Nodeless superconductivity in cuprates with Ba$_2$CuO$_3$-type structure

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Abstract. In this work, zero-temperature phase diagrams of cuprates with Ba$_2$CuO$_3$-type CuO chain structure are investigated. The projective symmetry group analysis is employed in the strong coupling limit, and the one-loop renormalization group with bosonization analysis is employed in the weak coupling limit. We find that in both of these two limits, large areas of the phase diagrams are filled with nodeless superconducting phases, instead of nodal $d$-wave phase mostly found in cuprates. This implies that nodeless superconducting phases are the dominant superconducting phases in cuprates with Ba$_2$CuO$_3$-type CuO chain structure in low temperature. Other phases are also found, including nodal superconducting phases and Luttinger liquid phases.

1 Introduction

CuO$_2$ plane [1,2] plays an important role in the cuprate superconductors with high transition temperature (high-$T_C$) [3–5], especially in the formation of $d$-wave pairing symmetry [6–9]. Traditionally, oxygen vacancies in CuO$_2$ planes are believed to be detrimental [10] to high-$T_C$. However, recent experiments [11,12] reported that in one kind of cuprates with a large amount of oxygen vacancies, Ba$_2$CuO$_{3+\delta}$ with $0 \leq \delta \leq 1$, high-$T_C$ ($T_C \approx 73 K$) superconductivity is still observed. These oxygen vacancies are located on CuO$_2$ plane and are important to possible novel superconductivity. Since this recently-discovered superconductivity is incorporated in a different family of high-$T_C$ cuprates, it is naturally important to investigate its electronic structure and superconducting mechanism. Various theoretical works [13–17] focusing on Ba$_2$CuO$_{3+\delta}$ have been proposed to determine the pairing symmetry and low-temperature phases in different crystal structures. Several models are suggested to describe this material and methods are proposed accordingly. Thomas Maier [14] and co-workers proposed a two-orbital ($d_{x^2-y^2}, d_{3z^2-r^2}$) tight-binding model and investigate by multi-orbital random phase approximation (RPA). One similar model is suggested by Kun Jiang [13] where effective $d_{x^2}$- and $d_{y^2}$-like orbitals are taken into account. In Ref. [15] oxygen vacancies are believed to effectively transform the original square lattice of CuO$_2$ and the authors present a $t-t'-J$ model on a brick wall lattice. Apart from these one or two orbital models, a so-called multi-orbital Lieb model is proposed by Kimihiro Yamazaki [16] which resembles the model considered by Lieb [18].

Liu [19] and co-workers showed by first principle calculation that Ba$_2$CuO$_{3+\delta}$ can be viewed as doped Ba$_2$CuO$_3$, which exhibits a CuO chain structure shown in Fig. 1 with one $E_g$ orbital (Cu 3$d_{z^2-r^2}$) active, and with strong intra-chain and weak inter-chain antiferromagnetic (AFM) coupling. In this work, we study the zero-temperature phases in Ba$_2$CuO$_{3+\delta}$ by investigating a single-orbital multi-chain $t$–$J$ model in both strong and weak coupling limits.

In both limits, we find that large areas of these phase diagrams are filled with nodeless and parity-even superconducting phases. These results indicate that the dominant superconducting phase in cuprates with Ba$_2$CuO$_3$-type CuO chain structure in low temperature is actually nodeless and parity-even superconducting phase, in contrast to the traditional nodal $d$-wave phase in cuprates with CuO$_2$ plane structure. This paper is organized as follows. In Sect. 2 the single-orbital [19] $t$–$J$ model is introduced to describe the system. In Sect. 3 and 4, the strong and weak coupling limits are investigated and corresponding phase diagrams are given, respectively. We draw the conclusions in Sect. 5. Details are listed in Appendix.
2 The model

As indicated in Ref. [19], the only active orbital is Cu 3d_{x,y,z}. Therefore, a single-orbital multi-chain t–J model is employed to describe the system. The Hamiltonian \( H = H_0 + H' \) reads

\[
H_0 = \sum_{x,y,z,s} -t(c_{x,y,z,s}^\dagger c_{x+1,y,z,s} + h.c.) -t_y(c_{x,y,z,s}^\dagger c_{x,y+1,z,s} + h.c.) -t'(c_{x,y,z,s}^\dagger c_{x,y+1,z+1,s} + c_{x,y,z,s}c_{x-1,y-1,z+1,s} + c_{x,y+1,z,1,s} + c_{x,y,z,s}c_{x,y-1,z+1,s} + h.c.) \tag{1}
\]

and

\[
H' = \sum_{x,y,z} JS_{x,y,z} \cdot S_{x+1,y,z} + J_yS_{x,y,z} \cdot S_{x,y+1,z} + J' S_{x,y,z} \cdot (S_{x+1,y,z+1} + S_{x-1,y,z+1} + S_{x,y+1,z+1} + S_{x,y-1,z+1}) \tag{2}
\]

where \( c \)'s (\( c^\dagger \)'s) are annihilation (creation) operators of electrons, parameters \( t, t_y, t_z, J \) are hopping amplitudes with \( t \) largest [19], \( J, J_y, J' \) are AFM couplings with \( J \) largest [19], and \( S_{x,y,z} = \sum_{s,s'} c_{x,y,z,s}^\dagger \sigma_{s,s'} c_{x,y,z,s'} \) with Pauli matrices \( \sigma = (\sigma^1, \sigma^2, \sigma^3) \). As illustrated in Fig. 2, \( c_{x,y,z,s}^\dagger \) represents an annihilation (creation) operator located at \( x\mathbf{e}_x + y\mathbf{e}_y + z\mathbf{e}_z \) with spin \( s \). Hopping and interaction on bonds perpendicular to \( xy \)-plane are neglected because of the large length [11,19] of these bonds. However, we have no reasons to ignore hopping and interaction along the \( y \) direction. Small \( J_y \) and \( t_y \) are introduced so that discussion here is closer to real materials. For all issues regarding the momentum space, we present results in an orthogonal coordinate system with reciprocal basis vectors \( \mathbf{e}_{k_x} \), \( \mathbf{e}_{k_y} \) and \( \mathbf{e}_{k_z} \), where \( \mathbf{e}_i \cdot \mathbf{e}_j = \delta_{ij} \) with \( i,j \in \{ x, y, z \} \). A point \( (k_x, k_y, k_z) \) in the lattice represents a momentum vector \( \mathbf{k} = k_x \mathbf{e}_{k_x} + k_y \mathbf{e}_{k_y} + k_z \mathbf{e}_{k_z} \).

In the following sections, the single-orbital multi-chain t–J model (Eqs. 1 and 2) is studied in strong and weak coupling limits.

3 Strong coupling limit

In the strong coupling limit \( (t \ll J) \), projective construction (slave particle) mean-field approach [20–22] is employed to analyze possible phases. The mean-field Hamiltonian is obtained for doping description through the SU(2) slave boson approach [22]. These phases are characterized by mean-field ansatzes classified by projective symmetry groups [20–22] (PSG’s). Numerical minimization of mean-field energy is employed to determine the phase diagram.

3.1 Mean-field Hamiltonian

A variation method is used in this section to analyze phases. A series of mean-field ansatzes are introduced representing different situations of ground states and are further optimized utilizing differential evolution algorithm.

