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Strong competition between $\Theta_{II}$-loop-current order and $d$-wave charge order along the diagonal direction in a two-dimensional hot spot model

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We study the fate of the so-called $\Theta_{II}$-loop-current order that breaks both time-reversal and parity symmetries in a two-dimensional hot spot model with antiferromagnetically mediated interactions, using Fermi surfaces relevant to the phenomenology of the cuprate superconductors. We start from a three-band Emery model describing the hopping of holes in the CuO$_2$ plane that includes two hopping parameters $t_{pp}$ and $t_{pd}$, local on-site Coulomb interactions $U_d$ and $U_p$ and nearest-neighbor $V_{pd}$ couplings between the fermions in the copper [Cu(3$d_{x^2-y^2}$)] and oxygen [O(2$p_x$) and O(2$p_y$)] orbitals. By focusing on the lowest-energy band, we proceed to decouple the local interaction $U_d$ of the Cu orbital in the spin channel using a Hubbard-Stratonovich transformation to arrive at the interacting part of the so-called spin-fermion model. We also decouple the nearest-neighbor interaction $V_{pd}$ to introduce the order parameter of the $\Theta_{II}$-loop-current order. In this way, we are able to construct a consistent mean-field theory that describes the strong competition between the composite order parameter made of a quadrupole-density-wave and $d$-wave pairing fluctuations proposed in Efetov et al. [Nat. Phys. 9, 442 (2013)] with the $\Theta_{II}$-loop-current order parameter that is argued to be relevant for explaining important aspects of the physics of the pseudogap phase displayed in the underdoped cuprates.

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I. INTRODUCTION

The physics of the pseudogap phase of cuprate superconductors remains one of the most enduring open problems of condensed matter physics. There are recent pervasive hints that the pseudogap phase in most underdoped cuprate superconductors might involve one or more symmetry-breaking “hidden” orders, whose precise microscopic mechanisms are still elusive to this date. State-of-the-art experiments such as nuclear magnetic resonance$^{11,12}$, pulsed-echo ultrasound experiments$^{4–6}$, x-ray scattering$^{7,8}$ and scanning tunneling microscopy$^{7,8}$ performed in non-Lanthanum-based materials established the emergence of a dome-shaped short-range incommensurate $d$-wave$^{9,10}$ charge-density-wave (CDW) at low hole doping with a modulation described by the wavevectors $\mathbf{Q}_x = (Q_0, 0)$ and $\mathbf{Q}_y = (0, Q_0)$ oriented along the principal axes of the CuO$_2$ unit cell (with $Q_0 \simeq 0.255$ in reciprocal lattice units$^{11,12}$). Quite surprisingly, the peak of this short-range charge order dome occurs approximately at the universal hole doping $x \simeq 0.12$ for several compounds$^{11,12}$, despite their differences in material-specific properties. This could suggest that simple, low-energy effective models may potentially capture the essence of the physics of these materials$^{11,12,13}$. We will follow this point of view in the present work. Moreover, by applying pressure on these systems, the charge order can be completely suppressed, while the pseudogap phase remains unaffected$^{13}$. This clearly indicates that such a CDW order emerges on top of an already-formed pseudogap phase, instead of being its driving force. On the other hand, at very high magnetic fields, the $d$-wave superconducting phase displayed by these materials is destroyed and the short-range CDW turns into a long-range order. In this context, it plays a central role in reconstructing the Fermi surface of these compounds into pockets, as is evidenced in quantum oscillation experiments$^{14,15}$.

In addition to these salient features taking place within the pseudogap phase, another form of “hidden” order representing potentially one of the driving forces of quantum criticality in these systems (that may even coexist with CDW order and $d$-wave superconductivity at lower temperature scales $T < T^*$) is suggested by a different set of equally groundbreaking experiments: spin-polarized neutron scattering$^{20,21}$ and Kerr-rotation experiments$^{22,23}$ indicate spontaneous breaking of both time-reversal and parity symmetries in this phase at temperatures that are reasonably close to $T^*$ over a wide doping range. This phase transition has thus been referred to as the Kerr transition in the literature. This transition was given a theoretical framework in the proposal by Varma$^{24}$ (see also an interesting, alternative proposal put forward in Ref.$^{25}$) that orbital loop current order – we shall specialize in the present work to the so-called $\Theta_{II}$-phase – may account for the observed properties in these materials, since it naturally preserves the translational symmetry of the lattice and, additionally, it leads to the breaking of the correct discrete symmetries consistent with spin polarized neutron scattering experiments$^{26}$. This theoretical description requires starting from at least a three-band model, in which one includes besides the usually considered copper $d_{x^2-y^2}$-orbital, also the oxygen $p_x$ and $p_y$-orbitals of the CuO$_2$ unit cell. Such a minimal model turns out to be essential to describe intra-unit-cell loop currents involving charge transfer between oxygen orbitals that appear in the afore-
mentioned $\Theta_{11}$-phase. This theoretical proposal is physically appealing but it has one potential disagreement with experiments: it is hard to obtain the result that the underlying Fermi surface gaps out at all, since the phase transition does not break translational symmetry near the hot spots (i.e. the points in momentum space where the Fermi surface intersects the antiferromagnetic Brillouin zone boundary). Moreover, it is important to mention that recently a quantum critical point (QCP) was revealed in the cuprates at a hole-doping $x_{crit} \simeq 0.18$ via an analysis of the quasiparticle mass enhancement using quantum oscillation experiments. Interestingly, this critical point may represent approximately the termination of the Kerr transition line, the charge-order dome and an as-yet-unidentified third phase competing with the previous two orders at a doping level reasonably close to optimal doping.

On the theoretical front, the hot spot model emerges as an interesting, minimal low-energy effective model that captures qualitative aspects of the physics of the high-$T_c$ cuprates from a weak-to-moderate coupling perspective. In this respect, an important work by Metlitski and Sachdev consisted in the elegant demonstration that, if the energy dispersion of this model is linearized, an exact emergent $SU(2)$ pseudospin symmetry relating a $d$-wave singlet superconducting (SSC) order to a $d$-wave quadrupole-density-wave (QDW) order at wavevectors along the Brillouin zone diagonal $(\pm Q_0, \pm Q_0)$ is verified at the spin-density-wave (SDW) quantum critical point. This degeneracy between these two orders effectively produces a composite order parameter (denoted by QDW/SSC) with both bond order and preformed pairs at high temperatures as shown by Efetov et al. and the properties of this state have been explored in connection with the physics of the cuprates using different approaches in many works. In addition to this fact, another emergent $SU(2)$ degeneracy relating two additional orders – a superconducting order with a finite Cooper-pair center of mass momentum (the so-called pair-density-wave (PDW)) and a $d$-wave CDW at the experimentally observed wavevectors $Q_x$ and $Q_y$ – has also been recently verified in the model in the work by Pépin et al. and explored further by Wang et al. This additional degeneracy generates another composite order parameter (denoted by PDW/CDW) with similar energy scales that also competes with the QDW/SSC order.

In the present work, we will consider the relevant scenario in which yet another order parameter (the $\Theta_{11}$-loop current order) competes with the QDW/SSC order in an effective hot spot model. The purpose of this study is to demonstrate the possibility that, due to this competition, QSW/SSC is strongly affected by the $\Theta_{11}$-order parameter that breaks both time-reversal and parity symmetries, but instead preserves their product. This opens an interesting avenue for future research and could be an explanation as to why the charge-order signal in the cuprates is always observed along the axial vectors (i.e. $Q_x$ and $Q_y$) and never along the diagonal direction. In order to perform this investigation, we will construct a novel mean-field theory by including both $\Theta_{11}$-loop current order and the QDW/SSC composite order parameter in such an effective model. As will become clear shortly, we will confirm in this analysis the strong competition between $\Theta_{11}$-loop current order and the QDW/SSC entangled order, with one order parameter being clearly always detrimental to the other. Then we proceed to discuss the physical implications of this strong competition for the physics of the underdoped cuprates, in light of the recent experiments performed in these materials.

Technically speaking, we will introduce a three-band model (Emery model) describing hopping of holes in the CuO$_2$ plane which includes two hopping parameters $t_{pp}$ and $t_{pd}$, on-site $U_d$ and $U_p$ local interactions and nearest-neighbor $V_{pd}$ couplings between the fermions in the copper ($d_{x^2-y^2}$) and oxygen ($p_x$ and $p_y$) orbitals. By focusing on the lowest-energy band, we will decouple the local interaction $U_d$ of the Cu orbital in the spin channel using a conventional Hubbard-Stratonovich transformation to arrive at the interacting part of the so-called spin-fermion model. Then, we will follow closely the methodology explained in full detail in the paper by Efetov et al. to define the composite order parameter associated with the QDW/SSC fluctuations. In addition to this, we will also decouple the nearest-neighbor interaction $V_{pd}$ of the model to introduce the order parameter associated with the $\Theta_{11}$-loop-current order. Lastly, we will proceed to derive analytically and then solve numerically the resulting mean-field equations, which describes the competition between these two order parameters.

This paper is organized as follows. In Section II, we define the three-band model that we will be interested in and show how to decouple the interactions to obtain the resulting mean-field equations describing the competition between the two orders. Since the interactions that promote QDW/SSC and $\Theta_{11}$-loop current order turn out to be different, this decoupling is unambiguous. In Section III, we solve numerically the self-consistent mean-field equations and then we discuss our main results. Finally, Section IV is devoted to our conclusions.

