Cooper problem in a cuprate lattice

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We solve the Cooper problem in a cuprate lattice by utilizing a three-band model. We determine
the ground state of a Cooper pair for repulsive on-site interactions, and demonstrate that the
Corresponding wave function has an orbital $d_{x^2−y^2}$ symmetry. We discuss the influence of next-
nearest-neighbor tunneling on the Cooper pair solution, in particular the necessity of next-nearest-
neighbor tunneling for having $d$-wave pairs for hole-doped systems. We also propose experimental
signatures of the $d$-wave Cooper pairs for a cold-atom system in a cuprate lattice.

I. INTRODUCTION

A cuprate lattice is a modified two-dimensional Lieb
lattice that is characterized by a square unit cell with
three sites [1–4]; see Fig. 1. In terms of single parti-
cles terms, we include potential energies for the $p$- and
d-orbitals, which have different values. The difference
of these potential energies modifies the charge-transfer
energy. Furthermore, we include a tunneling energy be-
tween the $p$-orbitals. The single-particle energy spectrum
of this lattice has two dispersive bands and one nearly flat
band in between. A large charge-transfer energy provides
a gap between the dispersive upper band and the other
two bands, where the dispersion of the latter is due to the
tunneling between $p$-orbitals, which is assumed to be smaller than the other energies; see Figs. 2(a) and 2(c). As we describe below, we will also assume the on-
site interaction of two particles to be different on $p$- and
d-orbitals. Realizations and proposals for this and rel-
ated lattices have been reported for cold atoms [5–11]
and photonic systems [12] as well as for solid-state sys-
tems [13, 14]. Phenomena that are associated with flat-
band or three-band systems have been reported in Refs.
[15–22].

The namesake realization of this lattice are the cuprate
materials, in particular the copper-oxide layers, which
are modeled as a cuprate lattice described above. These
layers of Cu and O atoms directly realize the lattice dis-
played in Fig. 1, where the Cu atoms are represented as
a $d_{x^2−y^2}$ orbital, and O atoms as $p_x$ and $p_y$ orbitals. It
is assumed that the CuO$_2$ layers are the location of the
electron pairs, and therefore contain the origin of super-
conductivity [23–26]. The mechanism of pairing is un-
der debate, with competing proposals reported in Refs.
[27–38]. ARPES measurements have provided insight
into the Fermi surface geometry in the relevant regime
[3, 4, 39–45], which can be captured by the three-band
model; see see Fig. 2(b) and 2(d). Numerous theoretical
studies on determining the ground state of the interac-
ting cuprate problem have been reported; see, e.g., Refs.
[46–55].

In the study of conventional superconductors, the
Cooper problem and its solution constituted a defining
insight that advanced the understanding of superconduc-
tivity in general. In its original formulation, the Cooper
problem assumes an effective electron-electron attraction
due to the dominance of the electron-phonon interaction
over the screened Coulomb repulsion, leading to a Cooper
pair with an orbital $s$-wave symmetry [4, 56–60]. This in-
sight paved the way for the subsequent development of BCS theory. Extensions of the Cooper problem to three-
body systems have been presented in Refs. [61, 62].

In this paper we solve the Cooper problem for a cuprate lattice. The Cooper problem is intrinsically suitable for the weak-coupling limit of a Fermi system, because a nearly-intact Fermi sea is assumed. Our proposal aims primarily at ultracold atom systems, specifically Fermi mixtures in cuprate optical lattices, which directly realizes the model that we describe. Utilizing the tunability of these systems, the interaction and density dependence of the pairing energy can be measured, to be compared to our predictions. In the weak-coupling limit, we expect these predictions to be quantitatively accurate. As we describe below, we formulate the Cooper problem for the cuprate lattice and solve it numerically, where we emphasize that these numbers suggest that the system is the case of academic completeness, because all available methods should be applied to an unsolved problem. Secondly, we point out that the resulting ground state properties are consistent with the typical findings in cuprate materials, with a ground state energy of the order of 100 K. Furthermore, we use the parameters for the three-level model of cuprates that were reported in Ref. [60]. We emphasize that these numbers suggest that the system is in the strongly correlated regime, and that therefore the Cooper problem approach cannot be expected to provide quantitatively correct predictions. We present this application of our calculation firstly for the sake of academic completeness, because all available methods should be applied to an unsolved problem. Secondly, we point out that the resulting ground state properties are consistent with the typical findings in cuprate materials, with a ground state energy of the order of 100 K.

This paper is organized as follows. In Sec. II we calculate the electronic band structure of the cuprate lattice for $t_{pp} \neq 0$. We define the Fermi sea, and demonstrate the effect of $t_{pp}$ on the Fermi-surface geometry. In Sec. III we consider the Cooper problem, and derive an eigenstate equation describing a Cooper pair on the submanifold $S$ of the upper band. In Sec. IV we calculate the ground-state energy and wave function, and determine its orbital symmetry. In Sec. V we propose experimental signatures of the $d$-wave Cooper pairs for a cold-atom system in a cuprate lattice. Finally, in Sec. VI we present the concluding remarks.

II. ELECTRONIC BAND STRUCTURE AND FERMI-HUBBARD MODEL

For the lattice configuration with three sites A, B, and C in the square unit cell displayed in Fig. 1, we assume the on-site potential to be $V_A \equiv V_d$ and $V_B \equiv V_C \equiv V_p$. We also define three sets of creation and annihilation operators $\{a_{nm}, a_{nm}\} \{b_{nm}, b_{nm}\}, \{c_{nm}, c_{nm}\}$ corresponding to the A-, B-, and C-site, respectively, where the indices $n$ and $m$ refer to the $x$- and $y$ direction in real space. These operators fulfill the fermionic algebra, and we refer to them as site operators. The spin index is suppressed.