In this approach operators of electrons are represented in spin-0 charged bosons (holons) \( h_i = (h_i, b_{2,i})^T \) and spin-1/2 neutral fermions (spinons) \( \psi_i = \psi_{i,s} \).
\[(f_{i,\uparrow}, f_{i,\downarrow})^T \text{ via [22]}
\]
\[c_{i,\uparrow} = \frac{1}{\sqrt{2}} b_{i}^{\dagger} \psi_{i},
\]
\[c_{i,\downarrow} = \frac{1}{\sqrt{2}} b_{i}^{\dagger} \tilde{\psi}_{i}, \quad (3)\]

where \(\tilde{\psi}_{i} = (f_{i,\downarrow}, -f_{i,\uparrow})^T\). In this representation, the mean-field Hamiltonian reads [22]

\[H_{MF} = \frac{3}{4} \sum_{<ij>} J_{ij} (\text{tr}(u_{ij}^\dagger u_{ij}) + (\psi_i^\dagger \psi_j + h.c.))
\]
\[- \sum_{<ij>} t_{ij} (b_i^\dagger b_j + h.c.) \quad (4)\]

where \(J\)'s and \(t\)'s are determined by Eqs. 1 and 2, \(u_{ij}\) is the mean-field ansatz [22]

\[u_{ij} = \left( \frac{-\langle f_{i,\alpha}^\dagger f_{j,\beta} \rangle^*}{\langle f_{i,\alpha} f_{j,\beta} \rangle} \right) \epsilon_{\alpha\beta} \langle f_{i,\alpha} f_{j,\beta} \rangle \right), \quad (5)\]

Here \(\epsilon_{\uparrow\uparrow} = -\epsilon_{\uparrow\downarrow} = 1\). There are two kinds of constraints [22], namely proper filling

\[\langle b_i^\dagger b_i \rangle = 2\delta \quad (6)\]

and physical states

\[\langle \psi_i^\dagger \tau^l \psi_i + b_i^\dagger \tau^l b_i \rangle = 0, \quad l = 1, 2, 3. \quad (7)\]

where \(\tau\)'s are Pauli matrices. In Ref. [22] these constraints are treated by the Lagrange-multiplier method. In this work, instead, an additional penalty term is introduced here to the mean-field Hamiltonian mentioned above so that the numerical variational method can be employed:

\[H_{\text{penalty}} = \sum_{i,l} P \left( \langle \psi_i^\dagger \tau^l \psi_i + b_i^\dagger \tau^l b_i \rangle \right)
\]
\[+ P \left( \frac{1}{N_x} \sum_i \langle b_i^\dagger b_i \rangle - 2\delta \right), \quad (8)\]

where \(P(x)\) is a penalty function, \(P(x) = Gx^2\) with \(G\) being huge (larger than \(10^9\) in practice). \(N_x\) indicates the number of lattice sites of the model. In the determination of mean-field ansatzes, it is required that \(P(x)\) does not contribute to mean-field energy in final solutions found.

### 3.2 Projective symmetry groups analysis and schematic phase diagram

Different phases characterized by mean-field ansatzes of different kinds of \(Z_2\) spin liquid are classified by PSG’s [20]. The PSG’s compose certain constraints on ansatzes, and at most 311 gauge inequivalent ansatzes are found. Details are presented in Appendix A. To further determine the phase diagram, the differential evolution algorithm is employed. With constraints from PSG’s, the number of optimizing variables is restricted to be 12, so that this global optimizing algorithm is sufficient.

\[J' / J\] and filling \(\delta\) are used as variables of the phase diagram. In what follows, the phase diagram is calculated in the case \(t = 2t' = 100t_y = 0.02J\) and \(J_y = 0.01J\). This set of coefficients satisfies that inter-chain hopping and coupling are smaller than intra-chain ones [19]. However, in the strong coupling limit, the hopping parameters are just perturbative renormalizations to the AFM coupling parameters in the mean-field calculation. The dependence of mean-field energy \(E_{MF}\) to \(t\) and \(J\) is roughly \(E_{MF} \sim t + J\). Therefore, the change of \(t\)'s will have a negligible impact on the results of the phase diagram, as long as their values remain much smaller than \(J\)'s. The practical calculation is performed on a \(16 \times 16 \times 16\) lattice with the periodic boundary condition. Numerical details are stated in Appendix B. With 25 choices of parameters investigated, the schematic phase diagram is obtained, as shown in Fig. 3. However, in region \(J' / J < 0.5, \delta < 0.1\), the numerical results are not reliable. This region of the phase diagram is left blank.

In the region of coefficients we choose, there are 4 phases in total. At zero temperature, the holons necessarily condense, and the system is consequently in superconducting phases.

(i) The nodeless superconducting phase, shown as “NL” in Fig. 3, described by

\[u_{i,i+\hat{z}} = \Delta_x \tau^1 - \chi_x \tau^3, \quad (9)\]
especially when the model to describe real materials will become worse, besides, we expect \( \Delta = 0.2 \). It should be noticed as \( \delta \rightarrow 0 \).

\[
\begin{align*}
\text{Density of states for } & \delta = 0.25, J'/J = 0.3 \text{ (upper)} \quad \text{and } \delta = 0.25, J'/J = 0.9 \text{ (lower).} \\
\text{The energy unit of } & \omega \text{ is } J. \end{align*}
\]

In both cases, two pairs of coherence peaks emerge and U-shape energy gaps appear in the low energy regime.

\[
\begin{align*}
u_{i,i+\hat{y}} & = \Delta_x \tau^1 - \chi_x \tau^3, \\
u_{i,i+\hat{z}} & = \Delta_z \tau^1 - \chi_z \tau^3 + i \chi_z' \tau^0. \\

\text{(9)}
\end{align*}
\]

In above formulas, \( \Delta_x \) is the pairing amplitude with \( \gamma = x, y, z \), \( \chi \) and \( \chi' \) indicate the real part and the imaginary part of hopping amplitude respectively. In this phase, for example, we have \( \Delta_x = c_{\alpha \beta}(f_{i,i+\hat{x}}, \gamma, \beta), \) \( \chi_{\alpha} = |\text{Re}(f_{i,i+\hat{z}}, \gamma, \alpha)| \) and \( \chi'_{\alpha} = |\text{Im}(f_{i,i+\hat{z}}, \gamma, \alpha)| \). Note that positive and negative signs in the formula are deliberately adjusted so that all order parameters, \( \Delta \)'s and \( \chi \)'s, are positive real numbers for all four phases mentioned here. In real materials \([11, 12]\), \( \delta \) is approximately 0.2. It should be noticed as \( \delta \) increases, the ability of the model to describe real materials will become worse, especially when \( \delta \) is close to 1. However, the results obtained from the model are still theoretically correct. Besides, we expect \( J' < J \) since the exchange path of \( J' \) is much longer. Taking these into considerations, we expect the real material is deeply inside the “NL” regime in the phase diagram as illustrated in Fig. 3. Results of density of states for \( \delta = 0.25, J'/J = 0.3 \) and \( \delta = 0.25, J'/J = 0.9 \) are presented in Fig. 4, respectively. As expected, U-shape energy gaps emerge in low energy regimes in both cases. Besides, both curves contain two pairs of coherence peaks since the superconducting order parameter is not uniform on Fermi surfaces.

The spinon Fermi surfaces and the zeros of superconducting gap of the nodeless superconducting phase we find are shown in Fig. 5. In this nodeless state, the superconducting order parameter doesn’t change sign on the same Fermi surface but does not necessarily have the same sign on different surfaces. In Fig. 5(b), as an example, the order parameter has + sign in the Fermi surface enclosing the origin but – sign in the other surface. Since holons condense in this phase, the spinon Fermi surfaces are the same as the electron Fermi surfaces after mean-field ansatzes are taken account.

(ii) The first nodal superconducting phase, shown as “N1” in Fig. 3 is described by

\[
\begin{align*}
u_{i,i+\hat{y}} & = \Delta_x \tau^1 - \chi_x \tau^3, \\
u_{i,i+\hat{z}} & = \Delta_z \tau^1 + \chi_z \tau^3, \\
u_{i,i+\hat{z}+\hat{y}} & = \Delta_z \tau^1 - \chi_z \tau^3. \\

\text{(10)}
\end{align*}
\]

(iii) The second nodal superconducting phase, shown as “N2” in Fig. 3 is described by

\[
\begin{align*}
u_{i,i+\hat{y}} & = \Delta_y \tau^1 - \chi_y \tau^3, \\
u_{i,i+\hat{z}} & = \Delta_z \tau^1 - \chi_z \tau^3, \\
u_{i,i+\hat{z}+\hat{y}} & = \Delta_z \tau^1 - \chi_z \tau^3 + i \chi_z' \tau^0. \\

\text{(11)}
\end{align*}
\]

As a comparison, we also find nodal superconducting phases, namely that the superconducting gaps have nodes on Fermi surfaces. All of the four ansatzes are consistent with the PSG analysis.