## II. THE THREE-BAND MODEL

We start this section by writing down both the non-interacting and interacting Hamiltonians of the so-called three-band (Emery) model following Refs. in order to describe the underdoped cuprates as follows

\begin{equation}
\mathcal{H}_0 = -t_{pd} \sum_{i,\sigma} \left( \hat{d}^\dagger_{i,\sigma} \hat{p}_{i+\hat{y}/2,\sigma} + H.c. \right) - t_{pp} \sum_{i,\sigma} \left( \hat{p}^\dagger_{i+\hat{y}/2,\sigma} \hat{p}_{i+\hat{y},\sigma} + H.c. \right) + (\epsilon_d - \mu) \sum_{i,\sigma} \hat{n}_{i,\sigma}^d + \frac{1}{2} (\epsilon_p - \mu) \sum_{i,\sigma} \sum_{\nu} \hat{n}_{i,\nu,2,\sigma}^p, \tag{1}
\end{equation}
This model describes the fermionic motion on the copper \([\text{Cu}(3d)\text{--}p^2]\) and oxygen \([O(2p_x)\text{ and } O(2p_y)]\) orbitals that are located in the CuO₂ unit cell (see Fig. 1). The quantities \(a^\dagger_i,\sigma, \hat{a}_{i,\sigma}\) and \(\hat{p}_{i,\sigma}\) correspond, respectively, to the fermionic number operators for particles located on the Cu and O orbitals. The model also takes into account pair hopping \((t_{pd} \text{ and } t_{pp})\), on-site \((U_d \text{ and } U_p)\) and nearest-neighbor \((V_{pd})\) interactions involving the fermions on the Cu and O orbitals. The parameters \(\varepsilon_d\) and \(\varepsilon_p\) are, respectively, the Cu and O orbital energies and \(\mu\) is the chemical potential which controls the electronic density in the system.

Following Abanov and Chubukov, we first decouple the \(U_d\) part of the interacting Hamiltonian in the spin channel using a conventional Hubbard-Stratonovich transformation. The resulting action becomes

\[
S_{\text{int}}[\phi] = \lambda \int d\tau \sum_i d^\dagger_{i,\sigma} \cdot \hat{d}_{i,\sigma} e^{iQ \cdot r_i}
+ \frac{1}{2} \int d\tau d^2 r \left[ \frac{1}{v_s^2} (\partial_\tau \hat{\phi})^2 + (\nabla \hat{\phi})^2 + m_\phi \hat{\phi}^2 + \frac{g}{2} (\hat{\phi})^2 \right],
\]

where the bosonic field \(\hat{\phi} = (\phi_x^\dagger, \phi_y^\dagger, \phi_z^\dagger)\) is the spin-density wave (SDW) order parameter at the antiferromagnetic wave vector \(Q = (\pi, \pi)\) and \(v_s\) is the spin-wave velocity, and \(m_\phi\) is the spin-wave bosonic mass which vanishes at the quantum critical point (QCP) of the theory. The \(\sigma^a\) \((a = x, y, z)\) are the usual Pauli matrices. Notice that in Eq. (3) we have partially integrated out the high-energy fermions in order to derive an effective theory \(S_{\text{int}}[\phi] \) that corresponds to the so-called spin-fermion model describing the coupling between the itinerant low-energy fermionic excitations and the antiferromagnetic SDW fluctuations. Another possibility in order to investigate the Emery model is to start from a more localized picture by mapping the model defined in Eqs. (1) and (2) onto an effective three-band \(t-J\) model. We, however, will not follow this latter route in the present work. For this reason, we would like to state clearly from the outset that our starting point here will be a more itinerant picture.

Now we turn our attention to the \(V_{pd}\) interaction term in Eq. (2). This can be rewritten as

\[
V_{pd} \sum_{i,\nu} \sum_{\sigma,\sigma'} \hat{n}^p_{i,\sigma} \hat{n}^p_{i+\nu/2,\sigma'} = -\lambda \sum_{i,j} A_{i,\sigma}^{(j)} A_{i,\sigma'}^{(j)},
\]

with the field operators on the right-hand-side of the above equality being

\[
A_{i,\sigma}^{(1,2)} = \frac{1}{2} [d^\dagger_{i,\sigma} \hat{p}_{i+\nu/2,\sigma} + d^\dagger_{i,\sigma} \hat{p}_{i-\nu/2,\sigma}],
\]

\[
A_{i,\sigma}^{(3,4)} = \frac{i}{2} [d^\dagger_{i,\sigma} \hat{p}_{i+\nu/2,\sigma} - d^\dagger_{i,\sigma} \hat{p}_{i-\nu/2,\sigma}],
\]

As first shown by Varma, only the order parameters associated with \(A_{i,\sigma}^{(2)}, A_{i,\sigma}^{(3)}, \text{ and } A_{i,\sigma}^{(4)}\) lead to states with the presence of stationary-loop currents on the CuO₂ plane and, of course, to time-reversal symmetry breaking. The loop-current order with order parameter defined in terms of \(A_{i,\sigma}^{(2)}\) is conventionally called the \(\Theta_2\)-loop current phase.

FIG. 1: (Color online) Orbital structure and the interactions of the three-band model in the CuO₂ unit cell.

FIG. 2: (Color online) Loop current pattern in the CuO₂ plane cell for the \(\Theta_2\) and \(\Theta_{12}\)-loop current phases [panels (a) and (b), respectively] proposed by Varma to explain the physical properties of the pseudogap state in high-\(T_c\) cuprate superconductors. The symbols \((\bigcirc)\) and \((\bigtriangleright)\) represent the orientation of the local magnetic moments generated by the loop currents.
superconductors as an evidence in favor of the Θ
rent phase (see Fig. 3). The mean-field value of the phase Θ
lows, we will choose for simplicity the positive value of
so-called hot spots which are defined as the intersection of
the Fermi surface with the antiferromagnetic zone bound-
the so-called hot spots which are defined as the intersection of
the Fermi surface with the antiferromagnetic zone boundary.
For instance, the hot spot labeled as 1 has a wavevector
the hot spot labeled as 1 has a wavevector
in momentum space with the constraint
K_+ + K_− = π. The wavevectors of all the other hot spots
in the Brillouin zone are obtained by simple symmetry oper-
the Brillouin zone are obtained by simple symmetry oper-
while the loop-current order with order parameter given
in terms of A_i,σ and A_i,σ are known as the Θ
2. In what fol-
we will analyze henceforth only this
type of order. In this way, the decoupling of the inter-
functionals.

where R_{1I}e^{i\Theta_I} = V_{pd} \sum \sigma (A_i^{(3)}(\Theta_I)) is a complex order param-
parameter. The mean-field value of the phase Θ_I was de-
terms of

At this point, we would like to point out that we will
we will consider only the lowest energy band of the noninter-
model, the low-energy band will naturally give rise to a Fermi
sequently, we will restrict the analysis of
in this effective model will arise from the points at
the Fermi surface shown in Fig. 3. The most singular contribu-
to the vicinity of these important hot
pot points in the considerations that follow. With this
in mind and to set up our notation, we now define the
resulting Hamiltonian defined in Eq. (1). For physically moti-
term, the low-energy band will naturally give rise to a Fermi

FIG. 3: (Color online) Representation of the Brillouin zone
the Brillouin zone with the underlying noninteracting Fermi surface (that en-
closes the blue area) which characterizes the underdoped
cuprate superconductors. The small black circles denote the
so-called hot spots which are defined as the intersection of
the Fermi surface with the antiferromagnetic zone bound-
ary. For instance, the hot spot labeled as 1 has a wavevec-

exactly in the Brillouin zone is obtained by simple symmetry oper-
the Fermi surface with the antiferromagnetic zone boundary.

that minimizes the energy for the present case.
where $\xi_p \equiv \varepsilon_p + \frac{2m}{\hbar^2}U_p - \mu$, $\xi_d \equiv \varepsilon_d - \mu$, and both time and space coordinates have been collected in terms of the variable $X = (\tau, \mathbf{r})$. The matrices $\hat{\Gamma}_1, \hat{\Gamma}_2, \hat{\Gamma}_{x(y)}$, and $\hat{\Gamma}_{2x(y)}$ appearing in Eq. (11) are diagonal in the $\Sigma \otimes \Lambda \otimes L$ pseudospin space and depend on all the parameters of the three-band model and also on the order parameter $R_{11}$ for the $\Theta_{11}$-loop current phase (see the Appendix A to check their definition). Here we follow Ref. [16] and introduce the 32-component fermionic spinors in the particle-hole space $\tau$ as

$$\Psi = \frac{1}{\sqrt{2}} \begin{pmatrix} d_x^\tau \\ i\sigma_d d_x^\tau \end{pmatrix}, \quad \Psi^\dagger = \frac{1}{\sqrt{2}} \begin{pmatrix} -d_x^\tau, -d^\tau i\sigma_2 \end{pmatrix},$$