The tight-binding Hamiltonian in momentum space is

$$H_{tb} = \sum_{k \in \text{1.BZ}} \begin{pmatrix} a_k^\dagger & b_k^\dagger & c_k^\dagger \end{pmatrix} \begin{pmatrix} a_k & b_k & c_k \end{pmatrix}$$

for all momentum points $k = (k_x, k_y)$ within the first Brillouin zone (1.BZ), where $k_x, k_y \in [-\pi/a, \pi/a]$ and $a$ denotes the lattice constant. The matrix $h_{tb}$ is

$$h_{tb} = \begin{pmatrix} V_d & f(k_x) & -g(k_y) \\ f^*(k_x) & V_p & -\tau f^*(k_x)g(k_y) \\ -g^*(k_y) & -\tau f(k_x)g^*(k_y) & V_p \end{pmatrix}$$

where $f(k_x) = t_{pd}(1 - e^{-ik_x})$, $g(k_y) = t_{pd}(1 - e^{-ik_y})$, and $\tau = t_{pp}/t_{pd}^2$. The parameters $t_{pd}$ and $t_{pp}$ show the nearest-neighbor and next-nearest-neighbor hopping, respectively. The functions $f^*$ and $g^*$ denote the complex conjugate of $f$ and $g$, respectively; see Appendix A.

The characteristic equation of the matrix $h_{tb}$ is cubic with three solutions $E_{kU}^F$, $E_{kF}^F$, and $E_{kL}^F$ that provide the electronic band structure of the lattice; see Appendix B for analytical solutions. Here the index U, F, and L stands for the upper-, flat-, and lower band, respectively. The dispersion $E_{kF}^F$ is exactly constant for vanishing $t_{pp}$, resulting in a flat band, but has a small momentum dependence for nonvanishing $t_{pp}$. However, we use the index F for both cases. Figures 2 a) and 2 c) show the band structure for vanishing and nonvanishing $t_{pp}$, respectively. For both cases there are two dispersive bands $E_{kU}^F$ and $E_{kL}^F$. For $t_{pp} = 0$ the dispersion is given by $E_{kU}^F = V_p$, between $E_{kU}^F$ and $E_{kL}^F$. For $t_{pp} \neq 0$ the dispersion is not constant, however, its momentum dependence is small compared to the other two bands.

To formulate the Cooper problem for the upper band, we consider two-particle states with vanishing total momentum. To find the interaction term of the Cooper problem, we use the three sets of creation and annihilation operators $\{\psi_{1,\sigma,k}\}$, $\{\psi_{F,\sigma,k}\}$, and $\{\psi_{L,\sigma,k}\}$, where $\sigma \in \{\uparrow, \downarrow\}$ is a spin index. These operators fulfill the fermionic algebra, and create or annihilate an electron in the the upper-, flat-, and lower band, respectively. In the following we refer to them as band operators. The band operators can be related to the site operators using the components of the eigenvectors of the matrix $h_{tb}$; see Appendix C. We assume that the charge-transfer energy, $V_{de} \equiv V_d - V_p$, is sufficiently large so that we neglect the interband pairings; cf. Figs. 2 a) and 2 c). We write the interaction Hamiltonian for the Cooper problem as

$$H_{int} = \frac{1}{A} \sum_{k,k' \in \text{1.BZ}} \sum_{\sigma\tau} V_{k,k'} \psi_{U,k',\sigma}^\dagger \psi_{U,-k,\sigma}^\dagger \psi_{U,-k',\tau} \psi_{U,k'}$$

see Appendix C for the derivation. Here, $A$ denotes the area of the first Brillouin zone and the interaction func-
Figure 2. Electronic band structure and Fermi surface of a cuprate lattice in the first Brillouin zone for $V_{dp} = 3.45\text{ eV}$ and $t_{pd} = 1.13\text{ eV}$: (a) Band structure for $t_{pp} = 0$; (b) the corresponding Fermi surface for $\mu \approx -0.679\text{ eV}$; (c) band structure for $t_{pp} = 0.8\text{ eV}$; and (d) the corresponding Fermi surface for $\mu \approx -0.679\text{ eV}$ in the upper band. The two lower bands are filled. For $t_{pp} \neq 0$ the flat band is deformed, and the curvature of the dispersive bands is changed. Blue and red dots in panels (b) and (d) correspond to the occupied and unoccupied states, respectively.

The on-site Coulomb interaction strength for $d_{x^2-y^2}$ orbitals is $U_d$, and for both $p_x$ and $p_y$ orbitals it is $U_p$.

Next, we define the Fermi sea by introducing a chemical potential, $\mu$. We define the interacting Fermi sea, $\text{FS}_{\text{int}}$, which includes corrections due to the interaction:

$$\text{FS}_{\text{int}} = \left\{ \mathbf{k} \in 1\text{BZ} : 2E^{(U)}_{\mathbf{k}} + \frac{1}{A} V_{\mathbf{k},\mathbf{k}} < 2\mu \right\},$$