In conclusion, in the strong coupling limit, the phase diagram is largely filled with a nodeless superconducting phase in the physically relevant regime of coefficients \( J'/J < 1 \). In principle, one can distinguish nodeless phases from nodal ones by measuring the density of states (DOS) and DOS of nodeless and nodal states exhibit different behaviours in low-energy regime \([23]\).

4 Weak coupling limit

In the weak coupling limit \( t \gg J \), one-loop renormalization group (RG) and bosonization analysis are employed to determine possible phases. A tight-binding model with anti-ferromagnetic interactions is employed, which has the same form as Eqs. 1 and 2 but with no-double-occupancy constraints loosed. This perspective of a \( t-J \) model is widely employed in the study of high-superconductivity \([24–26]\).

4.1 Quasi-1D model

An \( N = 2 \) chains \([27]\) model is considered, as shown in Fig. 6, where the periodic boundary condition is introduced along \( y \) and \( z \)-direction. One repeating unit contains one \( A \)-chain and one \( B \)-chain. In Fig. 6 four
Spinon Fermi surfaces are shown by yellow surfaces and zeros of the superconducting gap in the nodeless superconducting phase are shown by red surfaces. The superconducting gap on the spinon Fermi surfaces has indeed no node. \( k_x, k_y \) and \( k_z \) are described in the Cartesian system. (a) Plot for \( \delta = 0.25 \) and \( J'/J = 0.3 \). (b) Plot for \( \delta = 0.25 \) and \( J'/J = 0.9 \). It can be read from the comparison of the two figures that when \( J'/J \) is small, namely when inter-chain couplings are weak, the spinon Fermi surfaces are more quasi-1D.

In this coordinate, the non-interacting Hamiltonian \( H_0 \) can be diagonalized as

\[
H_0 = \sum_{\mathbf{k}, s, i=1,2} \epsilon_i(\mathbf{k}) \psi^\dagger_{i,s}(\mathbf{k}) \psi_{i,s}(\mathbf{k}),
\]

where

\[
\epsilon_{1,2}(\mathbf{k}) = -2 \left( \pm t' \left( \cos \left( \frac{k_x + k_y + k_z}{2} \right) + \cos \left( \frac{2b - k_y + k_z}{2} \right) + \cos \left( \frac{2b - k_y + k_z}{2} \right) \right) \right) + t \cos(k_x) + t_y \cos(k_y),
\]

where \( +(-) \) sign for \( \epsilon_{1(2)} \), respectively. For the \( N = 2 \) chains model, the summation over \( \mathbf{k} \) only contains those points with \( k_y = k_z = 0 \). Therefore, the Fermi points are determined via \[27\]

\[
\epsilon_i(k_{F,i}) = \mu, \quad i = 1, 2,
\]

for chemical potential \( \mu \). The Fermi points in this quasi-1D model can be viewed as a discrete set of points with \( k_y = k_z = 0 \) on the 3D Fermi surface of the \( N = +\infty \) model. As shown in Fig. 7. For clarity the \( k_y \) direction is neglected. For a generic filling, the Fermi points do not coincide, and there is no umklapp interaction. Only excitations around Fermi points are considered in long wave length limit. Field operators can be written

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**Fig. 5** Spinon Fermi surfaces are shown by yellow surfaces and zeros of the superconducting gap in the nodeless superconducting phase are shown by red surfaces. The superconducting gap on the spinon Fermi surfaces has indeed no node. \( k_x, k_y \) and \( k_z \) are described in the Cartesian system. (a) Plot for \( \delta = 0.25 \) and \( J'/J = 0.3 \). (b) Plot for \( \delta = 0.25 \) and \( J'/J = 0.9 \). It can be read from the comparison of the two figures that when \( J'/J \) is small, namely when inter-chain couplings are weak, the spinon Fermi surfaces are more quasi-1D.

**Fig. 6** The \( N = 2 \) chains model. Here four \( A \) chains are equivalent under the periodic boundary condition, while \( B \) chain is inequivalent to them. The unit cell is modified to be the conventional unit cell with two inequivalent atoms in one unit cell. These two inequivalent atoms are encircled by a dashed black line. The lattice vector is exactly \( e_x \).

Equivalent \( A \)-chains are depicted to have a better illustration of interactions between particles. Some previous work have focused on Luttinger liquids on two-leg ladders with [28–30] or without frustration [27,31–38]. However, the lattice structure in this model has not been investigated. Since the intra-chain coupling plays a more important role than that of the inter-chain coupling [19], and the translation symmetries of the conventional unit cells are presumably not destroyed, this quasi-1D model is believed to capture the most relevant physics. The unit cell is changed to be the conventional unit cell with two atoms in one unit cell.
in terms of chiral fermions (right/left movers) as [27]

\[ \psi^{L,R}_{i,s} \sim \psi^{R}_{i,s} e^{i k_F x} + \psi^{L}_{i,s} e^{-i k_F x}, \quad i = 1, 2, \]

with $\psi^{L,R}_{1,s}$, $\psi^{R}_{2,s}$ and $\psi^{R}_{2,s}$ corresponding to excitation around Fermi point 1L, 1R, 2L and 2R, respectively. The momenta of these chiral fermions are bounded by a momentum cut-off $A \ll k_{F,1,2}$. Therefore, the dispersion can be linearized within $A$. The effective non-interacting Hamiltonian reads

\[ H_0 = \sum_{i,s} \int dx v_i (\psi^{R}_{i,s} \partial_x \psi^{R}_{i,s} - \psi^{L}_{i,s} \partial_x \psi^{L}_{i,s}), \]

where $v_i = \delta v_i e(k)$ \mid $k_\parallel = k_F, k_y = k_x = 0$ is the Fermi velocity.

### 4.2 Renormalization group and bosonization analysis

A generic interaction Hamiltonian density subject to the constraint of momenta conservation reads

\[ \mathcal{H}' = \sum_{i,j=1}^{2} \left( f^R_{ij} T^R_{ij} T^L_{ij} - f^\sigma_{ij} T^R_{ij} \cdot T^L_{ij} \right) + \sum_{i=1}^{2} f_{i}^* T^R_{i,3-i} T^L_{i,3-i} - f_{i} \sigma T^R_{i,3-i} \cdot T^L_{i,3-i}, \]

where currents

\[ T^{L/R}_{ij} = \sum_s \psi^{L/R}_{i,s} \psi^{L/R}_{j,s}, \]

\[ T^{L/R}_{ij} = \frac{1}{2} \sum_{s,s'} \sigma_{ss'} \psi^{L/R}_{i,s} \psi^{L/R}_{j,s'}, \]

Coupling constants $f$’s and $(f^*)$’s represent intra-band and inter-band scattering, respectively. The relationship of their values are given by certain symmetries. Charge conjugation $T_{ij} \rightarrow T_{ji}$ gives $f^*_{ji} = f_{j-i,3-i}$, while reflection in $x$ direction gives $f_{ij} = f_{j-i,i}$. Details of the construction of this interaction Hamiltonian density is left in Appendix C.

