uncorrelated superconducting ground states. As shown in Eq. (37), the fidelity is equal to the product of N numbers with N being the number of $\boldsymbol{k}$, and thus we plot the geometric mean of the fidelity at the thermodynamic limit, i.e., $\lim_{N\to\infty} f(U)^{1/N}$. Black solid line: the half-filling case $n = 1$. Red dashed line: below half filling, $n = 0.8$.

Single-particle excitation gap Δ^{gap} When a single electron is added to or removed from the ground state, a single-particle excitation is created. Since the ground state is of even parity, the single-particle excited state must live in the odd sector. Thus, Δ^{gap} is equal to

$$\Delta^{\mathrm{gap}} = \min(E_{\boldsymbol{k},-} - E_{\boldsymbol{k},1}). \tag{38}$$

Here, $E_{\boldsymbol{k},-}$ denotes the lowest-lying eigenenergy of $\hat{H}^{\rm mf}_{\boldsymbol{k}}$ in the odd sector. As an example, in the 2D odd subspaces spanned by $\{|1000\rangle_{\boldsymbol{k}}, |1011\rangle_{\boldsymbol{k}}\}$, $\hat{H}^{\rm mf}_{\boldsymbol{k}}$ is written as

$$\begin{aligned}\hat{H}^{\rm mf}_{\boldsymbol{k}} &= \xi_{\boldsymbol{k}}(|1000\rangle\langle 1000| + (3\xi_{\boldsymbol{k}}+U)(|1011\rangle\langle 1011| \\ &\quad -\Delta\big(|1000\rangle\langle 1011| + |0100\rangle\langle 0111|\big), \qquad (39)\\ &= E_{\boldsymbol{k},-}|\psi^{(-)}_{\boldsymbol{k},1}\rangle\langle\psi^{(-)}_{\boldsymbol{k},1}| + E_{\boldsymbol{k},+}|\psi^{(+)}_{\boldsymbol{k},1}\rangle\langle\psi^{(+)}_{\boldsymbol{k},1}|, \qquad (40)\end{aligned}$$

and the forms of the Hamiltonian in the other three odd subspaces is of similar structure.

For the strongly correlated superconducting state as $U \gg \Delta$, if the energy of $|1000\rangle_{\boldsymbol{k}}$ is around zero, i.e., $\xi_{\boldsymbol{k}} \approx 0$, the energy of $|1011\rangle_{\boldsymbol{k}}$ will be well above zero with an energy difference of order U. The Δ term in Eq. (39) is negligible, and to the leading order we have $E_{\boldsymbol{k},-} = \xi_{\boldsymbol{k}}$. Similarly, if $\xi_{\boldsymbol{k}}+U$ is nearly zero, we have $E_{\boldsymbol{k},-} = 3\xi_{\boldsymbol{k}}+U$. Using these results for $E_{\boldsymbol{k},-}$ and for $E_{\boldsymbol{k},1}$ from Eqs. (29) and (32), we obtain $\Delta^{\rm gap} = \sqrt{2}\Delta$. This means that for strong correlated superconducting case, the pair potential as defined in Eq. (6) is not the single-particle excitation gap.

In summary, the HK model, which is an exactly solvable correlated electron model, provides us an ideal system to examining how superconductivity evolves as a function of U when the electron pairing is supported by a BCS-type electron-electron attraction. By employing the mean-field approximation, the pair potential is calculated self-consistently. The slightly counter-intuitive observation is that negative U suppresses superconductivity while not too strong positive U strengthens it. For strongly correlated superconductors, the single-particle superconducting energy gap is $\sqrt{2}$ times as large as the pair potential.

Appendix A: Exact results

To diagonalize $\hat{H}^{\rm mf}_{\boldsymbol{k}}$, we can rebuild the basis of the Fock subspace $\mathcal{H}_{\boldsymbol{k}}$ by employing the common eigenvectors of three conserved quantities, i.e., the electron-number parity $\hat{P}_{\boldsymbol{k}}$, the square of total spin $\hat{S}^2$, and the z component of total spin $\hat{S}_z$. Here the operator of electron-number parity is

$$\hat{P}_{\boldsymbol{k}} = (-1)^{\hat{N}_{\boldsymbol{k}}}, \qquad (A1)$$

where $\hat{N}_{\boldsymbol{k}}$ denotes the electron-number operator

$$\hat{N}_{\boldsymbol{k}} = \sum_{\alpha=\uparrow,\downarrow}\big(c^\dagger_{\boldsymbol{k}\alpha}c_{\boldsymbol{k}\alpha} + c^\dagger_{-\boldsymbol{k}\alpha}c_{-\boldsymbol{k}\alpha}\big). \qquad (A2)$$