where the interaction function $V_{\mathbf{k},\mathbf{k}'}$ is obtained as Eq. 4 for $\mathbf{k}' = \mathbf{k}$; see Fig. 4. We assume these states to be occupied with an inert Fermi sea. The unoccupied states that are considered in the Cooper problem are the Brillouin zone without the Fermi sea; i.e., $\mathbf{k} \in 1\text{BZ}\backslash\text{FS}_{\text{int}}$. Figures 2(b) and 2(d) show the Fermi surface for $t_{pp} = 0$ and $t_{pp} \neq 0$, respectively. The nonvanishing $t_{pp}$ changes the curvature of the dispersive bands, resulting in a Fermi-surface geometry that is in better agreement with the experimental data extracted from ARPES [3, 4, 39–45]. Moreover, we vary $\mu$ and calculate the corresponding electron density, $n_e$, for both $t_{pp} = 0$ and $t_{pp} \neq 0$, resulting in a chemical potential dependence of the density shown in Fig. 3. For a given value of $\mu$ we find that $n_e(t_{pp} \neq 0) \leq n_e(t_{pp} = 0)$. As a result, while the desired geometry of the Fermi surface is preserved, we can increase the hole doping for $t_{pp} \neq 0$ [63].
Figure 3. Electron density, \( n_e \), vs chemical potential, \( \mu \), in units of eV, of the upper band of the cuprate lattice, where \( V_{dp} = 3.45 \) eV and \( t_{pd} = 1.13 \) eV. The blue curve corresponds to \( t_{pp} = 0 \), and the red curve corresponds to \( t_{pp} = 0.8 \) eV. For a given value of \( \mu \), we have \( n_e(t_{pp} \neq 0) \leq n_e(t_{pp} = 0) \).

Finally, we include the kinetic energy, so that the total Hamiltonian of the Cooper problem is

\[
\hat{H}_{\text{tot}} = \sum_{\mathbf{k} \in \text{1.BZ}/\text{FS}_{\text{int}}} \xi_{\mathbf{k}}^{(U)} \psi_{\mathbf{U},\mathbf{k}\sigma}^\dagger \psi_{\mathbf{U},\mathbf{k}\sigma} + \frac{1}{A} \times \sum_{\mathbf{k},\mathbf{k}' \in \text{1.BZ}/\text{FS}_{\text{int}}} \mathcal{V}_{\mathbf{k},\mathbf{k}'} \psi_{\mathbf{U},\mathbf{k}\uparrow}^\dagger \psi_{\mathbf{U},-\mathbf{k}\downarrow}^\dagger \psi_{\mathbf{U},-\mathbf{k}\uparrow} \psi_{\mathbf{U},\mathbf{k}\downarrow},
\]

where \( \xi_{\mathbf{k}}^{(U)} = E_{\mathbf{k}}^{(U)} - \mu \) and \( \mathcal{V}_{\mathbf{k},\mathbf{k}'} \) is given by Eq. (4); see Appendix C.

### III. COOPER PROBLEM AND PAIRING EQUATION

The original Cooper problem and its solution show that two electrons that are immersed in an inert Fermi sea form a bound state with an orbital s-wave symmetry for an arbitrarily weak attractive interaction [4, 56–60]. The effective attraction models the phonon-mediated interaction that is dominant over the screened Coulomb repulsion. The interaction model that is used for conventional superconductors is a negative coupling constant in momentum space for the relative kinetic energy of the electrons smaller than the Debye energy; cf. e.g., Refs. [56, 59, 60]. Following the standard Cooper problem, we consider a singlet-state Cooper pair as

\[
\Psi = \sum_{\mathbf{k} \in \text{1.BZ}/\text{FS}_{\text{int}}} \phi_{\mathbf{k}} \psi_{\mathbf{U},\mathbf{k}\uparrow}^\dagger \psi_{\mathbf{U},-\mathbf{k}\downarrow}^\dagger |\text{FS}_{\text{int}}\rangle, \quad (7)
\]

where \( \phi_{\mathbf{k}} \) is the wave function of the Cooper pair in momentum space and \( |\text{FS}_{\text{int}}\rangle \) denotes the Fermi-sea state; cf. Eq. (5).

To find the ground-state energy and wave function, we consider the eigenvalue problem

\[
\hat{H}_{\text{tot}} |\Psi\rangle = E |\Psi\rangle, \quad (8)
\]

where \( E \) is the eigenenergy. We determine the operator \( \hat{H}_{\text{tot}} |\Psi\rangle \) and obtain an eigenequation describing the Cooper pair:

\[
\left( \epsilon_{\mathbf{k}}^{(U)} + \epsilon_{-\mathbf{k}}^{(U)} + \frac{1}{A} \mathcal{V}_{\mathbf{k},\mathbf{k}'} - E \right) \phi_{\mathbf{k}} = -\frac{1}{A} \sum_{\mathbf{k}' \neq \mathbf{k} \in \text{1.BZ}/\text{FS}_{\text{int}}} \mathcal{V}_{\mathbf{k},\mathbf{k}'} \phi_{\mathbf{k}'}; \quad (9)
\]

see Appendix D. In what follows we solve Eq. (9) numerically, and determine the ground-state energy, \( E_G < 0 \).

### IV. GROUND-STATE ENERGY AND WAVE FUNCTION

To solve Eq. (9) numerically, first we discretize the first Brillouin zone as \( \mathbf{k}_j = (k_{j,x}, k_{j,y}) \), where

\[
k_{j,x}, k_{j,y} = \frac{1}{a} \left[ -\pi + \frac{2\pi}{N} (j-1) \right] \text{ for } j = 1, 2, \ldots, N. \quad (10)
\]

Figure 4. Interaction function \( \mathcal{V}_{\mathbf{k},\mathbf{k}'} / N^2 \) in units of eV, cf. Eq. (4), for repulsive on-site interactions, where \( N = 100, V_{dp} = 3.45 \) eV, \( t_{pd} = 1.13 \) eV, \( t_{pp} = 0.8 \) eV, \( U_d = 10.3 \) eV, and \( U_p = 4.1 \) eV.
Here, \(a\) denotes the lattice constant and \(N \in \mathbb{N}\) is the number of grid points in \(x\)- and \(y\) direction, i.e., \(N_x = N_y = N\). We calculate the electronic band structure numerically and the interaction function \(V_{k,k'}\) at each grid point using Eq. (4). Next, for a given value of \(\mu\) we determine the Fermi surface following the relation (5). We note that the number of grid points within the first Brillouin zone is proportional to \(N_x N_y = N^2\), so the size of the matrix associated with \(\hat{H}_{\text{tot}}\) is proportional to \(N^4\), cf. Eq. (4). We choose the number of grid points sufficiently large to ensure convergence of the numerical results. We determine the Fermi sea numerically, and exclude it from the first Brillouin zone. We consider \(\hat{H}_{\text{tot}}\) on the reduced momentum space that corresponds to the unoccupied states; see Appendix E.