To construct a low energy effective theory, the interaction is renormalized and bosonized. In this work, the one-loop RG method is used. The derivation of the RG equations is left in Appendix D. There are four types of coupling constants, namely $f^R, f^{\sigma}, f^\sigma, f'^\sigma$ and RG equations are determined accordingly. Only 16 independent RG equations remain after the symmetry redundancy is eliminated. After solving RG equations numerically, in the region of coefficients adopted, we find that in all cases there are two coupling constants, $(f^R_{11}, f^\sigma_{11})$ or $(f'^R_{11}, f'^\sigma_{11})$, dominant. Since $f^R$ only contributes to gradient term after bosonization [27], they are simply dropped. Therefore, the interaction Hamiltonian after RG reads (take subscript 1 as an example)

\[ \mathcal{H}' = \sum_s \frac{1}{2} f^R_{11} \psi^{R}_{1,s} \psi^{R}_{1,s} \psi^{L}_{1,s} \psi^{L}_{1,s}, \]

where $\bar{s}$ means the opposite direction of spin $s$. After bosonization, in terms of the chiral boson fields, the Hamiltonian reads (take subscript 1 as an example)

\[ \mathcal{H}_0 \sim \frac{v_1}{2} (\partial_\tau \theta_{1,\sigma})^2 + (\partial_\tau \theta_{1,\sigma})^2, \]

\[ \mathcal{H}' \sim f^R_{11} \cos(\sqrt{8\pi} \theta_{1,\sigma}). \]

Purely free fields are neglected in $\mathcal{H}_0$. Therefore, the low energy effective theory of the system is a sine-Gordon theory. The bosonization dictionary is left in Appendix E, including the definition of $\theta_{1,\sigma}$.

### 4.3 Phase diagram

The global minima of Eq. (23) is

\[ \sqrt{2\pi} \theta_{i,\sigma} = 2l_i \pi \quad \text{or} \quad (2l_i + 1)\pi, \quad l_i \in \mathbb{Z}, \]

depending on the sign of $f^R_{11}$. Around a minimum, the interaction Hamiltonian can be expanded as $\mathcal{H}' \sim m(\delta \theta)^2$, which gives the field $\theta$ an effective mass. Therefore, when one $f^\sigma$ is dominant, there is one gapless spin mode and one gapped spin mode. The two charge modes are always gapless. To figure out the phase diagrams, the expectation values of different order parameters are calculated, including charge density wave (CDW), spin density wave (SDW), singlet superconductivity (SS) and triplet superconductivity (TS): [39]

\[ O_{CDW,\tau} = \sum_s \psi^{R}_{1,s} (x) \psi^{R}_{1,s} (0), \]

\[ O_{SDW,\tau} = \sum_{s,s'} \psi^{R}_{1,s} (x) \sigma_{ss'} \psi^{L}_{1,s'} (0), \]
only terms like $\phi, \theta$ the uncertainty principle in Appendix E. As indicated in Ref. [27], according to in terms of boson fields via the bosonization dictionary field of $\theta$ stands for Luttinger liquid phase with $n$ gapless superconducting phases [27]. NLSC stands for a nodeless superconducting phase $O_{SS,i} = \psi_{i,1}^{R}(x)\psi_{i,1}^{L}(0), \quad (27)$ $O_{TS,i} = \psi_{i,1}^{R}(x)\psi_{i,1}^{L}(0). \quad (28)$ Superscript “1” in $O_{TS,i}$ indicates the states of total spin being 1. Since no spin-orbital coupling arises in this system and no spontaneously symmetry breaking appears as it is a quasi-one-dimensional system, three components of spin-triplet order parameters with total spin 1, 0, $-1$ are degenerated, i.e., behaviours of the spin-triplet order parameter $O_{TS,i}$ and $O_{SS,i}$ are the same as $O_{1,i}$. These order parameters can be rewritten in terms of boson fields via the bosonization dictionary in Appendix E. As indicated in Ref. [27], according to the uncertainty principle $[\phi, \theta] = O(1)$, the conjugate field of $\theta_\sigma$, namely $\phi_\sigma$, fluctuates violently. Therefore, only terms like $e^{i\phi_\sigma(x)-\phi_\sigma(0)}$ can survive in the mean-field level. Applying these criteria, one can determine whether the order parameters are non-vanishing in certain phases.

Without losing generality, $f_{11}^{R}$ is supposed to be dominant. All the non-vanishing order parameters are $O_{CDW}$, $O_{SDW}$ and $O_{SS}$. When $f_{11}^{R}$ is negative, according to the Cooper instability, an attractive interaction will naturally induce superconductivity. Therefore, the system will be in an $s$-wave superconducting phase (with weak $d$-wave components due to the absence of four-fold rotation symmetry). When $f_{11}^{R}$ is positive, both CDW and SDW can exist in this system, due to the gaplessness of the charge modes and the spin mode. The system will present spin-charge separation and hence in a Luttinger liquid phase with two gapless charge modes and one gapless spin mode.

The phase diagram is shown in Fig. 8. We use $t'/t$ and filling $\delta$ as variables, and fix other coefficients as $t_y = 0.01t$ and $J = 3.0 = 6J_y = 0.03t$ to satisfy that inter-chain hopping and coupling are smaller than intra-chain ones [19]. The phase diagram is largely occupied by a nodeless superconducting phase denoted as NLSC in Fig. 8). Superconducting gaps on all four Fermi points (1L, 1R and 2L, 2R) are of the same sign, indicating a nodeless pairing state. For appropriate filling, one of the two bands is fully empty or fully occupied, leading to only two Fermi points, instead of four, participating in interactions. In this case, the only dominant coupling constants are $f_{15}$’s, implying all of the two charge modes and two spin modes are gapless in this Luttinger liquid phase denoted as [27] “C2S2” in Fig. 8. The other Luttinger liquid phase with two gapless charge modes and one spin mode is denoted as [27] “C2S1”.

5 Conclusions

In this work zero-temperature phases of cuprates with $Ba_2CuO_3$-type CuO chain structure are investigated in both strong and weak coupling limits of a single-orbital multi-chain $t-J$ model. We find that in both of the two limits, the phase diagrams are largely filled with nodeless superconducting phases. In this nodeless superconducting phase, the superconductivity will not be strongly suppressed by intra-band scattering, which connects Fermi surface points with equal-sign pairing order parameter [23]. Thus, we believe that the nodeless and parity-even superconducting pair studied in this work is more stable against disorder than other proposals with $d$-wave [14] or $d+id$ [15], where the order parameters change sign in the same Fermi surface. Details of the impurity potential in this material remain unclear. However, if the induced impurity scattering is intra-band favoured, the nodeless superconducting phases are more robust against disorder than nodal $d$-wave superconducting phases traditionally found in cuprates. Some previous theories [14,16] also proposed nodeless $s_\pm$-wave phases. However, they are based on multi-orbital models and developed on lattice structures apparently different from ours. $d$-wave superconductivity was also proposed in previous works [13,15]. Our proposed nodeless superconducting pairing symmetry can in principle be detected by spectroscopic [40,41] measurements.

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Author contributions

FW conceived of the presented idea and directed the project. Z-QG developed the theoretical framework. K-WS performed the large-scale numerical computation. All three workers contributed to the final manuscript.

Data Availability Statement This manuscript has no associated data or the data will not be deposited. [Author’s comment: This is a theoretical study and no experimental data.]

A Classification of $\mathbb{Z}_2$ spin liquids phases in Ba$_2$CuO$_{3+\delta}$

A.1 Projective symmetry groups

Under coordinates we choose in Sect. 3, space group symmetries, including translation, parity, and inversion, read

\[ T_x : (i_x, i_y, i_z) \mapsto (i_x + 1, i_y, i_z), \]
\[ T_y : (i_x, i_y, i_z) \mapsto (i_x, i_y + 1, i_z), \]
\[ T_z : (i_x, i_y, i_z) \mapsto (i_x, i_y, i_z + 1), \]
\[ P_x : (i_x, i_y, i_z) \mapsto (-i_x - i_z, i_y, i_z), \]
\[ P_y : (i_x, i_y, i_z) \mapsto (i_x, -i_y - i_z, i_z), \]
\[ I : (i_x, i_y, i_z) \mapsto (-i_x, -i_y, -i_z), \]

and the time-reversal symmetry is

\[ T : u_{ij} \mapsto -u_{ij}. \]

The symmetries above satisfy equalities

\[ T_x^{-1} T_y^{-1} T_x T_y = 1, \]
\[ T_y^{-1} T_z^{-1} T_y T_z = 1, \]
\[ T_z^{-1} T_x^{-1} T_z T_x = 1, \]
\[ T_x P_x T_x P_x = 1, \]
\[ T_y P_y T_y P_y = 1, \]
\[ T_z P_z T_z P_z = 1, \]
\[ P_x P_y P_z T_x P_y P_z = 1, \]
\[ P_y P_z P_x T_y P_z P_x = 1, \]
\[ P_z P_x P_y T_z P_x P_y = 1, \]

and translations. Unlike the 2D case [20], here we choose the gauge that

\[ G_s(i) = \tau^0, \]
\[ G_s(i) = \eta^{x_{i_y}} \tau^0, \]
\[ G_y(i) = \eta^{y_{i_x}} \tau^0, \]
\[ G_T(i) = g_T \eta^{x_{i_y}} \eta^{y_{i_x}} \tau^0, \]

where two gauge inequivalent choices of $g_T$ are $g_T = \tau^0$ or $i i \tau^1$, and seven $\eta$s are $\pm 1$.