(10)

where

$$P_x = \frac{1}{\sqrt{2}} \begin{pmatrix} p_x^\tau \\ io\sigma_2 p_x^\tau \end{pmatrix}, \quad P_y = \frac{1}{\sqrt{2}} \begin{pmatrix} p_y^\tau, -p_y^\tau i\sigma_2 \end{pmatrix}, \quad P_z = \frac{1}{\sqrt{2}} \begin{pmatrix} -p_z^\tau, -p_z^\tau i\sigma_2 \end{pmatrix}.$$  

(11)

In addition to the fermionic fields defined above, we also introduce the charge-conjugated vectors as

$$\tilde{\Psi} = \Psi^\dagger \tau_3, \quad \tilde{P}_x = P_x^\dagger \tau_3, \quad \tilde{P}_y = P_y^\dagger \tau_3,$$

(13)

where $\tau_3$ is the usual Pauli matrix defined in the $\tau$ space. Hence by making use of these last definitions, the action in Eq. (1) can be naturally rewritten as

$$S[\tilde{P}_x, \tilde{P}_y, \tilde{\Psi}, \tilde{\Phi}; n_p, R_{11}] = \int (\tilde{P}_x(X), \tilde{P}_y(X), \tilde{\Psi}(X)) \left( \begin{array}{ccc} -\partial_x + \xi_p \tau_3 & \hat{\Gamma}_1\tau_3 - \hat{\Gamma}_2(-i\nabla) \hat{\Gamma}_1 x \tau_3 + \hat{\Gamma}_2 x i\partial_x & \hat{\Gamma}_1 x \tau_3 + \hat{\Gamma}_2 x i\partial_x \\
\hat{\Gamma}_1 y \tau_3 + \hat{\Gamma}_2 y i\partial_y & -\partial_y + \xi_p \tau_3 & \hat{\Gamma}_1 y \tau_3 + \hat{\Gamma}_2 y i\partial_y \\
\hat{\Gamma}_1 \tau_3 + \hat{\Gamma}_2 i\partial_x & \hat{\Gamma}_1 \tau_3 + \hat{\Gamma}_2 i\partial_x & \hat{\Gamma}_1 i\tau_3 + \hat{\Gamma}_2 i\partial_x \end{array} \right) \left( \begin{array}{c} \tilde{P}_x(X) \\
\tilde{P}_y(X) \\
\tilde{\Psi}(X) \end{array} \right) dX + \lambda \int \left[ \frac{1}{2} (\partial_x \tilde{\phi})^2 + (\nabla \tilde{\phi})^2 + m_\sigma \tilde{\phi}^2 + \frac{g}{2} (\tilde{\phi})^2 \right] dX + \int \left( \frac{R_{11}^2}{V_{pd}} - \frac{n_p^2}{8} U_p \right) dX.$$  

(14)

In order to derive the thermodynamical properties of the present model, we should first integrate out the bosonic field in the functional integral

$$Z = \int \exp \left\{ -S[\tilde{P}_x, \tilde{P}_y, \tilde{\Psi}, \tilde{\Phi}; n_p, R_{11}] \right\} D[\tilde{P}_x, \tilde{P}_y, \tilde{\Psi}, \tilde{\Phi}]$$

$$= \int \exp \left\{ -S[\tilde{P}_x, \tilde{P}_y, \tilde{\Psi}; n_p; R_{11}] \right\} D[\tilde{P}_x, \tilde{P}_y, \tilde{\Psi}].$$

(15)

Here the function $D(X - X')$ that appears as a potential function in the fermionic quartic interaction is the bare bosonic propagator. Its Fourier transform is given by $D(\omega, \mathbf{k}) = (\omega^2/\nu_s^2 + |\mathbf{k}|^2 + m_s)^{-1}$ with $m_s$ standing for the spin-wave boson mass that vanishes at the QCP, $\nu_s$ is the spin-wave velocity and $\omega$ denotes the Matsubara bosonic frequency.

Next, we decouple the fermionic quartic term of the action in Eq. (14) by using a composite order parameter $M(X, X')$ for both the quadrupole density wave (QDW)
and the $d$-wave singlet superconducting (SSC) orders, as was described in full detail in Ref.\textsuperscript{15}. This is achieved by considering the renormalization of bosonic propagator $D(\omega, \mathbf{k})$ by the fermions at the hot spots which leads to the appearance of the effective spin-wave propagator

$$D_{\text{eff}}(\omega, \mathbf{k}) = (\gamma |\omega| + |\mathbf{k}|^2 + m_n)^{-1},$$

where $\gamma$ is naturally the Landau damping term. As a consequence, the low-energy effective action that describes the present system may be represented as follows

$$S_{\text{eff}}[P_x, P_y, \Psi; n_p, R_{\text{II}}, M]$$

$$= \int \left( \mathbf{P}_x(X), \mathbf{P}_y(X), \Psi(X) \right) \left( -\partial_t + \xi_p \tau \right) \tilde{\Gamma}_1 \tau_3 - \tilde{\Gamma}_2(-i\mathbf{V}) \Gamma_{1z} \tau_3 + \Gamma_{2x} \partial_x \Gamma_{1y} \tau_3 + \Gamma_{2y} \partial_y\right) \left( \mathbf{P}_x(X), \mathbf{P}_y(X) \right) dX$$

$$- i \int \Psi(X) M(X, X') \Psi(X')dXdX' + \frac{1}{2} \int J^{-1}(X - X')\text{Tr}[M(X, X') \Sigma_1 M(X', X) \Sigma_1]dXdX'$$

$$+ \int \left( \frac{R_{\text{II}}^2}{V_{pd}} - \frac{n_p^2}{8} U_p \right) dX,$$

where we have written $J(X - X') = 3\lambda^2 D_{\text{eff}}(X - X')$ instead of the spin-wave propagator in order to simplify the notation. The order parameter $M(X, X')$ for the QDW/SSC composite order is given by

$$M(X, X') = b(X, X')\Sigma_3 \left( \begin{array}{c} 0 \\ -\tilde{u}_x \\ 0 \end{array} \right),$$

with

$$\tilde{u}_x = \left( \begin{array}{c} \Delta_+ \\ \Delta_- \end{array} \right)_x.$$

Here $\Delta_+$ and $\Delta_-$ are, respectively, the $d$-wave singlet superconducting (SSC) and quadrupole density wave (QDW) components of the order parameter defined above. We also point out that the matrices $\tilde{u}_x$ belong to the $SU(2)$ group\textsuperscript{16} which lead to the constraint $|\Delta_+|^2 + |\Delta_-|^2 = 1$ involving both the SSC and QDW sectors. Although we have constructed an effective spin-fermion model for the CuO$_2$ unit cell by considering only the Cu atoms, we point out that the QDW/SSC order parameter in Eq. \textsuperscript{18} does not lead to a charge modulation located on the Cu orbitals. In fact, it can be shown\textsuperscript{15,20,22} that this composite order parameter generates a charge modulation with a checkerboard pattern residing on the oxygen O sites, which is described by incommensurate wavevectors with respect to the lattice.

The effective action in Eq. \textsuperscript{17} now has a quadratic form and the free energy of the system can be obtained as follows: First one has to integrate out the fermionic fields in the functional integral for the partition function and then apply the formulae $\text{Tr} \ln G^{-1} = \ln \text{det}(G^{-1})$. Following this procedure, we determine that the free energy in space-time coordinates evaluates to

$$F[T, n_p, R_{\text{II}}, M] = - \int \text{Tr} \ln [G^{-1}(X, X')]dXdX'$$

$$+ \frac{1}{2} \int J^{-1}(X - X')\text{Tr}[M(X, X') \Sigma_1 M(X', X) \Sigma_1]dXdX'$$

$$+ \int \left( \frac{R_{\text{II}}^2}{V_{pd}} - \frac{n_p^2}{8} U_p \right) dX,$$

where the matrix $G^{-1}(X, X')$ is the Fourier transform of $G^{-1}(\varepsilon_n, \mathbf{k})$. This latter function is given by

$$\left( \begin{array}{ccc} -i\varepsilon_n + \xi_p \tau_3 & \Gamma_{1z} \tau_3 - \Gamma_{2z} \mathbf{k} \\ \Gamma_{1z} \tau_3 - \Gamma_{2z} \mathbf{k} & -i\varepsilon_n + \xi_p \tau_3 & \Gamma_{1y} \tau_3 - \Gamma_{2y} \mathbf{k} \\ \Gamma_{1y} \tau_3 - \Gamma_{2y} \mathbf{k} & -i\varepsilon_n + \xi_p \tau_3 & \Gamma_{1x} \tau_3 - \Gamma_{2x} \mathbf{k} \end{array} \right).$$

The self-consistency equation for $b(X, X')$ is derived by minimizing the free energy $F[T, n_p, R_{\text{II}}, M]$ with respect to this order parameter. As a consequence, we obtain the following equation

$$- \text{Tr} \left\{ \frac{1}{G^{-1}(X, X')} \frac{\partial G^{-1}(X, X')}{\partial b(X, X')} \right\} + J^{-1}(X - X')b(X, X')$$

$$\times \text{Tr} \left\{ \Sigma_3 \left( \begin{array}{c} 0 \\ -\tilde{u}_x \end{array} \right) \Lambda \Sigma_3 \left( \begin{array}{c} 0 \\ -\tilde{u}_x \end{array} \right) \right\} = 0.$$