For the regime of attractive interactions, i.e., \(U_d, U_p < 0\), we find a Cooper pair with an approximate orbital \(s\)-wave symmetry; see Appendix F.

For repulsive on-site interactions, \(U_d, U_p > 0\), the interaction function \(V_{k,k'}\), cf. Eq. (4), has the momentum dependence shown in Fig. 3. The repulsive interaction suppresses the formation of pairs with \(s\)-wave symmetry. Instead, the ground state wave function has \(d\)-wave symmetry, as shown in Fig. 5, for the lattice parameters \(V_{dp} = 3.45\) eV, \(t_{pd} = 1.13\) eV, and \(t_{pp} = 0.8\) eV that follow approximately the values given by Ref. [46]. The orientation of the maxima and minima, and the location of the nodal points, indicates that the wave function supports an orbital symmetry of \(d_{x^2-y^2}\).

Finally, we vary the hole doping, \(\delta_h\), by changing the chemical potential, \(\mu\) [33]. We calculate the corresponding ground-state energy, \(E_G\), resulting in Fig. 6. We find that the largest absolute magnitude of the ground-state energy, \(E_G^{(\text{max})}\) \(\sim 0.01\) eV, occurs near the hole doping \(\delta_h \sim 0.35\). This converts to a critical temperature of the order of 100 K. The behavior of the ground-state energies consistent with Ref. [40] qualitatively.

V. EXPERIMENTAL SIGNATURE IN A COLD-ATOM SYSTEM

We propose to detect the predictions of our analysis in a system of ultracold atoms in an optical lattice. Specifically, we consider fermionic atoms in higher bands of optical lattices. Lattice geometries that resemble the cuprate lattice and related geometries have been realized experimentally for bosonic atoms in Refs. [7–9]. Utilizing a Feshbach resonance, the whole range of repulsive interactions is accessible, from weak to strong coupling. In particular, our predictions can be tested quantitatively in the weak-coupling regime.

We propose to use noise correlations of time-of-flight images as an observable to detect the symmetry of the Cooper pair in the far-field limit, which is achieved for expansions in which the expanded cloud is much larger than the in-situ cloud, the density correlations of the atoms of different spins include the correlations of \(\hat{n}(\mathbf{k}, \sigma)\) and \(\hat{n}(-\mathbf{k}, -\sigma)\), where \(\hat{n}(\mathbf{k}, \sigma)\) is the occupation of the momentum state \(\mathbf{k}\) and spin-state \(\sigma\) of the in-situ system; see Refs. [64–67]. This quantity gives access to the square of the pair wave function, depicted in Fig. 5. In particular the angular dependence of its magnitude and the nodal points of the wave function are observable in this quantity.

As a second measurement, we propose to use stirring
We find that the solution of Cooper problem predicts the
ity, primarily for the purpose of academic completeness.
of the Cooper problem on the study of superconductiv-
ble in the weak-coupling limit. However, we present the
 materials. We emphasize that the interaction strengths
calculation to the three-band model reported for cuprate
our predictions. As a second platform, we apply our cal-
try mapped out. We pointed out noise correlations and
the interaction strength and the Fermi surface geome-
tems, and the dependence on system parameters such as
lattice. Here, the weak-coupling regime can be imple-
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VI. CONCLUSIONS

In conclusion, we have presented the solution of the
Cooper problem for a cuprate lattice, for repulsive in-
teractions. The band structure of the cuprate lattice
consists of three bands, where we focus on densities for
which the two lower bands are filled, and the Fermi sur-
face is in the highest band. For these densities, and for
repulsive on-site interactions, we demonstrate that the
ground state solution of the Cooper problem has a $d_{x^2-y^2}$
orbital symmetry. The binding energy of the Cooper
pair depends strongly on the shape of the Fermi sur-
face. We show that it is small for a connected surface
of the shape of a deformed circle, while it is large for
surfaces that break up into four disconnected arcs. As
a primary, quantitative implementation of our results we
propose to create an ultracold Fermi gas in a cuprate
lattice. Here, the weak-coupling regime can be imple-
mented naturally due to the tunable nature of these sys-
tems, and the dependence on system parameters such as
the interaction strength and the Fermi surface geometry
mapped out. We pointed out noise correlations and
stirring experiments as experimental methods to detect
our predictions. As a second platform, we apply our cal-
culation to the three-band model reported for cuprate
materials. We emphasize that the interaction strengths
of this model suggests that it is in the strongly correlated
regime, whereas the Cooper problem is primarily applicable
in the weak-coupling limit. However, we present the
predictions of the Cooper problem here, given the impact
of the Cooper problem on the study of superconductiv-
ity, primarily for the purpose of academic completeness.
We find that the solution of Cooper problem predicts the
experimentally observed $d_{x^2-y^2}$ symmetry of the electron
pairs, a sharp increase of the binding energy with increas-
ring hole doping when the Fermi surface breaks up into
four disconnected arcs, and a maximal binding energy of
approximately 100 K. This study and its experimental
implementation provides a direct analogy between cold-
atom systems and the three-band model that is utilized in
cuprate materials, and therefore advances the exchange
between cold-atom and condensed-matter systems.