Then we consider parities $P_x$ and $P_y$. The PSG equations given by Eq. (39) to (46) read

\[ G_z(P_x(i)) G_{z_x}^{-1}(i + \hat{x}) G_x(i + \hat{x}) G_{r_x} P_x(i) \in G, \]
\[ G_y^{-1}(P_x(i)) G_{y_x}^{-1}(i) G_y(i) G_{r_y} P_x(i) \in G, \]
\[ G_y^{-1}(P_y(i)) G_{y_y}^{-1}(i) G_y(i) G_{r_y} P_y(i) \in G, \]
\[ G_y(P_y(i)) G_{y_y}^{-1}(i + \hat{y}) G_y(i + \hat{y}) G_{r_y} P_y(i) \in G, \]
\[ G_y P_y G_y P_x G_y P_x G_y P_y(i) \in G, \]
\[ G_y P_y G_y P_x G_y P_y(i) \in G, \]
\[ G_y P_y G_y P_x G_y P_y(i) \in G. \]

Since $P_x$ and $P_y$ do not change $i_z$, in our gauge Eq. (57) to (60) reduce to

\[ G_x^{i_y}(i + \hat{x}) G_x(i) = \eta^{y_{i_x}} \tau^0, \]
\[ G_y^{i_x}(i + \hat{y}) G_y(i) = \eta^{y_{i_x}} \tau^0, \]
\[ G_y^{i_y}(i + \hat{y}) G_y(i) = \eta^{y_{i_x}} \tau^0, \]
\[ G_y^{i_y}(i + \hat{y}) G_y(i) = \eta^{y_{i_x}} \tau^0, \]

which give $G_P(i)$ and $G_y(i)$ the generic form

\[ G_P(i) = g_T \Theta P_x(i) \eta^{y_{i_x}} \eta^{y_{i_y}} \eta_{i_xy}, \]
\[ G_y(i) = g_T \Theta P_y(i) \eta^{y_{i_x}} \eta^{y_{i_y}} \eta_{i_xy}, \]

where $\Theta$s are ($\pm 1$)-valued functions of $i_z$. Eq. (61) to (65) then reduce to

\[ g_T^2 \Theta P_x(i) \Theta P_x(i + 1) \eta^{y_{i_y}} G_x(i) = \eta^{y_{i_y}} \tau^0, \]
\[ g_T^2 \Theta P_y(i) \Theta P_y(i + 1) \eta^{y_{i_y}} G_y(i) = \eta^{y_{i_y}} \tau^0, \]
\[ g_T g_y g_T g_y \eta^{y_{i_y}} \eta_{i_xy} = \pm \tau^0, \]
\[ g_T^2 \eta^{y_{i_y}} \eta_{i_xy} = \pm \tau^0, \]
\[ g_T^2 \eta^{y_{i_y}} \eta_{i_xy} = \pm \tau^0, \]

for all sites $i$. Eq. (74). to (76) require that

\[ \eta_{i_xy} = \eta_{i_xy}, \eta_{i_y} = \eta_{i_y} = \eta_{i_y} = 1, \]

while Eqs. (72) and (73) give two $\Theta$s a specific form. All gauge inequivalent $\Theta$s are

\[ \Theta P_x(i) = \eta^{y_{i_y}} \eta_{i_y}, \]
\[ \Theta P_y(i) = \eta^{y_{i_y}} \eta_{i_y}. \]
\[ \Theta P_x(i_z) = \eta_{i_z} \sqrt{2} \sin(\frac{\pi}{2} i_z + \frac{\pi}{4}), \]

for \( G_x(i) = (-1)^i \tau^0 \), (80)

\[ \Theta P_y(i_z) = \eta_{i_z} \sqrt{2} \sin(\frac{\pi}{2} i_z + \frac{\pi}{4}), \]

for \( G_y(i) = (-1)^i \tau^0 \). (81)

Finally, we consider inversion \( I \). Equations (47) to (49) induce PSG equations

\[ G_x(I(i))G_{I(i)} + G_x(i)G_{I(i)} \in \mathcal{G}, \]

(82)

\[ G_y(I(i))G_{I(i)} + G_y(i)G_{I(i)} \in \mathcal{G}, \]

(83)

\[ G_x(I(i))G_{I(i)} + G_x(i)G_{I(i)} \in \mathcal{G}. \] (84)

Under our gauge, \( G_I(i) \) has the generic form

\[ G_I(i) = g_{i1} \eta_{i1} \eta_{i1}^* \eta_{i1}. \] (85)

According to Eqs. (50) and (51),

\[ G_I(P_x(i))G_{P_x(I(i))}G_{P_x(i)} \in \mathcal{G}, \]

(86)

\[ G_I(P_y(i))G_{P_y(I(i))}G_{P_y(i)} \in \mathcal{G}, \] (87)

we have

\[ g_{i1}g_{P_x}^{-1} g_{i1}g_{P_x} \eta_{i1}^* = \pm \tau^0, \] (88)

\[ g_{i1}g_{P_y}^{-1} g_{i1}g_{P_y} \eta_{i1}^* = \pm \tau^0, \] (89)

for all sites \( i \). Therefore, \( \eta_{i1} = \eta_{P_x} = 1. \) From just the same argument, \( \eta_{i2} = \eta_{P_y} = 1. \). Then, Eqs. (56), (70), (71) and (85) reduce to

\[ G_{I(i)} = g_{i1} \eta_{i1}^*, \] (90)

\[ G_{P_x(i)} = g_{P_x} \Theta P_x(i_z) \eta_{P_x}^*, \]

(91)

\[ G_{P_y(i)} = g_{P_y} \Theta P_y(i_z) \eta_{P_y}^*, \]

(92)

\[ G_I(i) = g_{i1} \eta_{i1}^*, \] (93)

where \( \eta_x, \eta_y \) and \( \eta_z \) can take value of \( \pm 1 \), and \( \Theta P_x(i_z) \) and \( \Theta P_y(i_z) \) are determined above. The constraints of \( g_s \) reduce to

\[ g_{i1}^2 = g_{P_x}^2 = g_{P_y}^2 = \pm \tau^0, \]

(94)

\[ g_{P_x}g_{P_y}g_{P_x}g_{P_y} = \pm \tau^0, \]

(95)

\[ g_{i1}g_{P_x}^{-1} g_{i1}g_{P_x} = \pm \tau^0, \] (96)

\[ g_{i1}g_{P_y}^{-1} g_{i1}g_{P_y} = \pm \tau^0, \] (97)

\[ g_{i1}g_{P_x}^{-1} g_{i1}g_{P_x} = \pm \tau^0, \] (98)

\[ g_{i1}g_{P_y}^{-1} g_{i1}g_{P_y} = \pm \tau^0, \] (99)

\[ g_{i1}g_{P_x}^{-1} g_{i1}g_{P_x} = \pm \tau^0. \] (100)

All gauge equivalent choices of \( g_s \) are

\[ g_I = \tau^0, \]

(101)

\[ g_{P_x} = \tau^0, \]

(102)

\[ g_{P_y} = \tau^0, \]

(103)

\[ g_I = \tau^0, \]

(104)

\[ g_{P_x} = \tau^0, \]

(105)

\[ g_{P_y} = \tau^0, \]

(106)

\[ g_I = \tau^0, \] (107)

\[ g_{P_x} = \tau^0, \]