The square of the total spin is $\hat{S}^2 = \hat{S}^2_x + \hat{S}^2_y + \hat{S}^2_z$, with

$$\hat{S}_{x,y,z} = \frac{1}{2}\sum_{\alpha,\beta}\big(c^\dagger_{\boldsymbol{k}\alpha}\sigma^{x,y,z}_{\alpha,\beta}c_{\boldsymbol{k}\beta} + c^\dagger_{-\boldsymbol{k}\alpha}\sigma^{x,y,z}_{\alpha,\beta}c_{-\boldsymbol{k}\beta}\big), \qquad (A3)$$

where $\sigma^{x,y,z}$ are the Pauli matrices. Table A1 shows the 16 basis vectors classified according to the eigenvalues of $\hat{P}_{\boldsymbol{k}}$, $\hat{N}_{\boldsymbol{k}}$, $\hat{S}^2$, and $\hat{S}_z$. According to this table, $\mathcal{H}_{\boldsymbol{k}}$ are divided into even ($P=1$) and odd ($P=-1$) sectors, each of which is in 8 dimensions (8D).

Table A1. Basis vectors built according to their quantum numbers. P, N, S and S_z denote the eigenvalues of of $\hat{P}_{\boldsymbol{k}}$, $\hat{N}_{\boldsymbol{k}}$, $\hat{S}$ and $\hat{S}_z$, respectively.

P	N	S	S_z	Basis vectors
$+1$	0	0	0	$\|0_{\boldsymbol{k}}\rangle$
	2			$\|s_{\boldsymbol{k}}\rangle = (\|1100\rangle_{\boldsymbol{k}} + \|0011\rangle_{\boldsymbol{k}})/\sqrt{2}$
	4			$\|f_{\boldsymbol{k}}\rangle = \|1111\rangle_{\boldsymbol{k}}$
	2			$\|1001\rangle_{\boldsymbol{k}}$
				$\|0110\rangle_{\boldsymbol{k}}$
		1	1	$\|t_1\rangle_{\boldsymbol{k}} = \|1010\rangle_{\boldsymbol{k}}$
			0	$\|t_0\rangle_{\boldsymbol{k}} = (\|1100\rangle_{\boldsymbol{k}} - \|0011\rangle_{\boldsymbol{k}})/\sqrt{2}$
			-1	$\|t_{\bar{1}}\rangle_{\boldsymbol{k}} = \|0101\rangle_{\boldsymbol{k}}$
-1	1	$\frac{1}{2}$	$\frac{1}{2}$	$\|1000\rangle_{\boldsymbol{k}}$
				$\|0010\rangle_{\boldsymbol{k}}$
			$-\frac{1}{2}$	$\|0100\rangle_{\boldsymbol{k}}$
				$\|0001\rangle_{\boldsymbol{k}}$
	3		$\frac{1}{2}$	$\|1011\rangle_{\boldsymbol{k}}$
				$\|1110\rangle_{\boldsymbol{k}}$
			$-\frac{1}{2}$	$\|0111\rangle_{\boldsymbol{k}}$
				$\|1101\rangle_{\boldsymbol{k}}$

The even sector Five of the eight basis vectors of the even sector are obviously the eigenkets of $\hat{H}^{\rm mf}_{\boldsymbol{k}}$. Namely, they are the spin-triplet states, i.e., $|t_1\rangle_{\boldsymbol{k}}$, $|t_0\rangle_{\boldsymbol{k}}$ and $|t_{\bar{1}}\rangle_{\boldsymbol{k}}$, and the Pauli-blocking states $|1001\rangle_{\boldsymbol{k}}$ and $|0110\rangle_{\boldsymbol{k}}$. The eigenenergies of the spin-triplet and Pauli-blocking states are $2\eta_1$ and η_2, respectively; η_1 and η_2 are defined in Eq. (2) with relation $2\eta_1 \le \eta_2$.

The remaining three eigenstates of $\hat{H}^{\rm mf}_{\boldsymbol{k}}$ in the even sector seats in the subspace spanned by $|0_{\boldsymbol{k}}\rangle$, $|s_{\boldsymbol{k}}\rangle$, and $|f_{\boldsymbol{k}}\rangle$, i.e., the empty, spin singlet and fully occupied states. The corresponding 3×3 Hermitian matrix is shown in Eq. (12) and the three eigenvalues are

$$E_{\boldsymbol{k},i} = 2\xi_{\boldsymbol{k}} + \frac{2U}{3} + 2E^{\rm even}_{\boldsymbol{k}}\frac{\cos\left(\theta_{\boldsymbol{k}} + \frac{2\pi}{3}{\rm i}\right)}{\cos\frac{\pi}{6}}, \qquad (A4)$$

where $i = 1,2,3$ and

$$E^{\rm even}_{\boldsymbol{k}} = \sqrt{\frac{U^2}{3} + U\xi_{\boldsymbol{k}} + \xi^2_{\boldsymbol{k}} + \Delta^2}, \qquad (A5)$$

$$\theta_{\boldsymbol{k}} = \frac{1}{3}\arccos\left[\frac{q_{\boldsymbol{k}}}{(\sqrt{3}E^{\rm even}_{\boldsymbol{k}})^3}\right], \qquad (A6)$$

$$q_{\boldsymbol{k}} = U\left(U^2 + \frac{9}{2}U\xi_{\boldsymbol{k}} + \frac{9}{2}\xi^2_{\boldsymbol{k}} - \frac{9}{4}\Delta^2\right). \qquad (A7)$$