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APPENDIX A. DERIVATION OF THE
TIGHT-BINDING HAMILTONIAN (1)

We consider the cuprate lattice, see Fig. [1] and write
the spinless tight-binding Hamiltonian in terms of the
site operators in real space:

$$
\hat{H}_{tb} = \sum_{n,m} \left[ V_d a_{nm}^\dagger a_{nm} + V_p b_{nm}^\dagger b_{nm} + V_d c_{nm}^\dagger c_{nm} 
+ t_p d_{nm}^\dagger d_{nm} + t_p d_{nm}^\dagger b_{nm} + t_p d_{nm}^\dagger c_{nm} 
- t_p d_{nm} a_{nm}^\dagger - t_p d_{nm} b_{nm} - t_p d_{nm} c_{nm} 
+ t_p d_{nm} c_{nm-1} + t_p d_{nm-1} a_{nm} - t_p d_{nm-1} b_{nm} 
- t_p d_{nm} c_{nm} - t_p d_{nm} b_{nm-1} + t_p d_{nm} c_{nm-1} 
- t_p d_{nm} a_{nm-1} + t_p d_{nm-1} b_{nm-1} - t_p d_{nm} c_{nm-1} 
+ t_p d_{nm} c_{nm} + t_p d_{nm-1} b_{nm-1} \right],
$$

where $n$ and $m$ are two indices for the $x$- and $y$ direction, respectively. Next, we take the Fourier transform of each
operator, and obtain the tight-binding Hamiltonian in momentum space:

$$
\hat{H}_{tb} = \sum_{\mathbf{k} \in \mathbb{BZ}} \left[ V_d a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + V_p b_{\mathbf{k}}^\dagger b_{\mathbf{k}} + V_d c_{\mathbf{k}}^\dagger c_{\mathbf{k}} 
+ t_p d_{\mathbf{k}}^\dagger d_{\mathbf{k}} + t_p d_{\mathbf{k}}^\dagger b_{\mathbf{k}} + t_p d_{\mathbf{k}}^\dagger c_{\mathbf{k}} 
- t_p d_{\mathbf{k}} a_{\mathbf{k}} - t_p d_{\mathbf{k}} b_{\mathbf{k}} - t_p d_{\mathbf{k}} c_{\mathbf{k}} 
+ t_p d_{\mathbf{k}} b_{\mathbf{k}}^\dagger + t_p d_{\mathbf{k}} c_{\mathbf{k}}^\dagger 
- t_p d_{\mathbf{k}}^\dagger (1 - e^{-ikx} + e^{ikx} e^{-iky} - e^{-iky}) b_{\mathbf{k}}^\dagger c_{\mathbf{k}} 
- t_p d_{\mathbf{k}}^\dagger (1 - e^{-ikx} + e^{ikx} e^{iky} - e^{iky}) c_{\mathbf{k}}^\dagger b_{\mathbf{k}} \right].
$$

Finally, we define $f(k_x) = t_p d(1 - e^{-ikx})$, $g(k_x) = t_p d(1 - e^{ikx})$, and $\tau = t_p / t_p^2$, and arrive at Eq. [1].

APPENDIX B. ANALYTICAL DESCRIPTION
OF THE BAND STRUCTURE OF THE CUPRATE
LATTICE

The characteristic equation associated with Eq. [4]
reads as
\[ s^3 + c(k_x, k_y)s^2 + d(k_x, k_y)s + e(k_x, k_y) = 0, \quad (B1) \]

where

\[ c(k_x, k_y) = -V_d - 2V_p, \quad (B2) \]

\[ d(k_x, k_y) = -|f(k_x)|^2 - |g(k_y)|^2 - \tau^2 |f(k_x)|^2 |g(k_y)|^2 \]
\[ + V_p^2 + 2V_dV_p, \quad (B3) \]

\[ e(k_x, k_y) = V_p|f(k_x)|^2 + V_p|g(k_y)|^2 + \tau(V_d - 2) \times |f(k_x)|^2 |g(k_y)|^2 - V_dV_p, \quad (B4) \]

and \( \tau = t_{pp}/t_{pd} \). Next, we define a variable \( S = s - c(k_x, k_y)/3 \), and rewrite Eq. (B1) as

\[ S^3 + 3p(k_x, k_y)S + 2q(k_x, k_y) = 0, \quad (B5) \]

where

\[ p(k_x, k_y) = \frac{1}{3}d(k_x, k_y) - \frac{1}{9}[c(k_x, k_y)]^2, \quad (B6) \]

\[ q(k_x, k_y) = \frac{1}{27}[c(k_x, k_y)]^3 - \frac{1}{6}c(k_x, k_y)d(k_x, k_y) \]
\[ + \frac{1}{2}e(k_x, k_y). \quad (B7) \]

Following the mathematical formalism represented in Ref. [69], we calculate the three roots of Eq. (B1), revealing the band structure of the cuprate lattice:

\[ \tilde{E}_k^{(U)} = \frac{V_d + V_p}{2} + 2t_{pd}\sqrt{\sin^2\left(\frac{k_x}{2}\right) + \sin^2\left(\frac{k_y}{2}\right) + \left(\frac{V_d}{4t_{pd}}\right)^2}, \quad (B11) \]

\[ \tilde{E}_k^{(F)} = V_p, \quad (B12) \]

\[ \tilde{E}_k^{(L)} = \frac{V_d + V_p}{2} - 2t_{pd}\sqrt{\sin^2\left(\frac{k_x}{2}\right) + \sin^2\left(\frac{k_y}{2}\right) + \left(\frac{V_d}{4t_{pd}}\right)^2}, \quad (B13) \]

respectively; see Fig. [2](a). By comparing Eqs. [B8]-[B13] we find that the next-nearest-neighbor hopping, \( t_{pp} \), deforms the flat band \( \tilde{E}_k^{(F)} \), and changes the curvature of the dispersive bands \( \tilde{E}_k^{(U)} \) and \( \tilde{E}_k^{(L)} \).