(108)

\[ g_{P_y} = \tau^0, \]

(109)

\[ g_I = \tau^0, \]

(110)

\[ g_{P_x} = \tau^0, \]

(111)

\[ g_{P_y} = \tau^0, \]

(112)

\[ g_I = \tau^0, \]

(113)

\[ g_{P_x} = \tau^0, \]

(114)

\[ g_{P_y} = \tau^0, \]

(115)

\[ g_I = \tau^0, \]

(116)

\[ g_{P_x} = \tau^0, \]

(117)

\[ g_{P_y} = \tau^0, \]

(118)

\[ g_I = \tau^0, \]

(119)

\[ g_{P_x} = \tau^0, \]

(120)

\[ g_{P_y} = \tau^0, \]

(121)

\[ g_I = \tau^0, \]

(122)

\[ g_{P_x} = \tau^0, \]

(123)

\[ g_{P_y} = \tau^0, \]

(124)

\[ g_I = \tau^0, \]

(125)

\[ g_{P_x} = \tau^0, \]

(126)

\[ g_{P_y} = \tau^0, \]

(127)

\[ g_I = \tau^0, \]

(128)

\[ g_{P_x} = \tau^0, \]

(129)

\[ g_{P_y} = \tau^0, \]

(130)

\[ g_I = \tau^0, \]

(131)

\[ g_{P_x} = \tau^0, \]

(132)

\[ g_{P_y} = \tau^0, \]

(133)

\[ g_I = \tau^0, \]

(134)

\[ g_{P_x} = \tau^0, \]

(135)

\[ g_{P_y} = \tau^0, \]

(136)

\[ g_I = \tau^0, \]

(137)

\[ g_{P_x} = \tau^0, \]

(138)

\[ g_{P_y} = \tau^0, \]

(139)

\[ g_I = \tau^0, \]

(140)

\[ g_{P_x} = \tau^0, \]

(141)

\[ g_{P_y} = \tau^0, \]

(142)

\[ g_I = \tau^0, \]

(143)

\[ g_{P_x} = \tau^0, \]

(144)

\[ g_{P_y} = \tau^0, \]

(145)

\[ g_I = \tau^0, \]

(146)

\[ g_{P_x} = \tau^0, \]

(147)

\[ g_{P_y} = \tau^0. \]

(148)

There are 48 different gauge inequivalent choices of \( g_s \). Therefore, the total number of PSGs is \( 48 \times 2^3 \times 4 = 6144 \). However, when \( g_{I} = \tau^0 \), to acquire non-vanishing anosotets, \( \eta_I \) must be identical to [20] -1. Therefore, \( 15 \times 2 \times 4 = 960 \).
PSGs are killed and the total number of PSGs reduces to 5184.

### A.2 Ansatzes of the nearest-neighbour spin model

In this section we assume that only \( u_{i,i+z}, u_{i,i+y}, u_{i,i+z}, \) \( u_{i,i-x+z}, u_{i,i-y+z} \) and \( u_{i,i-x-y+z} \) are non-vanishing. First, an ansatz \( u_{i,i+m} \) under \( T_x G_x, T_y G_y \) and \( T_z G_z \) reads

\[
    u_{i,i+m} = \frac{\eta_{i,m}}{\eta_{y,i,m}} w_{i}^{m_l} \eta_{i,m}^{r_l}, \quad l = 0, 1, 2, 3, \tag{149}
\]

where \( u_{i,m} \), \( i = 1, 2, 3 \) is real and \( u_{0}^{m} \) is pure imaginary. \( T \) and \( I \) further give constraints

\[
    \eta_{i,m}^{m_l} g_{i} w_{i}^{m_l} g_{i} = -u_{i,m}^{r_l}; \quad \eta_{i,m}^{m_l} g_{i} w_{i}^{m_l} g_{i} = u_{i,m}^{r_l}. \tag{150}
\]

Using \( u_{i,m} = u_{i,0} \), we can conclude that when

\[
    \eta_{i,m}^{m} g_{i} = -u_{i,m}^{r} \quad \text{and} \quad \eta_{i,m}^{m} g_{i} = u_{i,m}^{r}, \tag{152}
\]

all \( u_{m} \) vanish. This kills \( 10 \times 2^{3} \times 4 = 320 \) PSGS and the totally number of PSGS is 5184 – 320 = 4864. When

\[
    \eta_{i,m}^{m} g_{i} = -u_{i,m}^{r} \quad \text{and} \quad \eta_{i,m}^{m} g_{i} = -u_{i,m}^{r}, \tag{153}
\]

all \( u_{m}^{r} \) vanish for odd \( m \), namely only \( u_{i,i+z} \) and \( u_{i,i+y} \) remain non-zero. These ansatzes degenerate todescribe spin liquids in a rectangular lattice in 2D plane, which is irrelevant to us. There is another similar case. When \( G_{x} = (-)^{z} \rho_{z}^{0} \), \( G_{p} \) will give the constraint

\[
    \left( \cos \left(\frac{\pi}{2} m_{x} \right) + (-)^{z} \sin \left(\frac{\pi}{2} m_{x} \right) \right), \tag{154}
\]

For odd \( m_{x} \), \( l.h.s. \) is a function of \( i_{x} \) while \( r.h.s. \) is not, which indicates that all the \( u_{m} \) for odd \( m_{x} \) must vanish to satisfy the equation. As indicated in the previous argument, we do not take consideration of these ansatzes. Therefore, only \( G_{x}(i) = G_{y}(i) = \tau_{0} \) case will be under consideration. The number of PSGS left is \( (4864 - (9 + 14) \times 2^{3} \times 4) / 4 = 1032. \)

When \( G_{x}(i) = G_{y}(i) = \tau_{0} \), \( P_{x} \) and \( P_{y} \) give constraints on ansatzes

\[
    g_{P_{x}} w_{i}^{r_l} g_{P_{x}} = u_{i}^{r_l}; \tag{155}
\]

\[
    \eta_{i,m}^{m_l} g_{i} w_{i}^{m_l} g_{i} = -u_{i,m}^{r_l}; \tag{156}
\]

\[
    \eta_{i,m}^{m} g_{i} w_{i}^{m} g_{i} = u_{i,m}^{r_l}; \tag{157}
\]

\[
    \eta_{i,m}^{m} g_{i} w_{i}^{m} g_{i} = u_{i,m}^{r_l}; \tag{158}
\]

\[
    \eta_{i,m}^{m} g_{i} w_{i}^{m} g_{i} = -u_{i,m}^{r_l}; \tag{159}
\]

\[
    \eta_{i,m}^{m} g_{i} w_{i}^{m} g_{i} = u_{i,m}^{r_l}; \tag{160}
\]

\[
    \eta_{i,m}^{m} g_{i} w_{i}^{m} g_{i} = -u_{i,m}^{r_l}; \tag{161}
\]

\[
    \eta_{i,m}^{m} g_{i} w_{i}^{m} g_{i} = u_{i,m}^{r_l}. \tag{162}
\]

These equations determine the constraints of ansatzes in numerical calculation. Two of the constraints are employed. One is the periodic condition, that the periodicity of all the ansatzes is 1, and the other is the sector condition, that the ansatzes satisfy

\[
    u_{z} = s_{z} u_{x+z} = s_{y} u_{y+z} = s_{z+y} u_{x+y+z} \tag{163}
\]

with \( s_{x}, s_{y}, s_{x+y} = \pm 1 \). According to numerical results, there are at most 311 inequivalent ansatzes.

### B Numerical method and data for strong coupling case

Differential evolution (DE), originally developed by Storn and Price [42], is a meta-heuristic algorithm that globally optimizes a given objective function in an iterative manner. Usually, the objective function is treated as a black box and no assumptions are needed. For example, unlike traditional gradient descent, conjugate gradient and quasi-Newton methods, derivatives are not needed. Evaluation of derivatives of mean-field energy defined previously is time-consuming for which DE is suitable. Besides, another algorithm, the Nelder-Mead method is also tested but doesn’t perform as well as DE.