By performing the trace operation over the space $\Sigma \otimes \Lambda \otimes L \otimes \tau$ for the second term on the left-hand-side of the equation above, the order parameter $b(X, X')$ can be
simply expressed as
\[
b(X, X') = \frac{1}{16} J(X - X') \text{Tr} \left\{ \mathcal{G}(X, X') \frac{\partial G^{-1}(X, X')}{\partial b(X, X')} \right\}
\]
\[
= \frac{1}{16} J(X - X') \text{Tr} \left\{ \mathcal{G}(X, X') i \Pi_3 \Sigma_3 \left( \begin{array}{cc} 0 & \tilde{u}_+ \\ -\tilde{u}_+ & 0 \end{array} \right) \right\},
\]
where \( \Pi_3 \) is a projector for the three-band-model space which is defined as
\[
\Pi_3 = \left( \begin{array}{ccc} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{array} \right).
\]
At this point, we will make use of the ansatz \( b(X, X') = b(X - X') \) and Fourier transform Eq. (23) to momentum-frequency space. As a result, we get the expression
\[
b(\varepsilon_n, k) = \frac{T}{16} \sum_{\varepsilon_n} \int J(\varepsilon_n - \varepsilon_n', k - k') \text{Tr} \left\{ \left[ G^{-1}(i \varepsilon_n', k') \right]^{-1} \right\} \frac{\partial G^{-1}(i \varepsilon_n', k')}{\partial b(\varepsilon_n', k')} \frac{1}{(2\pi)^2}.
\]
In order to express \( b(\varepsilon_n, k) \) in a convenient form, we need to evaluate the trace that appears in the above equation. This problem can be circumvented by using the following identity
\[
\text{Tr} \left\{ \left[ G^{-1}(i \varepsilon_n', k') \right]^{-1} \right\} \frac{\partial G^{-1}(i \varepsilon_n', k')}{\partial b(\varepsilon_n', k')} \frac{1}{(2\pi)^2} = \frac{1}{\det[ G^{-1}(i \varepsilon_n', k') ]} \frac{\partial \det[ G^{-1}(i \varepsilon_n', k') ]}{\partial b(\varepsilon_n', k')} \frac{1}{(2\pi)^2}.
\]
Then, by substituting Eq. (20) into Eq. (25), we finally arrive at the self-consistency equation
\[
b(\varepsilon_n, k) = \frac{3\lambda^2 T}{16} \sum_{\varepsilon_n} \int \frac{D_{\text{eff}}(\varepsilon_n - \varepsilon_n', k - k')}{\det[ G^{-1}(i \varepsilon_n', k') ]} \frac{\partial \det[ G^{-1}(i \varepsilon_n', k') ]}{\partial b(\varepsilon_n', k')} \frac{1}{(2\pi)^2} \frac{dk'}{(2\pi)^2},
\]
where we have set \( J(\varepsilon_n - \varepsilon_n', k - k') = 3\lambda^2 D_{\text{eff}}(\varepsilon_n - \varepsilon_n', k - k') \).

We now turn our attention to the evaluation of \( \det[ G^{-1}(i \varepsilon_n, k) ] \). In order to do this, we will need to use the set of determinant formulas
\[
\text{det} \left( \begin{array}{cc} \hat{A} & \hat{B} \\ \hat{C} & \hat{D} \end{array} \right) = \text{det}(\hat{A}) \text{det}(\hat{D} - \hat{C} \hat{A}^{-1} \hat{B}),
\]
\[
\text{det}(\hat{A} \otimes \hat{D}) = [\text{det}(\hat{A})]^m [\text{det}(\hat{D})]^n,
\]
where \( \hat{A} \) and \( \hat{D} \) are, respectively, \( n \)- and \( m \)-square matrices and \( \text{det}(\hat{A}) \) is different from zero. In this way, by

III. MEAN-FIELD RESULTS

In order to investigate the interplay between both \( \Theta_{11} \)-loop-current (LC) and QDW orders in the present three-

where \( \Delta_+ = 0 \) and applying these reduction formulas to the matrix \( G^{-1}(i \varepsilon_n, k) \), we obtain, after some algebraic manipulations, that \( \det[ G^{-1}(i \varepsilon_n, k) ] \) evaluates formally to
\[
\det[ G^{-1}(i \varepsilon_n, k) ] = \prod_{l=1}^{D_l(m)} (i \varepsilon_n, k),
\]
where \( D_l(m)(i \varepsilon_n, k) \) are well-behaved functions of the three-band-model parameters, which are computed in detailed form in Appendices B and C. Thus, by inserting the result displayed in Eq. (30) into Eq. (27), the mean-field equation for \( b(\varepsilon_n, k) \) in terms of \( D_l(m)(i \varepsilon_n, k) \) finally reads
\[
b(\varepsilon_n, k) = \frac{3\lambda^2 T}{16} \sum_{l,m=1}^{2} \sum_{\varepsilon_n} \int \frac{D_{\text{eff}}(\varepsilon_n - \varepsilon_n', k - k')}{{D_l(m)(i \varepsilon_n, k')}} \frac{\partial D_l(m)(i \varepsilon_n, k')}{{\partial b(\varepsilon_n', k')}} \frac{dk'}{(2\pi)^2}.
\]
We note that, since we have set \( \Delta_+ = 0 \), the above self-consistency equation describes only the QDW sector of the fluctuations in the present system.

As a consequence of the result in Eq. (30), we determine after Fourier transforming the right-hand-side of Eq. (20) that the free energy of the present model has the following analytical form
\[
\begin{align*}
F[T, n_p, R_{II}, b] &= -T \sum_{l,m=1}^{2} \sum_{\varepsilon_n} \int \ln \left[ \frac{1}{{D_l(m)(i \varepsilon_n, k)}} \right] \frac{dk}{(2\pi)^2} \\
&+ \frac{8T}{3\lambda^2} \sum_{\varepsilon_n} \int b(\varepsilon_n, k) \frac{dk}{(2\pi)^2} \left[ \sum_{\varepsilon_n} \int b(\varepsilon_n', k') \right]
\end{align*}
\]
\[
\times D_{\text{eff}}^{-1}(\varepsilon_n - \varepsilon_n', k - k') \frac{dk'}{(2\pi)^2} + \frac{R_{II}^2}{V_{pd}} - \frac{n_p^2}{8} U_p,
\]
where we have set the volume of the system to unity. In order to self-consistently determine the mean-field order parameter \( R_{II} \), we need also minimize the free energy with respect to it. In this way, the self-consistency equation for \( R_{II} \) in turn reads
\[
R_{II} = \frac{V_{pd} T}{2} \sum_{l,m=1}^{2} \sum_{\varepsilon_n} \int \frac{1}{{D_l(m)(i \varepsilon_n, k)}} \frac{\partial D_l(m)(i \varepsilon_n, k)}{{\partial R_{II}}} \frac{dk}{(2\pi)^2}.
\]
The solutions of both Eqs. (31) and (33) will be obtained in the next section, following a numerical procedure described in great detail in Appendices B and C.
band model, we solve numerically the mean-field equations for $R_{II}$ and $b$. The present numerical approach consists in the discretization of the Brillouin zone with a mesh of $320 \times 320$ points. We also make the assumption that the order parameter $b(\varepsilon_n, \mathbf{k})$ does not depend crucially on the frequency and momentum. In this way, we will only investigate the ground state properties of the present model, which therefore allows us to evaluate the Matsubara sums that appear in the mean-field equations exactly. We perform this calculation by either varying the ratio of the critical parameters is given approximately

$$m_a = 10^{-2}, \gamma = 10^{-5}$$

and the other interactions are set to $t_{pd} = 1, t_{pp} = 0.5, U_p = 3,$ and $\varepsilon_d - \varepsilon_p = 3$. The fermionic density on the O orbital is given by $n_p = 0.6$ and the position of the hot spots is such that $\delta = 0.93$.

spin-polarized neutron scattering experiments. In Fig. (a), it can also be seen that the QDW order parameter $b$, by contrast, vanishes as the interaction $V_{pd}$ becomes stronger. Moreover, one can note in the same figure a narrow region where both order parameters can be finite for moderate $V_{pd}$, indicating that the present three-band model could in principle accommodate a coexisting phase involving both time-reversal (LC order) and translational symmetry breaking (QDW order), but as can be inferred from Fig. (a) this apparently occurs for somewhat fine-tuned interactions.

We can also analyze the behavior of the same order parameters as a function of spin-fermion coupling $\lambda$, when we keep instead the interaction $V_{pd}$ fixed. The corresponding results are depicted in Fig. (b). As a result, we find that the LC order parameter $R_{II}$ is finite below a threshold of $\lambda$ and then is clearly suppressed when this interaction becomes larger. Once more, the behavior of the QDW order parameter $b$ is essentially the opposite one, namely, it grows from zero to finite values as the spin-fermion interaction becomes stronger. In an analogous way to the previous case, there is also a very narrow window where both phases may coexist for moderate $\lambda$ and $V_{pd}$. Despite this, the generic behavior which can be inferred from both figures is that the LC order appears to be detrimental to the QDW order and vice-versa. In other words, we may conclude at this point that, for a large majority of initial choices for the couplings $V_{pd}$ and $\lambda$ within the present three-band model, there is a strong tendency for the above two orders not to coexist, at least at mean-field level.