**APPENDIX C. DERIVATION OF THE HAMILTONIANS [3] AND [6]**

For the cuprate lattice, see Fig. [1] the interaction Hamiltonian of the Fermi-Hubbard model reads in general as

\[ \hat{H}_{\text{int}} = U_C \sum_{k,p,q \in 1.BZ} \alpha_{k+p\sigma}^\dagger \alpha_{k-q\sigma}^\dagger \alpha_{k+p\sigma} \alpha_{k+q\sigma}, \quad (C1) \]

where \( \alpha^\dagger \in \{a^\dagger, b^\dagger, c^\dagger\} \) and \( \alpha \in \{a, b, c\} \) denote the creation and annihilation site operators, respectively, \( q \) is the momentum transfer [70], and \( U_C \) is an on-site Coulomb interaction strength. We notice that for each eigenvalue of \( h_{\text{int}} \), cf. Eq. (2), there exists a corresponding normalized eigenvector, which we denote as \( \psi_k^{(U)} = (\psi_{k(1;U)}, \psi_{k(2;U)}, \psi_{k(3;U)}) \), \( \psi_k^{(F)} = (\psi_{k(1;F)}, \psi_{k(2;F)}, \psi_{k(3;F)}) \), and \( \psi_k^{(L)} = (\psi_{k(1;L)}, \psi_{k(2;L)}, \psi_{k(3;L)}) \). The index \( U, F, \) and \( L \) corresponds to the upper-, flat-, and lower band, respectively. The site operators can be related to the band operators using the following relation:

\[
\begin{pmatrix}
\alpha_{k\sigma}^\dagger \\
\beta_{k\sigma}^\dagger \\
c_{k\sigma}^\dagger
\end{pmatrix} =
\begin{pmatrix}
\psi_{k(1;U)}^\dagger \\
\psi_{k(2;F)}^\dagger \\
\psi_{k(3;L)}^\dagger
\end{pmatrix}^{-1} =
\begin{pmatrix}
\psi_{k(1;U)} \\
\psi_{k(2;F)} \\
\psi_{k(3;L)}
\end{pmatrix}
\begin{pmatrix}
\psi_{U,k\sigma} \\
\psi_{F,k\sigma} \\
\psi_{L,k\sigma}
\end{pmatrix},
\]

(C2)

We can rewrite the interaction Hamiltonian [C1] corresponding to three sites A, B, and C in terms of the band
Hamiltonian (3) is obtained as
\[ \hat{H}_{\text{int}}(d) = \sum_{k,k' \in \text{1.BZ}} V_{k,k'}^{(d)} \psi_{U,k}^\dagger \psi_{U,k'}, \]
(C3)
where the label \( \Omega \) denotes an orbital configuration which can be \( d \equiv d_{x^2-y^2}, p_x, \) and \( p_y \). The on-site Coulomb interaction strengths for \( d_{x^2-y^2} \) and \( p_x \) (\( p_y \)) orbitals are assumed to be \( U_d \) and \( U_p \), respectively, and the interaction functions are

\[ V_{k,k'}^{(d)}(\Omega) = v_{11}(k') v_{11}(-k') v_{11}^*(k), \]
(C4)

\[ V_{k,k'}^{(p_x)} = v_{21}(k') v_{21}(-k') v_{21}^*(k), \]
(C5)

\[ V_{k,k'}^{(p_y)} = v_{31}(k') v_{31}(-k') v_{31}^*(k). \]
(C6)

The functions \( v_{ij} \) have been introduced in Eq. (C2), and \( v_{ij}^\dagger \) denotes the complex conjugate of \( v_{ij} \). The interaction Hamiltonian \( \hat{H}_{\text{int}} \) is obtained as
\[ \hat{H}_{\text{int}} = \hat{H}_{\text{int}}^{(d)} + \hat{H}_{\text{int}}^{(p_x)} + \hat{H}_{\text{int}}^{(p_y)}, \]
where \( V_{k,k} = V_{k,k}^{(d)} + V_{k,k}^{(p_x)} + V_{k,k}^{(p_y)} \) and the Fermi sea has been excluded from the first Brillouin zone.

We note that the tight-binding Hamiltonian \( \hat{H} \) in the basis spanned by the band operators is diagonal. For the submanifold \( S \) of the upper band, we find the kinetic energy to be
\[ \hat{H}_{\text{kin}} = \sum_{k \in \text{1.BZ}} \sum_{\sigma \in \{\uparrow, \downarrow\}} E_k^{(U)} \psi_{U,k\sigma}^\dagger \psi_{U,k\sigma}, \]
(C7)
where the Fermi sea will be excluded from the first Brillouin zone by introducing a chemical potential, \( \mu \). Finally, the total Hamiltonian \( \hat{H}_{\text{tot}} \) is obtained as \( \hat{H}_{\text{tot}} = \hat{H}_{\text{kin}} + \hat{H}_{\text{int}} \).