DE works with a group (called population) of solution candidates (called agents), which is initialized randomly. In each iterative step, a certain agent is selected and a new agent is generated from this agent and two other randomly selected agents in a random, linear way. If the new agent is better that the old agent, the old agent is replaced by the new one. If not, the trial agent is simply discarded. This procedure continues until some certain accuracy is reached.

In this paper, DE is used to optimize the mean-field energy with respect to ansatzes. Constrained by PSG’s, the number of optimizing variables is restricted to be 12. The number of agents is set to be 120, 10 times the number of variables, with differential weight being 0.9 and cross-over probability being 0.5.

#### B.1 Fourier transformation of the mean-field Hamiltonian

The mean-field Hamiltonian reads

\[
    H_{MF} = H_{MF}^{f} - H_{MF}^{b} \tag{164}
\]

with

\[
    H_{MF}^{f} = \frac{3}{4} \sum_{\alpha} \sum_{\alpha} \sum_{\alpha} J_{\alpha} H_{\alpha}^{1} U_{\alpha} \psi_{\alpha} \psi_{\alpha} \tag{165}
\]

and

\[
    H_{MF}^{b} = \sum_{\alpha} \sum_{\alpha} \sum_{\alpha} U_{\alpha} \psi_{\alpha} \psi_{\alpha} \tag{166}
\]

Here superscripts \( f \) and \( b \) mean fermion and boson respectively. \( r \) refers to the coordinate of one certain super-cell. \( \alpha \) refers to the index of one certain bond in a cell. \( \alpha_{1} \) is the index of the first end of bond \( \alpha \), \( \alpha_{2} \) is the other end. They are assigned for each bond \( \alpha \) before practical calculation. Order of these two sites, \( \alpha_{1} \) and \( \alpha_{2} \), matters, which means they are not symmetric in formulas. \( U_{\alpha} \) is defined to be \( u_{\alpha_{1}, \alpha_{2}} \), so it becomes a bond-dependent quantity. Note that \( u_{\alpha_{1}, \alpha_{2}} \) not necessarily equals to \( u_{\alpha_{2}, \alpha_{1}} \). In this holon-condensed case, bosons are treated as scalars.

Only derivation of Fourier-transformed form for the fermion Hamiltonian is shown in detail. The Fourier-transformed form of the boson Hamiltonian can be obtained by just replacing \( \psi \) with \( b \) since commutation relations are not included in derivation.
Take substitutions
\[ \psi_{\alpha_i}(r) = \frac{1}{\sqrt{N_{\text{cell}}}} \sum_k \psi_{\alpha_1}(k) e^{i k \cdot (r + l_{\alpha_1})} \]  
(167)
and
\[ \psi_{\alpha_2}(r) = \frac{1}{\sqrt{N_{\text{cell}}}} \sum_k \psi_{\alpha_2}(k) e^{i k \cdot (r + l_{\alpha_2})}, \]  
(168)
we further have
\[ H_{MF}^I = \frac{3}{4} \sum_\alpha \sum_{k} J_\alpha [\psi_{\alpha_1}^\dagger(k) U_{\alpha} e^{i k \cdot (l_{\alpha_2} - l_{\alpha_1})} \psi_{\alpha_2}(k) + \psi_{\alpha_2}^\dagger(k) U_{\alpha}^* e^{-i k \cdot (l_{\alpha_2} - l_{\alpha_1})} \psi_{\alpha_1}(k)]. \]  
(169)
It should be noted that this Hamiltonian is block-diagonalized with respect to \( k \). So we can calculate eigenvalues and eigenvectors of each block-matrix individually to reduce calculation workload.
\[ \mathcal{H}_{MF}^b = \sum_\alpha \sum_{k} t_{\alpha} [b_{\alpha_1}^\dagger(k) U_{\alpha} e^{i k \cdot (l_{\alpha_2} - l_{\alpha_1})} b_{\alpha_2}(k) + b_{\alpha_2}^\dagger(k) U_{\alpha}^* e^{-i k \cdot (l_{\alpha_2} - l_{\alpha_1})} b_{\alpha_1}(k)]. \]  
(170)
These two equations can be rephrased in matrix form:
\[ H_{MF}^I = \sum_k \psi^\dagger(k) Q_{MF}^I(k) \psi(k) \]  
(171)
with
\[ \psi(k) = \begin{pmatrix} \psi_{1,\alpha_1}(k) \\ \psi_{2,\alpha_1}(k) \\ \vdots \\ \psi_{N_{\text{site}},\alpha_1}(k) \\ \psi_{1,\alpha_2}(k) \\ \vdots \\ \psi_{N_{\text{site}},\alpha_2}(k) \end{pmatrix}. \]  
(172)
Here \( N_{\text{site}} \) means the number of sites in one unit cell. And the number of cells is indicated by \( N_{\text{cell}} \).
The \( Q_{MF}^I \) can be diagonalized as
\[ Q_{MF}^I(k) = S^I(k) D^I(k) S^I(k). \]  
(173)
Denote \( \phi(k) = S^I(k) \psi(k) \), we further have
\[ H_{MF}^I = \sum_k \sum_{l=1}^{2N_{\text{site}}} \lambda_l^I(k) \phi_l^I(k) \phi_l(k). \]  
(174)
To obtain energy of the original Hamiltonian, we need to evaluate the average \( \langle \psi_{\alpha_1}^\dagger(k_1) \psi_{\alpha_2}(k_2) \rangle_0 \). The subscript 0 means that average is taken in a Gaussian level. These two averages can be expressed as
\[ \langle \psi_{\alpha_1}^\dagger(k_1) \phi_l(k_2) \rangle_0 = \delta_{k_1, k_2} \sum_{l=1}^{2N_{\text{site}}} S^I_{l, \alpha_1} S^I_{l, \alpha_2} \phi_l(k_1) \phi_l(k_2), \]  
(175)
where
\[ \langle \phi_l^\dagger(k) \phi_l(k) \rangle_0 = \begin{cases} 0, & \lambda_l^I(k) > 0 \\ 1, & \lambda_l^I(k) < 0. \end{cases} \]  
(176)
For simplicity, we define several functions:
\[ n_f(i, s) = \sum_k \langle \psi_{\alpha_1}^\dagger(k) \psi_{\alpha_2}(k) \rangle_0, \]  
(177)
\[ n_b(i, s) = \sum_k \langle \phi_{\alpha_1}^\dagger(k) \phi_{\alpha_2}(k) \rangle_0, \]  
(178)
\[ O_f(\alpha, s_1, s_2) = \sum_k e^{i k \cdot (l_{\alpha_2} - l_{\alpha_1})} \langle \psi_{\alpha_1}^\dagger(k) \psi_{\alpha_2}(k) \rangle_0. \]  
(179)
\[ O_b(\alpha, s_1, s_2) = \sum_k e^{i k \cdot (l_{\alpha_2} - l_{\alpha_1})} \langle \phi_{\alpha_1}^\dagger(k) \phi_{\alpha_2}(k) \rangle_0. \]  
(180)
Here \( i \) is the site index in one super-cell, \( s, s_1 \) and \( s_2 \) can be up or down.