FIG. 4: (Color online) (a) Mean-field values of $R_{II}$ and $b$ as a function of the nearest-neighbor interaction $V_{pd}$ in the limit of zero temperature for $\lambda = 20$. (b) Mean-field values of $R_{II}$ and $b$ as a function of the spin-fermion interaction $\lambda$ in the limit of zero temperature for $V_{pd} = 14$. Both solutions in (a) and (b) were obtained by performing numerical integration in momentum space of the self-consistency equations given by Eqs. (31) and (33) with a mesh of $320 \times 320$ points in the Brillouin zone. Here $m_a = 10^{-2}, \gamma = 10^{-5}$ and the other interactions are set to $t_{pd} = 1, t_{pp} = 0.5, U_p = 3,$ and $\varepsilon_d - \varepsilon_p = 3$. The fermionic density on the O orbital is given by $n_p = 0.6$ and the position of the hot spots is such that $\delta = 0.93$. 

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In order to analyze the sensitivity of the above mean-field results to changes in the physical parameters of the three-band model, we have also investigated its properties with respect to varying both the spin-wave bosonic mass \( m_a \) and the orbital-energy transfer \( \varepsilon_d - \varepsilon_p \). As the strength of \( m_a \) becomes larger (which corresponds naturally to shorter SDW correlation lengths), we obtain a clear tendency for both critical interactions (i.e. \( \lambda_c \) and \( V_{pq} \)) to increase even further in our numerical data. This result would of course lie beyond the regime of applicability of a mean-field approach to the present model and other complementary methods that include quantum fluctuation effects should be used to describe such a regime. In addition to this, we have also examined the dependence of our results with respect to changes in the orbital-energy transfer of the model. As a consequence, we were able to establish numerically that, as the difference \( \varepsilon_d - \varepsilon_p \) is reduced towards zero, the critical interactions \( \lambda_c \) and \( V_{pq} \) also display a tendency to increase further within the present approach.

IV. CONCLUSIONS

In the present work, we have performed a consistent mean-field calculation for the three-band (Emery) model relevant to the phenomenology of the underdoped cuprates. We have shown that a low-energy effective description of this model may indeed exhibit both the \( \Theta_{11} \)-loop-current order first proposed by Varma \cite{Varma99} and the so-called QDW which arises from an emergent \( SU(2) \) pseudospin symmetry that exists in the spin-fermion model \cite{De丑04,De丑06}. As a result, we have obtained that the above two order parameters have a tendency to be detrimental to each other, at least at mean-field level.

We would like to point out that the mean-field values of the critical interactions to obtain these two phases are relatively large compared with some physical parameters of the three-band model. This is expected to be an artifact of the mean-field approach and, for this reason, other complementary methods (such as, e.g., renormalization group techniques that include quantum fluctuation effects) should be used in order to establish a quantitative agreement between the present model and the experimental data. It is also important to mention that there are other works in the literature, which analyzed three-band model techniques that include quantum fluctuation effects. It is also important to mention that the present model and the experimental data to changes in the critical interactions to obtain these two phases are relatively large compared with some physical parameters of the three-band model. This is expected to be an artifact of the mean-field approach and, for this reason, other complementary methods (such as, e.g., renormalization group techniques that include quantum fluctuation effects) should be used in order to establish a quantitative agreement between the present model and the experimental data. It is also important to mention that there are other works in the literature, which analyzed three-band model techniques that include quantum fluctuation effects.

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Appendix A: Definition of the \( \hat{\Gamma} \), matrices

The matrices \( \hat{\Gamma}_1, \hat{\Gamma}_2, \hat{\Gamma}_{1x}, \hat{\Gamma}_{2x}, \hat{\Gamma}_{1y}, \) and \( \hat{\Gamma}_{2y} \) that appear throughout this work are defined by linearizing the functions of the three-band model around the hot spots depicted in Fig. 3. The structure of the resulting matrices can then be simplified by resorting to a representation based on Pauli matrices defined in distinct pseudospin spaces \cite{Hasegawa01}, which are denoted by \( \Sigma, \Lambda, \) and \( L \). Technically speaking, the pseudospin space \( \Sigma \) connects hot spots that can be mapped onto each other by the antiferromagnetic wavevector \( \mathbf{Q} = (\pi, \pi) \). Different pairs of hot spots connected by the wavevector \( \mathbf{Q} \) are mapped onto each other by the pseudospin space \( \Lambda \). Lastly, the pseudospin space \( L \) connects orthogonal quartet of hot spots. Following these definitions, the matrices of the three-band model can be simply written as

\[
\hat{\Gamma}_1 = -2t_{pp} \cos \delta \, \mathbb{1}_\Sigma \otimes \mathbb{1}_\Lambda \otimes \mathbb{1}_L, \quad \text{(A1)}
\]
\[
\hat{\Gamma}_2 = t_{pp}(\sin \delta \Lambda_3 \otimes L_3 - \Sigma_3 \otimes \Lambda_3) i \partial_x
\]
\[
- t_{pp}(\sin \delta \Lambda_3 + \Sigma_3 \otimes \Lambda_3 \otimes L_3) i \partial_y, \quad \text{(A2)}
\]
\[
\hat{\Gamma}_{1x} = \gamma_1 e^{-i\varphi \Lambda_3 \otimes L_3} + \gamma_2 e^{i\theta \Lambda_3 \otimes L_3} \Sigma_3 \otimes L_3, \quad \text{(A3)}
\]
\[
\hat{\Gamma}_{2x} = -\frac{1}{2} \gamma_1 e^{-i\varphi \Lambda_3 \otimes L_3} \Sigma_3 \otimes L_3 + \frac{1}{2} \gamma_2 e^{i\theta \Lambda_3 \otimes L_3} \Lambda_3 \otimes L_3, \quad \text{(A4)}
\]
\[
\hat{\Gamma}_{1y} = \gamma_1 e^{i\varphi \Lambda_3} - \gamma_2 e^{-i\theta \Lambda_3} \Sigma_3 \otimes L_3, \quad \text{(A5)}
\]
\[
\hat{\Gamma}_{2y} = -\frac{1}{2} \gamma_1 e^{i\varphi \Lambda_3 \otimes L_3} \Sigma_3 \otimes L_3 + \frac{1}{2} \gamma_2 e^{-i\theta \Lambda_3} \Lambda_3, \quad \text{(A6)}
\]
where \( \delta = (K_+ - K_-)/2 \) and \( \mathbb{1} \Sigma, \mathbb{1} \Lambda, \) and \( L \) are, respectively, the identity matrices in the \( \Sigma, \Lambda, \) and \( L \) pseudospin spaces. The parameters \( \varphi, \theta, \gamma_1, \) and \( \gamma_2 \) are defined as

\[
\tan \varphi = \frac{R_{II} \tan \left( \frac{\delta}{2} \right)}{2t_p}, \quad (A7)
\]

\[
\tan \theta = \frac{R_{II} \cot \left( \frac{\delta}{2} \right)}{2t_p}, \quad (A8)
\]

\[
\gamma_1 = \left[ 2t_{pd} \cos \left( \frac{\delta}{2} \right) + \frac{R_{II}^2}{2} \sin^2 \left( \frac{\delta}{2} \right) \right]^{1/2}, \quad (A9)
\]

\[
\gamma_2 = \left[ 2t_{pd} \sin \left( \frac{\delta}{2} \right) + \frac{R_{II}^2}{2} \cos^2 \left( \frac{\delta}{2} \right) \right]^{1/2}. \quad (A10)
\]

Appendix B: Evaluation of the Matsubara sums for the mean-field equations

1. Quadrupole density wave (QDW) order parameter

In order to compute the Matsubara sum in Eq. 10, we will consider that the QDW order parameter does not depend on both the frequency and the momentum. In this manner, we can rewrite this equation as

\[
b(T) = \frac{3 \lambda^2 T}{16} \sum_{l,m=1}^2 \sum_{\varepsilon_n} \int \frac{D_{\text{eff}}(\varepsilon_n, k)}{D_{\text{eff}}^{(m)}(i\varepsilon_n, k)} \frac{dk}{(2\pi)^2}, \quad (B1)
\]

where we have not written explicitly the full dependence of \( b(T) \) to not clutter up the notation.

There is a subtlety to obtain the analytic continuation of the effective bosonic propagator \( D_{\text{eff}}(\varepsilon_n, k) \) since this function depends on \( |\omega| \) which is not well-defined for complex numbers. To circumvent that, we make use of the two integral formulas

\[
|\omega| = -\frac{i \omega}{\pi} \int_{-\infty}^{\infty} \frac{dx}{x - i \omega}, \quad (B2)
\]

\[
sgn(\omega) = -\frac{i \pi}{\pi} \int_{-\infty}^{\infty} \frac{dx}{x - i \omega}. \quad (B3)
\]

As a result, the analytic continuation of \( D_{\text{eff}}(\varepsilon_n, k) \) becomes

\[
D_{\text{eff}}(-iz, k) = \frac{1}{-i \gamma z sgn[\text{Im}(z)] + |k|^2 + m_a}. \quad (B4)
\]

As may be easily concluded, \( D_{\text{eff}}(-iz, k) \) is not analytic in the entire complex plane. Indeed, it possesses a branch cut (see Fig. 5 which must be avoided when performing complex integration. As a result, we obtain that Eq. [B1] may be rewritten as

\[
b(T) = \frac{3 \lambda^2 T}{16} \sum_{l,m=1}^2 \sum_{\varepsilon_n} \int \frac{D_{\text{eff}}(\varepsilon_n, k)}{D_{\text{eff}}^{(m)}(i\varepsilon_n, k)} \frac{dk}{(2\pi)^2} \left\{ \frac{-1}{2\pi i} \oint_{C_1} \frac{dz}{z} D_{\text{eff}}(-iz, k) \right\}, \quad (B5)
\]

where we have used the result \( D_{\text{eff}}^{(m)}(z, k) = h_{l,m}(z, k) f_{l,m}(z, k) \) (see the Appendix C for details).