**APPENDIX D. DERIVATION OF THE EIGENEQUATION (9)**

To derive the pairing equation we calculate the resulting operator \( \hat{H}_{\text{tot}} |\Phi\rangle \), where \( \hat{H}_{\text{tot}} = \hat{H}_{\text{kin}} + \hat{H}_{\text{int}} \) subject to the interacting Fermi sea. For that, first we apply \( \hat{H}_{\text{kin}} \) on \( |\Phi\rangle \). The part corresponding to spin-up, \( \hat{H}_{\text{kin}}^{(\uparrow)} |\Phi\rangle \), is obtained to be

\[ \hat{H}_{\text{kin}}^{(\uparrow)} |\Phi\rangle = \sum_{k \in \text{1.BZ} \backslash \text{FS}} \xi_k^{(\uparrow)} \psi_{U,k\uparrow}^\dagger \sum_{\kappa \in \text{1.BZ} \backslash \text{FS}} \phi(\kappa) \psi_{U,k\uparrow} |\Phi\rangle, \]
(D1)

where \( \delta_{k\kappa} \) denotes the Kronecker delta. To find the effect of the spin-down part, \( \hat{H}_{\text{kin}}^{(\downarrow)} |\Phi\rangle \), we define \( \kappa' \equiv -\kappa \), and rewrite the singlet-state Cooper pair \( |\kappa\rangle \) in terms of \( \kappa' \). We obtain that

\[ \hat{H}_{\text{kin}}^{(\downarrow)} |\Phi\rangle = \sum_{\kappa' \in \text{1.BZ} \backslash \text{FS}} \delta_{k\kappa'} \xi_{k'}^{(\uparrow)} |\Phi\rangle. \]
(D2)

Equations (D1) and (D2) result in:

\[ \hat{H}_{\text{kin}} |\Phi\rangle = \sum_{k \in \text{1.BZ} \backslash \text{FS}} \left( \xi_k^{(\uparrow)} + \xi_{-k}^{(\uparrow)} \right) |\Phi\rangle. \]
(D3)

Next, we apply \( \hat{H}_{\text{int}} \) on \( |\Phi\rangle \). Here we split up the interaction Hamiltonian to the diagonal and off-diagonal parts. For the diagonal part we obtain:
\[
\hat{H}_{\text{int}}^{(\text{diag})} |\Phi\rangle = \frac{1}{\mathcal{A}} \sum_{k \in 1 \text{BZ} \setminus \text{FS}_{\text{int}}} \nu_{k,k} \psi_{U,k}^\dagger \psi_{U,k}^\dagger \sum_{\kappa \in 1 \text{BZ} \setminus \text{FS}_{\text{int}}} \phi(\kappa) \psi_{U,\kappa}^\dagger \psi_{U,\kappa}^\dagger |\text{FS}_{\text{int}}\rangle
\]

\[
= \frac{1}{\mathcal{A}} \sum_{k \in 1 \text{BZ} \setminus \text{FS}_{\text{int}}} \nu_{k,k} \sum_{\kappa \in 1 \text{BZ} \setminus \text{FS}_{\text{int}}} \phi(-k) \psi_{U,-k}^\dagger \psi_{U,k}^\dagger |\text{FS}_{\text{int}}\rangle
\]

\[
+ \frac{1}{\mathcal{A}} \sum_{k \in 1 \text{BZ} \setminus \text{FS}_{\text{int}}} \nu_{k,k} \sum_{\kappa \in 1 \text{BZ} \setminus \text{FS}_{\text{int}}} \delta_{k,-\kappa} \phi(\kappa) \psi_{U,k}^\dagger \psi_{U,-k}^\dagger \psi_{U,\kappa}^\dagger \psi_{U,\kappa}^\dagger |\text{FS}_{\text{int}}\rangle
\]

\[
= \frac{1}{\mathcal{A}} \sum_{k \in 1 \text{BZ} \setminus \text{FS}_{\text{int}}} \nu_{k,k} |\Phi\rangle ,
\]

where \(\mathcal{A}\) denotes the area of the first Brillouin zone. For the off-diagonal part we obtain:

\[
\hat{H}_{\text{int}}^{(\text{off-diag})} |\Phi\rangle = \frac{1}{\mathcal{A}} \sum_{k,k',\in 1 \text{BZ} \setminus \text{FS}_{\text{int}}} \nu_{k,k'} \psi_{U,k'}^\dagger \psi_{U,k}^\dagger \sum_{\kappa \in 1 \text{BZ} \setminus \text{FS}} \phi(\kappa) \psi_{U,k}^\dagger \psi_{U,k'}^\dagger |\text{FS}_{\text{int}}\rangle
\]

\[
= -\frac{1}{\mathcal{A}} \sum_{k,k',\in 1 \text{BZ} \setminus \text{FS}_{\text{int}}} \nu_{k,k'} \psi_{U,k'}^\dagger \psi_{U,k}^\dagger \sum_{k' \in 1 \text{BZ} \setminus \text{FS}} \phi(k') \left(1 - \psi_{U,k'}^\dagger \psi_{U,k}\right) |\text{FS}_{\text{int}}\rangle
\]

\[
= \frac{1}{\mathcal{A}} \sum_{k,k' \in 1 \text{BZ} \setminus \text{FS}_{\text{int}}} \nu_{k,k'} |\Phi\rangle .
\]

Equations (D4) and (D5) result in

\[
\hat{H}_{\text{int}} |\Phi\rangle = \frac{1}{\mathcal{A}} \sum_{k,k' \in 1 \text{BZ} \setminus \text{FS}_{\text{int}}} \nu_{k,k'} |\Phi\rangle . \quad (D6)
\]

Finally, we insert Eqs. (D3) and (D6) into the eigenvalue problem (8), and arrive at the pairing equation (9).