Since $0 \le \theta_{\boldsymbol{k}} \le \pi/3$ according to Eq. (A6), we have $E_{\boldsymbol{k},1} \le E_{\boldsymbol{k},2} \le E_{\boldsymbol{k},3}$ from Eq. (A4). $E_{\boldsymbol{k},1} = E_{\boldsymbol{k},2}$ or $E_{\boldsymbol{k},2} = E_{\boldsymbol{k},3}$ occur when $\theta_{\boldsymbol{k}} = 0$ or $\pi/3$, which is satisfied if and only if $\Delta = 0$ and $\xi_{\boldsymbol{k}}(\xi_{\boldsymbol{k}}+U)(2\xi_{\boldsymbol{k}}+U) = 0$. As a result, the three eigenenergies are arranged in strictly ascending order, i.e., $E_{\boldsymbol{k},1} < E_{\boldsymbol{k},2} < E_{\boldsymbol{k},3}$, when $\Delta \neq 0$ for any U and $\xi_{\boldsymbol{k}}$.

Furthermore, according to the variational principle, the minimum of the three eigenvalues, i.e., $E_{\boldsymbol{k},1}$, is less than

the minimum of the three diagonal elements of the Hermitian matrix in Eq. (12) when $\Delta \neq 0$. Namely, $E_{\boldsymbol{k},1} < \min(0, 2\eta_1, 2\eta_2) \leq 2\eta_1$. Therefore, $E_{\boldsymbol{k},1}$ is the lowest eigenvalue in the even sector.

The odd sector The 8D odd sector of $\mathcal{H}_{\boldsymbol{k}}$ can be decomposed into four 2D subspaces spanned by $\{|1000\rangle_{\boldsymbol{k}}, |1011\rangle_{\boldsymbol{k}}\}$, $\{|0100\rangle_{\boldsymbol{k}}, |0111\rangle_{\boldsymbol{k}}\}$, $\{|0010\rangle_{\boldsymbol{k}}, |1110\rangle_{\boldsymbol{k}}\}$ and $\{|0001\rangle_{\boldsymbol{k}}, |1101\rangle_{\boldsymbol{k}}\}$, respectively. In each of the four 2D subspaces, $\hat{H}^{\rm mf}_{\boldsymbol{k}}$ takes the similar form. In the 2D odd subspaces spanned by $\{|1000\rangle_{\boldsymbol{k}}, |1011\rangle_{\boldsymbol{k}}\}$, $\hat{H}^{\rm mf}_{\boldsymbol{k}}$ can be written as Eq. (39). The two eigenenergies are

$$E_{\boldsymbol{k},\pm} = 2\xi_{\boldsymbol{k}} + \frac{U}{2} \pm E^{\rm odd}_{\boldsymbol{k}}, \tag{A8}$$

where

$$E^{\rm odd}_{\boldsymbol{k}} = \sqrt{\left(\xi_{\boldsymbol{k}} + \frac{U}{2}\right)^2 + \Delta^2}. \tag{A9}$$

For the other three 2D subspaces, the eigenenergies are exactly the same as Eq. (A8). Therefore, $E_{\boldsymbol{k},\pm}$ are both four-fold degenerate, and $E_{\boldsymbol{k},-}$ is the lowest eigenvalue in the odd sector.

The minimal eigenvalue Comparing Eq. (A5) to Eq. (A9), we have

$$\frac{2}{\sqrt{3}} E^{\rm even}_{\boldsymbol{k}} \geq E^{\rm odd}_{\boldsymbol{k}} + \frac{1}{6}U. \tag{A10}$$

Since $0 \leq \theta_{\boldsymbol{k}} \leq \pi/3$ according to Eq. (A6), we have $\cos(\theta_{\boldsymbol{k}} + 2\pi/3) \leq -1/2$, and therefore from Eq. (A4) we have

$$E_{\boldsymbol{k},1} \leq 2\xi_{\boldsymbol{k}} + \frac{2}{3}U - \frac{2}{\sqrt{3}} E^{\rm even}_{\boldsymbol{k}}. \tag{A11}$$

Making use of the above two inequalities, we have

$$E_{\boldsymbol{k},1} \leq E_{\boldsymbol{k},-}, \tag{A12}$$

where equality will occur if and only if $\Delta = 0$ and $\xi_{\boldsymbol{k}}(\xi_{\boldsymbol{k}} + U)(2\xi_{\boldsymbol{k}} + U) = 0$. Thus, when $\Delta \neq 0$, we always have $E_{\boldsymbol{k},1} < E_{\boldsymbol{k},-}$, i.e., the mean-field superconducting ground state is in the 3D subspace of the even sector.

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