Here \( h_{l,m}(z, k) \) and \( f_{l,m}(z, k) \) are both polynomials with respect to \( z \) and the relation between their degrees is the following

\[
\deg \left[ \frac{\partial h_{l,m}(z, k)}{\partial b} \right] < \deg[\partial h_{l,m}(z, k)]. \quad (B6)
\]

As expected, a similar inequality holds for \( f_{l,m}(z, k) \) and \( \partial f_{l,m}(z, k)/\partial b \). The main consequence of the result in Eq. (B5) is that we can have a series expansion of the form

\[
\sum_{n=1}^{N} \frac{\Delta_{l,n}^{(m)}(k)}{z - \zeta_{l,n}^{(m)}}, \quad (B7)
\]

where \( N = \frac{3}{2} \dim(\Sigma \otimes \Lambda \otimes L \otimes \tau) \) is equal to twelve and \( \zeta_{l,n}^{(m)} \) represent both the roots of \( h_{l,m}(z, k) \) \((1 \leq l \leq N/2) \) and \( f_{l,m}(z, k) \) \((N/2 + 1 \leq l \leq N) \). The coefficients \( \Delta_{l,n}^{(m)}(k) \) are calculated as

\[
\Delta_{l,n}^{(m)}(k) = \left. \frac{\partial h_{l,m}(z, k)}{\partial b} \right|_{z = \zeta_{l,n}^{(m)}(k)}, \quad 1 \leq l \leq \frac{N}{2}, \quad (B8)
\]

\[
\Delta_{l,n}^{(m)}(k) = \left. \frac{\partial f_{l,m}(z, k)}{\partial b} \right|_{z = \zeta_{l,n}^{(m)}(k)}, \quad \frac{N}{2} + 1 \leq l \leq N. \quad (B9)
\]

Then by substituting Eq. (B7) into Eq. (B5), we obtain that the mean-field equation for \( b(T) \) assumes the
form

\[
b(T) = \frac{3\lambda^2}{16} \left[ \sum_{l,m=1}^{2N} \sum_{n=1}^{N} \int_{\mathcal{C}_1} \Delta^{(m)}_{l,n}(k) \left[ -\frac{1}{2\pi i} \oint_{\mathcal{C}_1} dz n_F(z) \right. \right.
\]
\[
\times \left. \left. \frac{D_{\text{eff}}(-iz,k)}{z - \xi^{(m)}_{l,n}(k)} \right] \frac{dk}{(2\pi)^2}. \right\] \tag{B10}
\]

The complex integral between brackets is computed by changing the integration contour from \(\mathcal{C}_1\) to \(\mathcal{C}_2\) (see Fig. 5), i.e.,
\[
-\frac{1}{2\pi i} \oint_{\mathcal{C}_1} dz n_F(z) \frac{D_{\text{eff}}(-iz,k)}{z - \xi^{(m)}_{l,n}(k)}
\]
\[
= -\frac{1}{2\pi i} \int_{-\infty}^{\infty} dx n_F(x) \left[ \frac{1}{-i\gamma x + |k|^2 + ma x^+ - \xi^{(m)}_{l,n}(k)} \right.
\]
\[
- \frac{1}{i\gamma x + |k|^2 + ma x - \xi^{(m)}_{l,n}(k)} \left. \right] \tag{B11}
\]

where \(x^\pm = x \pm i\eta\) and \(\eta \to 0^+\). At this point, we employ the Dirac identity
\[
\frac{1}{x \pm i\eta} = \mp i\pi \delta(x) + \mathcal{P} \left( \frac{1}{x} \right), \tag{B12}
\]

with \(\mathcal{P}\) standing for the Cauchy principal value in order to obtain the following
\[
-\frac{1}{2\pi i} \oint_{\mathcal{C}_1} dz n_F(z) \frac{D_{\text{eff}}(-iz,k)}{z - \xi^{(m)}_{l,n}(k)}
\]
\[
= \frac{\sqrt{|k|^2 + ma}}{\sqrt{|k|^2 + ma^2 + \gamma^2 \xi^{(m)}_{l,n}(k)^2}} n_F^{(m)}_{l,n}(k)
\]
\[
- \frac{2\sqrt{|k|^2 + ma}}{\pi} \int_{-\infty}^{\infty} dx n_F(x) \frac{x}{|k|^2 + ma^2 + \gamma^2 x^2} \frac{1}{x - \xi^{(m)}_{l,n}(k)}. \tag{B13}
\]

Finally after inserting the result in Eq. (B13) into Eq. (B10), the mean-field equation for the QDW order parameter at finite temperature can be simply expressed as
\[
b(T) = \frac{3\lambda^2}{16} \left[ \sum_{l,m=1}^{2N} \sum_{n=1}^{N} \int \left\{ \frac{|k|^2 + ma}{|k|^2 + ma^2 + \gamma^2 \xi^{(m)}_{l,n}(k)^2} \right. \right.
\]
\[
\times n_F^{(m)}_{l,n}(k) - \frac{\gamma}{\pi} \mathcal{P} \int_{-\infty}^{\infty} dx \frac{x n_F(x)}{|k|^2 + ma^2 + \gamma^2 x^2} \frac{1}{x - \xi^{(m)}_{l,n}(k)} \right\} \Delta^{(m)}_{l,n}(k) \right. \tag{B14}
\]
\[
\left. \left. \frac{dk}{(2\pi)^2}. \right. \right\]

In the limit of \(T \to 0\), the Fermi-Dirac distribution function \(n_F(x)\) becomes the step function \(\theta(-x)\). As a result, the integral in Eq. (B14) involving the Cauchy principal value evaluates to
\[
\lim_{T \to 0} \mathcal{P} \int_{-\infty}^{\infty} dx \frac{x n_F(x)}{|k|^2 + ma^2 + \gamma^2 x^2} \frac{1}{x - \xi^{(m)}_{l,n}(k)}
\]
\[
= \frac{\pi}{2\gamma} \frac{|k|^2 + ma}{\sqrt{|k|^2 + ma^2 + \gamma^2 \xi^{(m)}_{l,n}(k)^2}} \ln \left[ \frac{\gamma \xi^{(m)}_{l,n}(k)}{|k|^2 + ma} \right], \tag{B15}
\]

where now \(ma = ma(T = 0)\) is the zero-temperature bosonic mass. Hence in this limit the mean-field equation

\[
\int_{-\infty}^{\infty} dx \frac{x n_F(x)}{|k|^2 + ma^2 + \gamma^2 x^2} \frac{1}{x - \xi^{(m)}_{l,n}(k)}
\]

\[
= \frac{\pi}{2\gamma} \frac{|k|^2 + ma}{\sqrt{|k|^2 + ma^2 + \gamma^2 \xi^{(m)}_{l,n}(k)^2}} \ln \left[ \frac{\gamma \xi^{(m)}_{l,n}(k)}{|k|^2 + ma} \right], \tag{B15}
\]

which was the statement of the mean-field equation.
for the QDW order parameter is given by
\[
b(T = 0) = -\frac{3\lambda^2}{32} \sum_{l,m=1}^2 \sum_{n=1}^N \left\{ \frac{|k|^2 + m_a}{(|k|^2 + m_a)^2 + \gamma^2 |\xi^{(m)}_{l,n}(k)|^2} \right\} \times \text{sgn}[\xi^{(m)}_{l,n}(k)] + \frac{2}{\pi} \frac{\gamma \xi^{(m)}_{l,n}(k)}{|k|^2 + m_a^2 + \gamma^2 |\xi^{(m)}_{l,n}(k)|^2} \times \log \left( \frac{|\xi^{(m)}_{l,n}(k)|}{|k|^2 + m_a} \right) \Delta^{(m)}_{l,n}(k) \frac{dk}{2\pi^2},
\]
where we have used the identity \( \theta(-x) = \frac{1}{2} [1 - \text{sgn}(x)] \) in order to simplify the above equation.

2. \( \Theta_{II} \)-loop-current (LC) order parameter

The mean-field equation for the loop-current order parameter can be simplified following the same procedure outlined above. First of all, we transform the Matsubara sum in Eq. (B13) into an integral over the complex plane. This leads to
\[
R_{II}(T) = V_{pd} \sum_{l,m=1}^2 \int \left\{ -\frac{1}{2\pi i} \oint_{C_l} dz n_F(z) \left[ \frac{1}{h_1^{(m)}(z,k)} \partial h_1^{(m)}(z,k) \right] \frac{\partial R_{II}}{\partial h_1^{(m)}(z,k)} \right\} \frac{dk}{2\pi^2}.
\]

Then we expand the terms between brackets in the above equation in a series of partial fractions, i.e.,
\[
\frac{1}{h_1^{(m)}(z,k)} \frac{\partial h_1^{(m)}(z,k)}{\partial R_{II}} + \frac{1}{h_1^{(m)}(z,k)} \frac{\partial h_1^{(m)}(z,k)}{\partial R_{II}} = \sum_{n=1}^N \Xi^{(m)}_{l,n}(k),
\]
with \( n_F(z) \) being the Fermi-Dirac distribution function in this case.