**APPENDIX E. NUMERICAL CALCULATION OF Eqs. (9)**

As discussed in the text, to solve Eq. (9) numerically we discretize the first Brillouin zone equidistantly following the relation (10). In order to increase the number of the grid points in each direction and to achieve the numerical stability, first we calculate the interacting Fermi surface using the relation

\[
\text{FS}_{\text{int}} = \left\{ k^{(j)} \in 1 \text{BZ} : 2E_{k^{(j)}}^{(U)} + \frac{1}{N^2} \nu_{k^{(j)},k^{(j)}} < 2\mu \right\},
\]

and exclude it from the first Brillouin zone. Next, we constitute the pairing equation (9) on the reduced momentum space as

for \(j = 1,2,\ldots,N\). Finally, we diagonalize Eq. (E2), and obtain the eigenenergies \(E_j\). Among \(E_j\), the desired ground-state energy, \(E_G\), is the one which is negative and has the largest absolute value.

Finally, we notice that the behavior of the desired eigenvalues as a function of the chemical potential, \(\mu\), might display a zigzag effect due to the finite discretization of the momentum space. To prevent this behavior, for the noninteracting regime, we calculate the smallest value of the eigenenergy, \(E_0\), of Eq. (E2), for the occupied states. Next, for the interacting regime, we add \(E_0\) within the first bracket of Eq. (E2), and calculate the ground-state energy for the unoccupied states.
APPENDIX F. GROUND-STATE SOLUTION FOR THE ATTRACTIVE REGIME

As expected, for the attractive regime, $U_d, U_p < 0$, the ground-state solution supports an orbital $s$-wave symmetry. Figure 7 shows the wave function for $U_d = -2$ eV and $U_p = -1$ eV.

Figure 7. Ground-state wave function of the Cooper pair in the attractive regime of the Fermi-Hubbard model (6), where $N = 100$, $V_{dp} = 3.45$ eV, $t_{pd} = 1.13$ eV, $t_{pp} = 0.8$ eV, $\mu \approx -0.679$ eV, $U_d = -2$ eV, and $U_p = -1$ eV. The wave function supports an orbital $s$-wave symmetry.

[1] E. H. Lieb, Phys. Rev. Lett. 62, 1201 (1989).
[2] M. Niţă, B. Ostahie, and A. Aldea, Phys. Rev. B 87, 125428 (2013).
[3] N. Plakida, High-Temperature Cuprate Superconductors: Experiment, Theory, and Applications (Springer, Berlin, 2010), Chaps. 2 and 3.
[4] A. J. Leggett, Quantum Liquids (Oxford University Press, New York, 2006), Chaps. 5 and 7.
[5] C. J. Pethick and H. Smith, Bose–Einstein Condensation in Dilute Gases (Cambridge University Press, New York, 2008), Chap. 5.
[6] J. Fortágh and C. Zimmermann, Rev. Mod. Phys. 79, 235 (2007).
[7] R. Shen, L. B. Shao, B. Wang, and D. Y. Xing, Phys. Rev. B 81, 041410(R) (2010).
[8] V. Apaja, M. Hyrkäis, and M. Manninen, Phys. Rev. A 82, 041402(R) (2010).
[9] S. Tuie, H. Ozawa, T. Ichinose, T. Nishio, S. Nakajima, and Y. Takahashi, Sci. Adv. 1, e1500854 (2015).
[10] M. R. Slot, T. S. Gardenier, P. H. Jacobse, G. C. P. van Miert, S. N. Kempkes, S. J. M. Zevenhuizen, C. M. Smith, D. Vannemelbergh, and I. Swart, Nat. Phys. 13, 672 (2017).
[11] R. Drost, T. Ojanen, A. Harju, and P. Liljeroth, Nat. Phys. 13, 668 (2017).
[12] S. Mukherjee, A. Spracklen, D. Choudhury, N. Goldman, P. Öhberg, E. Andersson, and R. R. Thomson, Phys. Rev. Lett. 114, 245504 (2015).
[13] W. Jiang, H. Huang, and F. Liu, Nat. Comm. 10, 2207 (2019).
[14] B. Cui, X. Zheng, J. Wang, D. Liu, S. Xie, and B. Huang, Nat. Comm. 11, 66 (2020).
[15] J. D. Bodyfelt, D. Leykam, C. Danieli, X. Yu, and S. Flach, Phys. Rev. Lett. 113, 236403 (2014).
[16] D. Leykam, A. Andreanov, and S. Flach, Adv. Phys. X 3, 1473052 (2018).
[17] N. B. Kopnin, T. T. Heikkilä, and G. E. Volovik, Phys. Rev. B 83, 220503(R) (2011).
[18] V. I. Iglovikov, F. Hébert, B. Grémaud, G. G. Batrouni, and R. T. Scalettar, Phys. Rev. B 90, 094506 (2014).
[19] S. Peotta and P. Törmä, Nat. Comm. 6, 8944 (2014).
[20] A. Julku, S. Peotta, T. I. Vanhala, D. -H. Kim, and P. Törmä, Phys. Rev. Lett. 117, 045303 (2016).
[21] K. Kobayashi, M. Okumura, S. Yamada, M. Machida, and H. Aoki, Phys. Rev. B 94, 214501 (2016).
[22] M. Tovmasyan, S. Peotta, P. Törmä, and S. D. Huber, Phys. Rev. B 94, 245149 (2016).
[23] J. R. Schrieffer and J. S. Brooks (eds.), Handbook of High-Temperature Superconductivity: Theory and Experiment (Springer, New York, 2007), Chap. 1.