**B.2 Evaluation of the energy**

With the assistance with definitions above, the energy of the original mean-field Hamiltonian (Eq. 164) can be expressed as
\[ \langle H_{MF}^0 \rangle_0 = \langle H_{MF}^I \rangle_0 - \langle H_{MF}^b \rangle_0. \]  
(181)
\[ \langle H_{MF}^I \rangle_0 = \sum_\alpha \frac{3J_\alpha}{4} \left[ \frac{N_{\text{cell}}}{4} - \frac{1}{4} n_f(\alpha, \uparrow) - \frac{1}{4} n_f(\alpha, \downarrow) \right. \]  
\[ - \frac{1}{4} n_b(\alpha, \downarrow) - \frac{1}{4} n_f(\alpha, \downarrow) \]  
\[ - \frac{1}{4} n_f(\alpha, \uparrow) O_f(\alpha, \uparrow, \downarrow) \]  
\[ + \frac{1}{4} n_f(\alpha, \uparrow) O_f(\alpha, \uparrow, \downarrow) \]  
\[ + \frac{1}{4} n_f(\alpha, \downarrow) O_f(\alpha, \uparrow, \downarrow) \]  
\[ + \frac{1}{4} n_f(\alpha, \downarrow) O_f(\alpha, \downarrow, \uparrow) \]  
\[ - \frac{1}{4} n_f(\alpha, \downarrow) O_f(\alpha, \downarrow, \uparrow) \]  
\[ + \frac{1}{4} n_f(\alpha, \downarrow) O_f(\alpha, \downarrow, \downarrow) \]  
\[ - \frac{1}{4} n_f(\alpha, \downarrow) O_f(\alpha, \downarrow, \downarrow) \]  
\[ + \frac{1}{4} n_f(\alpha, \downarrow) O_f(\alpha, \uparrow, \downarrow) \]  
\[ - \frac{1}{4} n_f(\alpha, \downarrow) O_f(\alpha, \downarrow, \downarrow) \]  
\[ + \frac{1}{4} n_f(\alpha, \uparrow) O_f(\alpha, \downarrow, \downarrow) \]  
\[ - \frac{1}{4} n_f(\alpha, \uparrow) O_f(\alpha, \downarrow, \downarrow) \]  
\[ + \frac{1}{4} n_f(\alpha, \uparrow) O_f(\alpha, \uparrow, \downarrow) \]  
\[ \left. - \frac{1}{4} n_f(\alpha, \uparrow) O_f(\alpha, \uparrow, \downarrow) \right]. \]  
(182)
When spin is included, we define charge and spin current
\[ \psi^* \] normalization at leading order [27] and thus are neglected. The current algebra reads [27]
\[ T_{ij}^{R}(x, \tau)T_{lm}^{R}(0,0) \sim \frac{\delta_{il}\delta_{jm}}{2\pi z_j}, \]
\[ T_{ij}^{R}(x, \tau)T_{lm}^{R}(0,0) \sim \frac{\delta_{il}\delta_{jm}}{2\pi z_i}, \]

where \( T^{Ra} \) is the components of the vector current \( T^R \).

\[ T_{ij}^{R}(x, \tau)T_{lm}^{R}(0,0) \sim \frac{\delta_{il}\delta_{jm}}{2\pi z_j}, \]

\[ T_{ij}^{R}(x, \tau)T_{lm}^{R}(0,0) \sim \frac{\delta_{il}\delta_{jm}}{2\pi z_i}, \]

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where \( T^{Ra} \) is the components of the vector current \( T^R \).

\[ T_{ij}^{R}(x, \tau)T_{lm}^{R}(0,0) \sim \frac{\delta_{il}\delta_{jm}}{2\pi z_j}, \]

\[ T_{ij}^{R}(x, \tau)T_{lm}^{R}(0,0) \sim \frac{\delta_{il}\delta_{jm}}{2\pi z_i}, \]

Employing the standard method [39] and using the current algebra above, we obtain the RG equations
\[ \dot{f}_{ii}^{R} = -\frac{16(f_{ii}^{R})^2 + 3(f_{i}^{\sigma})^2}{32\pi v_{i}}, \]
\[ \dot{f}_{ii}^{\sigma} = -\frac{2(f_{i}^{R})^2 + 4f_{i}^{R}f_{i}^{\sigma} + (f_{i}^{\sigma})^2}{4\pi v_{i}}, \]
\[ \dot{f}_{i,3}^{R} = \frac{16(f_{i}^{R})^2 + 3(f_{i}^{\sigma})^2}{16\pi (v_{i} + v_{3,i})}, \]
\[ \dot{f}_{i,3}^{\sigma} = \frac{2(f_{i}^{R})^2 + 4f_{i}^{R}f_{i}^{\sigma} - (f_{i}^{\sigma})^2}{2\pi (v_{i} + v_{3,i})}, \]
\[ \dot{f}_{ii}^{R} = \frac{16f_{ii}^{R}f_{ii}^{\alpha} + 3f_{ii}^{R}f_{ii}^{\sigma}}{8\pi (v_{i} + v_{3,i})} - \sum_{s} \frac{16f_{ss}^{R}f_{ii}^{\alpha} + 3f_{ss}^{R}f_{ii}^{\sigma}}{32\pi v_{i}}, \]
\[ \dot{f}_{ii}^{\sigma} = \frac{2f_{ij}^{R}f_{ij}^{\alpha} + 2f_{ij}^{R}f_{ij}^{\sigma} - f_{ij}^{\alpha}f_{ij}^{\sigma}}{\pi (v_{i} + v_{3,i})} - \sum_{s} \frac{2f_{ss}^{R}f_{ss}^{\alpha} + 2f_{ss}^{R}f_{ss}^{\sigma} + f_{ss}^{R}f_{ss}^{\alpha}}{4\pi v_{i}}. \]

\[ \dot{f}_{ij,0}^{R} = \frac{1}{4}f_{ij,0}^{R} = J' \left( 1 - (-1)^{i+j} \cos \left( \frac{k_{F1} + k_{F2}}{2} \right) \right) + \frac{1}{4}J \left( 1 - \cos(k_{F1} + k_{F2}) \right) + \delta_{ij}J_{y}, \]
\[ \dot{f}_{i,0}^{\sigma} = \frac{1}{4}f_{i,0}^{\sigma} = J \sin(k_{F1}) \sin(k_{F2}) \]
\[ -2J' \sin \left( \frac{k_{F1}}{2} \right) \sin \left( \frac{k_{F2}}{2} \right) = J_{y}. \]

Symmetry of the coupling constants are employed in the derivation of the equations above. The initial value of these coupling constants are
\[ f_{ij,0}^{R} = \frac{1}{4}f_{ij,0}^{R} = J' \left( 1 - (-1)^{i+j} \cos \left( \frac{k_{F1} + k_{F2}}{2} \right) \right) + \frac{1}{4}J \left( 1 - \cos(k_{F1} + k_{F2}) \right) + \delta_{ij}J_{y}, \]
\[ f_{i,0}^{\sigma} = \frac{1}{4}f_{i,0}^{\sigma} = J \sin(k_{F1}) \sin(k_{F2}) \]
\[ -2J' \sin \left( \frac{k_{F1}}{2} \right) \sin \left( \frac{k_{F2}}{2} \right) = J_{y}. \]

The RG flows are calculated numerically.
E Bosonization dictionary [39]

The bosonization dictionary [39] reads

$$\psi_R^{i,s} \sim \eta_i, \sigma \sqrt{\pi \phi_R^{i,s}},$$

(203)

where the chiral boson fields satisfy commutation relation [27]

$$[\phi_R^{i,s}(x), \phi_R^{i',\sigma'}(y)] = -[\phi_L^{i,s}(x), \phi_L^{i',\sigma'}(y)] = \frac{i}{4} \delta_{ii'} \delta_{\sigma \sigma'} \delta(x-y) \delta_{s's''},$$

(204)

and $$\eta$$ are Klein factors satisfying $$\{\eta_i, \sigma \eta_{i', \sigma'}\} = 2 \delta_{ii'} \delta_{ss'}$$. To describe spin and charge modes, we further define

$$\phi_{i,\rho} = \frac{1}{\sqrt{2}} (\phi_R^{i,1} + \phi_L^{i,1} + \phi_L^{i,4}),$$

(206)

$$\theta_{i,\rho} = \frac{1}{\sqrt{2}} (\phi_R^{i,1} + \phi_L^{i,1} - \phi_L^{i,4}),$$

(207)

$$\phi_{i,\sigma} = \frac{1}{\sqrt{2}} (\phi_R^{i,1} - \phi_L^{i,1} + \phi_L^{i,4}),$$

(208)

$$\theta_{i,\sigma} = \frac{1}{\sqrt{2}} (\phi_R^{i,1} - \phi_L^{i,1} - \phi_L^{i,4}),$$

(209)

where subscript $$\rho$$ represents charge mode and $$\sigma$$ represents spin mode, respectively.

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