Having in mind the result in Eq. (B18), we evaluate the complex integral in Eq. (B17) as
\[
-\frac{1}{2\pi i} \sum_{n=1}^N \Xi^{(m)}_{l,n}(k) \oint_{C_l} dz n_F(z) \frac{dk}{(2\pi)^2} = \sum_{n=1}^N \Xi^{(m)}_{l,n}(k) n_F[\xi^{(m)}_{l,n}(k)].
\]

Lastly the mean-field equation for the loop-current order parameter at finite temperature is obtained by inserting Eq. (B21) into Eq. (B17). Therefore this yields
\[
R_{II}(T) = \frac{V_{pd}}{2} \sum_{l,m=1}^2 \sum_{n=1}^N \int \Xi^{(m)}_{l,n}(k) n_F[\xi^{(m)}_{l,n}(k)] \frac{dk}{(2\pi)^2},
\]
with \( n_F(z) \) being the Fermi-Dirac distribution function in this case.

Appendix C: Form of the functions \( D^{(m)}_l(i\varepsilon_n, k) \)

In order to compute the determinant \( \det[G^{-1}(i\varepsilon_n, k)] \) that appears in the main text of this work, we need to make use of the Eqs. (C4) and (C5). Then as we are interested in the interplay between loop-current and quadrupole density wave orders, we also neglect the superconducting sector of the matrix \( \hat{u}_r \). As a result, this determinant evaluates to
\[
\det[G^{-1}(i\varepsilon_n, k)] = 2 \prod_{l=1}^2 \prod_{m=1}^2 D^{(m)}_l(i\varepsilon_n, k),
\]
where \( D^{(m)}_l(i\varepsilon_n, k) \) are functions whose form will be determined in this appendix.

Before proceeding with that, let us define the following coefficients
\[
c_1(k_x) = \sqrt{2} \left( -t_{pd} + i \frac{R_{II}}{4} k_x \right),
\]
\[
c_1(k_y) = \sqrt{2} \left( -t_{pd} + i \frac{R_{II}}{4} k_y \right),
\]
\[
c_2(k_x) = \sqrt{2} \left( -t_{pd} k_x - i R_{II} \right),
\]
\[
c_2(k_y) = \sqrt{2} \left( -t_{pd} k_y - i R_{II} \right),
\]
which are written as a function of Cu-O hopping \( t_{pd} \), the loop-current order parameter \( R_{II} \), and the the momentum distance \( k \) to the hot spots. The purpose of defining

\[
\Xi^{(m)}_{l,n}(k) = \frac{\partial h_1^{(m)}(z,k)}{\partial R_{II}} \bigg|_{z = \xi^{(m)}_{l,n}(k)}, \quad 1 \leq n \leq N/2,
\]
\[
\Xi^{(m)}_{l,n}(k) = \frac{\partial h_1^{(m)}(z,k)}{\partial z} \bigg|_{z = \xi^{(m)}_{l,n}(k)}, \quad N/2 + 1 \leq n \leq N.
\]

In the limit of zero temperature, this equation becomes
\[
R_{II}(T = 0) = \frac{V_{pd}}{2} \sum_{l,m=1}^2 \sum_{n=1}^N \int \Xi^{(m)}_{l,n}(k) \theta[-\xi^{(m)}_{l,n}(k)] \frac{dk}{(2\pi)^2},
\]
which appears in the main text of this work, we need to make use of the Eqs. (C1) and (C2). Then as we are interested in the interplay between loop-current and quadrupole density wave orders, we also neglect the superconducting sector of the matrix \( \hat{u}_r \). As a result, this determinant evaluates to
\[
\det[G^{-1}(i\varepsilon_n, k)] = 2 \prod_{l=1}^2 \prod_{m=1}^2 D^{(m)}_l(i\varepsilon_n, k),
\]
where \( D^{(m)}_l(i\varepsilon_n, k) \) are functions whose form will be determined in this appendix.

Before proceeding with that, let us define the following coefficients
\[
c_1(k_x) = \sqrt{2} \left( -t_{pd} + i \frac{R_{II}}{4} k_x \right),
\]
\[
c_1(k_y) = \sqrt{2} \left( -t_{pd} + i \frac{R_{II}}{4} k_y \right),
\]
\[
c_2(k_x) = \sqrt{2} \left( -t_{pd} k_x - i R_{II} \right),
\]
\[
c_2(k_y) = \sqrt{2} \left( -t_{pd} k_y - i R_{II} \right),
\]
which are written as a function of Cu-O hopping \( t_{pd} \), the loop-current order parameter \( R_{II} \), and the the momentum distance \( k \) to the hot spots. The purpose of defining
these four coefficients is of course to write down the functions $D_i^{(m)}(i\varepsilon_n, \mathbf{k})$ in a compact form.

We then construct the set of basis functions shown in Table II from the hot-spot parameter $\delta = (K_+ - K_-)/2$

and the $c_i(k_x, k_y)$ ($i = 1, 2$). As a consequence, we can write explicitly the $D_i^{(m)}(i\varepsilon_n, \mathbf{k})$ as

$$D_1^{(1)}(i\varepsilon_n, \mathbf{k}) = \{(i\varepsilon_n + \xi_\delta)[(i\varepsilon_n + \xi_p)^2 - t_{pp}^2(a_1(k) + b_1(k))] - P_1^{(0)}(k)(i\varepsilon_n + \xi_p) - t_{pp}P_1^{(1)}(k)\}$$

$\times \{(i\varepsilon_n + \xi_\delta)[(i\varepsilon_n + \xi_p)^2 - t_{pp}^2(a_2(k) + b_2(k))] - P_2^{(0)}(k)(i\varepsilon_n + \xi_p) - t_{pp}P_2^{(1)}(k)\}$

$- \xi^2[(i\varepsilon_n + \xi_p)^2 - t_{pp}^2(a_1(k) + b_1(k))][(i\varepsilon_n + \xi_p)^2 - t_{pp}^2(a_2(k) + b_2(k))]^2,$

(C6)

$D_1^{(2)}(i\varepsilon_n, \mathbf{k}) = \{(i\varepsilon_n + \xi_\delta)[(i\varepsilon_n + \xi_p)^2 - t_{pp}^2(a_1(k) - b_1(k))] - M_1^{(0)}(k)(i\varepsilon_n + \xi_p) - t_{pp}M_1^{(1)}(k)\}$

$\times \{(i\varepsilon_n + \xi_\delta)[(i\varepsilon_n + \xi_p)^2 - t_{pp}^2(a_2(k) - b_2(k))] - M_2^{(0)}(k)(i\varepsilon_n + \xi_p) - t_{pp}M_2^{(1)}(k)\}$

$- \xi^2[(i\varepsilon_n + \xi_p)^2 - t_{pp}^2(a_1(k) - b_1(k))][(i\varepsilon_n + \xi_p)^2 - t_{pp}^2(a_2(k) - b_2(k))]^2,$

(C7)

$D_2^{(1)}(i\varepsilon_n, \mathbf{k}) = \{(i\varepsilon_n + \xi_\delta)[(i\varepsilon_n + \xi_p)^2 - t_{pp}^2(a_1(k) + b_3(k))] - P_3^{(0)}(k)(i\varepsilon_n + \xi_p) - t_{pp}P_3^{(1)}(k)\}$

$\times \{(i\varepsilon_n + \xi_\delta)[(i\varepsilon_n + \xi_p)^2 - t_{pp}^2(a_4(k) + b_4(k))] - P_4^{(0)}(k)(i\varepsilon_n + \xi_p) - t_{pp}P_4^{(1)}(k)\}$

$- \xi^2[(i\varepsilon_n + \xi_p)^2 - t_{pp}^2(a_3(k) + b_3(k))][(i\varepsilon_n + \xi_p)^2 - t_{pp}^2(a_4(k) + b_4(k))]^2,$

(C8)

$D_2^{(2)}(i\varepsilon_n, \mathbf{k}) = \{(i\varepsilon_n + \xi_\delta)[(i\varepsilon_n + \xi_p)^2 - t_{pp}^2(a_1(k) + b_3(k))] - M_3^{(0)}(k)(i\varepsilon_n + \xi_p) - t_{pp}M_3^{(1)}(k)\}$

$\times \{(i\varepsilon_n + \xi_\delta)[(i\varepsilon_n + \xi_p)^2 - t_{pp}^2(a_4(k) - b_4(k))] - M_4^{(0)}(k)(i\varepsilon_n + \xi_p) - t_{pp}M_4^{(1)}(k)\}$

$- \xi^2[(i\varepsilon_n + \xi_p)^2 - t_{pp}^2(a_3(k) - b_3(k))][(i\varepsilon_n + \xi_p)^2 - t_{pp}^2(a_4(k) - b_4(k))]^2,$

(C9)

where we have used a second set of basis functions defined in Table II as well as the new functions

$$P_i^{(0)}(k) = a_{ix}(k_x) + a_{iy}(k_y) + b_{ix}(k_x) + b_{iy}(k_y),$$

(C10)

$$P_i^{(1)}(k) = [\bar{a}_i(k) + \bar{b}_i(k)][a_{ixy}(k) + b_{ixy}(k)],$$

(C11)

$$M_i^{(0)}(k) = a_{ix}(k_x) + a_{iy}(k_y) - b_{ix}(k_x) - b_{iy}(k_y),$$

(C12)

$$M_i^{(1)}(k) = [\bar{a}_i(k) - \bar{b}_i(k)][a_{ixy}(k) - b_{ixy}(k)],$$

(C13)

which depend on the basis functions of both tables.

In the main text of this paper, we have to perform the analytic continuation $\varepsilon_n \rightarrow -i\varepsilon$ for $D_i^{(m)}(i\varepsilon_n, \mathbf{k})$. By observing the results in Eqs. (C6)-(C9), we conclude that each $D_i^{(m)}(i\varepsilon_n, \mathbf{k})$ could be written as a product of a function times its complex conjugate. Therefore we can make the analytic continuation as follows

$$D_i^{(m)}(z, \mathbf{k}) = h_i^{(m)}(z, \mathbf{k})\overline{h}_i^{(m)}(z, \mathbf{k}),$$

(C14)

where the functions on the right-hand side of the above equality are given by

$$h_1^{(1)}(z, \mathbf{k}) = \{(z - \xi_\delta)[(z - \xi_p)^2 - t_{pp}^2(a_1(k) + b_1(k))] - P_1^{(0)}(k)(z - \xi_p) + t_{pp}P_1^{(1)}(k)\}$$

$\times \{(z - \xi_\delta)[(z - \xi_p)^2 - t_{pp}^2(a_2(k) + b_2(k))] - P_2^{(0)}(k)(z - \xi_p) + t_{pp}P_2^{(1)}(k)\}$

$- \xi^2[(z - \xi_p)^2 - t_{pp}^2(a_1(k) + b_1(k))][(z - \xi_p)^2 - t_{pp}^2(a_2(k) + b_2(k))]\},

(C15)

$$\overline{h}_1^{(1)}(z, \mathbf{k}) = \{(z + \xi_\delta)[(z + \xi_p)^2 - t_{pp}^2(a_1(k) + b_1(k))] - P_1^{(0)}(k)(z + \xi_p) - t_{pp}P_1^{(1)}(k)\}$$

$\times \{(z + \xi_\delta)[(z + \xi_p)^2 - t_{pp}^2(a_2(k) + b_2(k))] - P_2^{(0)}(k)(z + \xi_p) - t_{pp}P_2^{(1)}(k)\}$

$- \xi^2[(z + \xi_p)^2 - t_{pp}^2(a_1(k) + b_1(k))][(z + \xi_p)^2 - t_{pp}^2(a_2(k) + b_2(k))]\},

(C16)

$$h_1^{(2)}(z, \mathbf{k}) = \{(z - \xi_\delta)[(z - \xi_p)^2 - t_{pp}^2(a_1(k) - b_1(k))] - M_1^{(0)}(k)(z - \xi_p) + t_{pp}M_1^{(1)}(k)\}$$

$\times \{(z - \xi_\delta)[(z - \xi_p)^2 - t_{pp}^2(a_2(k) - b_2(k))] - M_2^{(0)}(k)(z - \xi_p) + t_{pp}M_2^{(1)}(k)\}$

$- \xi^2[(z - \xi_p)^2 - t_{pp}^2(a_1(k) - b_1(k))][(z - \xi_p)^2 - t_{pp}^2(a_2(k) - b_2(k))]\},

(C17)
TABLE I: First set of basis functions used to represent the free energy of the three-band model. Here these functions are written in terms of the hot-spot parameter $\delta = (K_+ - K_-)/2$ and the coefficients $c_i(k_x)$ and $c_i(k_y)$ ($i = 1, 2$).

<table>
<thead>
<tr>
<th>Basis function</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a_{1x}(k_x)$</td>
<td>$c_1(k_x) + c_2(k_x)$</td>
</tr>
<tr>
<td>$a_{2x}(k_x)$</td>
<td>$c_1(k_x) + c_2(k_x)$</td>
</tr>
<tr>
<td>$a_{3x}(k_x)$</td>
<td>$c_1(k_x) + c_2(k_x)$</td>
</tr>
<tr>
<td>$a_{4x}(k_x)$</td>
<td>$c_1(k_x) + c_2(k_x)$</td>
</tr>
<tr>
<td>$b_{1x}(k_x)$</td>
<td>$\delta c_1(k_x) + c_2(k_x)$</td>
</tr>
<tr>
<td>$b_{2x}(k_x)$</td>
<td>$\delta c_1(k_x) + c_2(k_x)$</td>
</tr>
<tr>
<td>$b_{3x}(k_x)$</td>
<td>$\delta c_1(k_x) + c_2(k_x)$</td>
</tr>
<tr>
<td>$b_{4x}(k_x)$</td>
<td>$\delta c_1(k_x) + c_2(k_x)$</td>
</tr>
</tbody>
</table>

TABLE II: Second set of basis functions needed to evaluate the free energy of the present three-band model. In our notation, the indices $l$ and $\tilde{l}$ refer respectively to the functions $a_l(k)$ and $b_l(k)$ and $\tilde{a}_l(k)$ and $\tilde{b}_l(k)$.

<table>
<thead>
<tr>
<th>$l$</th>
<th>$a_l(k)$</th>
<th>$b_l(k)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$(k_x + k_y)^4 + \sin^2(\delta k_y - k_x + 2 \cot \delta)^2$</td>
<td>$2 \sin(\delta k_y + \cot \delta - k_x - \cot \delta)^2$</td>
</tr>
<tr>
<td>2</td>
<td>$(k_x + k_y)^4 + \sin^2(\delta k_y - k_x + 2 \cot \delta)^2$</td>
<td>$2 \sin(\delta k_y - \cot \delta)^2$</td>
</tr>
<tr>
<td>3</td>
<td>$(k_x - k_y)^4 + \sin^2(\delta k_y - k_x + 2 \cot \delta)^2$</td>
<td>$2 \sin(\delta k_y + \cot \delta)^2$</td>
</tr>
<tr>
<td>4</td>
<td>$(k_x - k_y)^4 + \sin^2(\delta k_y - k_x + 2 \cot \delta)^2$</td>
<td>$2 \sin(\delta k_y - \cot \delta)^2$</td>
</tr>
</tbody>
</table>

$\mathbf{\tilde{T}}_1^{(2)}(z, k) = \{(1 + \xi_d)[(z + \xi_p)^2 - t_{pp}^2(a_1(k) - b_1(k))] - M_1^{(0)}(k)(z + \xi_p) - t_{pp}M_1^{(1)}(k)\}$

$\mathbf{\tilde{h}}_2^{(1)}(z, k) = \{(1 + \xi_d)[(z - \xi_p)^2 - t_{pp}^2(a_3(k) + b_3(k))] - P_3^{(0)}(k)(z - \xi_p) + t_{pp}P_3^{(1)}(k)\}$

$\mathbf{\tilde{h}}_2^{(2)}(z, k) = \{(1 + \xi_d)[(z + \xi_p)^2 - t_{pp}^2(a_3(k) + b_3(k))] - P_3^{(0)}(k)(z + \xi_p) - t_{pp}P_3^{(1)}(k)\}$
\[ h^{(2)}_2(z, k) = \{(z - \xi_d)(z - \xi_p)^2 - t_{pp}^2(a_3(k) - b_3(k)) - M_{3}^{(0)}(k)(z - \xi_p) + t_{pp}M_{4}^{(1)}(k)\} \times \{(z - \xi_d)(z + \xi_p)^2 - t_{pp}^2(a_4(k) - b_4(k)) - M_{4}^{(0)}(k)(z - \xi_p) + t_{pp}M_{4}^{(1)}(k)\} - b^2[(z - \xi_p)^2 - t_{pp}^2(a_3(k) - b_3(k))][(z - \xi_p)^2 - t_{pp}^2(a_4(k) - b_4(k))], \]

\[ \overline{h}^{(2)}_2(z, k) = \{(z + \xi_d)(z + \xi_p)^2 - t_{pp}^2(a_3(k) - b_3(k)) - M_{3}^{(0)}(k)(z + \xi_p) - t_{pp}M_{4}^{(1)}(k)\} \times \{(z + \xi_d)(z + \xi_p)^2 - t_{pp}^2(a_4(k) - b_4(k)) - M_{4}^{(0)}(k)(z + \xi_p) - t_{pp}M_{4}^{(1)}(k)\} - b^2[(z + \xi_p)^2 - t_{pp}^2(a_3(k) - b_3(k))][(z + \xi_p)^2 - t_{pp}^2(a_4(k) - b_4(k))]. \]

According to the approach developed in the Appendix B for solving the LC and QDW mean-field equations, we need to determine first the roots of \( h^{(m)}_i(z, k) \) and \( \overline{h}^{(m)}_i(z, k) \) which are denoted here as \( \xi^{(m)}_i(k) \) \((n = 1, \ldots, N)\). As \( h^{(m)}_i(z, k) \) and \( \overline{h}^{(m)}_i(z, k) \) are both sixth-order polynomials in the variable \( z \), their roots will be determined by means of numerical methods.

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