Superconductivity model for a spin-vortex checkerboard

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(Dated: April 12, 2017)

We introduce a microscopic model aimed at describing superconductivity that can possibly exist in the background of a magnetic texture called “spin-vortex checkerboard”. This texture was proposed previously as a possible alternative to stripes to interpret the experimental phenomenon of spin and charge modulations in 1/8-doped lanthanum cuprates. The model involves two kinds of interacting fermionic excitations residing in spin-rich and spin-poor regions of the modulated structure. It is a generalization of another model developed earlier for the so-called “grid checkerboard”. We present the mean-field solution of the model, from which we obtain model’s predictions for the temperature evolution of the superconducting gap, compare these predictions with available experiments on high-T_c cuprate superconductors and find a good overall agreement.

I. INTRODUCTION

Interplay between superconductivity and the onset of electronic spin and charge modulations in cuprate superconductors remains one of the intriguing and unresolved issues in the field of high-temperature superconductivity. Manifestations of electronic modulations are reported in a broad doping range for several families of cuprates — most noticeably around the doping level of 1/8 [1,2]. For 1/8-doped lanthanum cuprates, the modulated structure is widely believed to exhibit one-dimensional pattern often referred to as “stripes” [1,2]. Yet the principal aspects of the same experimental evidence are also consistent with the possibility of two-dimensional modulations called “checkerboards” [3,4].

The experiment-based arguments discriminating between stripes and checkerboards in 1/8-doped lanthanum cuprates are at present rather indirect. At the same time, the issue cannot be resolved on purely theoretical grounds, because it requires accuracy of the calculations of the ground state energy not achievable by first-principles theories. The checkerboard was, initially, less popular as an interpretation of experiments, in part, because of the perception that it inhibits the electronic transport in all lattice directions and hence prevents the onset of superconductivity as well. The latter point, however, was challenged by a model of superconductivity in the background of a checkerboard modulation [20]. That model was based on a particular version of a checkerboard called “grid”. Later, the grid checkerboard was shown to be inconsistent with the results of spin-polarized neutron scattering experiment of Ref. [21]. This experiment, however, did not rule out another version of a checkerboard representing a two-dimensional arrangement of spin vortices [12], shown in Fig. 1(a). Somewhat similar noncollinear spin textures were also considered in Refs. [22,27]. The general properties of spin-vortex checkerboard were analyzed in Refs. [11,15]. So far, however, the superconductivity model developed for grid [20] has not been generalized to the spin-vortex checkerboard. In the present article, we introduce such a generalized model, find its mean-field solution and compare it with experiments.

It should be remarked here that, experimentally, the onset of static spin modulations in 1/8-doped lanthanum cuprates — spin vortices or stripes — largely suppresses three-dimensional superconductivity but appears to coexist with two-dimensional superconductivity [22,20]. For both spin vortices and stripes, the suppression of the three dimensional superconductivity can be explained by the displacement of the modulation patterns in the adjacent CuO_2 planes. Beyond 1/8-doped lanthanum cuprates, the generic situation possibly involves the fluctuating counterpart of the static spin-vortex texture used in the present work. These fluctuations are likely caused by system’s proximity to the threshold of electronic phase separation [32]. They are expected to couple spin, charge and lattice degrees of freedom — see e.g. [33]. In this respect, the spin-vortex checkerboard just suggests us the coupling connectivity between low-energy fermionic states. As it stands, the model illustrates the potential of the general two-component scenario [21,23] in the limit of initially localized components for describing the superconductivity in cuprates.

II. SUPERCONDUCTIVITY MODEL

The model to be considered has two different kinds of fermionic states physically located in magnetic and non-magnetic parts of the underlying spin texture. The general reasoning for constructing the model is the same as in Ref [20]. Namely, the entire texture is divided into plaquettes having different kind of spin background, and then, for each plaquet, only one-particle fermionic states closest to the chemical potential are retained for the model description. Given that plaquettes are rather small, it can be estimated [20] that the spacing of one-particle energies within each plaquet is of the order of 40 meV, which implies that, for temperatures much smaller than 400K, it is appropriate to retain only the levels closest to the chemical potential.

We expect that the lowest one-particle states in spin-polarized plaquettes are non-spin-degenerate, and hence we include exactly one state per plaquet. As can be seen in Fig. 1(a), the texture has four kinds of spin-polarized pla-
FIG. 1. (color online). (a) Spin-vortex checkerboard. Each arrow represents average spin polarization on a square lattice formed by Cu atoms within CuO$_2$ planes. (b) Partition of the spin-vortex checkerboard into plaquettes associated with a-, b-, and c-states. Thick lines indicate the borders of unit cells of the modulated structure. Each unit cell (also shown in Fig. 2) includes two a-states, two c-states and four b-states.

FIG. 2. (color online). Unit cell from Fig. 1(b) with labels $\alpha$, $\eta$ and $\zeta$ as introduced in the text. Colors represent different quasiparticle states as follows: b-states with $\alpha = 1$ (pink), $\alpha = 2$ (yellow), $\alpha = 3$ (green), and $\alpha = 4$ (gray); even a-state $[\eta = 1]$ (orange), odd a-state $[\eta = -1]$ (brown); even c-state $[\zeta = 1]$ (blue), odd c-state $[\zeta = -1]$ (cyan).

We refer to two of the resulting states as “a-states” and to the remaining two as “c-states”. Two different kinds a-states are distinguished by index $\eta = \pm 1$, and c-states — by index $\zeta = \pm 1$. Two a-states or two c-states with different values of $\eta$ or $\zeta$ respectively are expected to have orthogonal spin wave functions that can be obtained from each other by spin inversion. The lowest-energy states of spin-unpolarized plaquets around the cores of spin vortices are expected to be spin-degenerate. We, therefore, place two fermionic states on each such plaquet with spins “up” or “down” along any chosen direction. We call them “b-states”. Since the spin texture contains four nonequivalent kinds of spin-vortex cores, we distinguish the corresponding b-states by index $\alpha = 1, 2, 3, 4$ and by spin index $\uparrow$ or $\downarrow$ — see Fig. 2.

We now construct the low-energy Hamiltonian following the same reasoning as in Ref. We assume that the direct one-fermion hopping between different plaquets is suppressed due to the differences of spin textures and due to the expected texture fluctuations. At the same time, we assume that fast fluctuations of the texture around the average pattern shown in Fig. 1(a) induce pair transitions that do not change the center-of-mass position of the two fermions involved. This leaves us only with terms representing on-site energies $\epsilon_a$, $\epsilon_b$ and $\epsilon_c$ (with $\epsilon_a = \epsilon_c$) and with the following two-kinds of effective interaction terms, namely: two a-states or two c-states adjacent to a given spin vortex core making transitions to the two b-states inside the core or vice versa.
The resulting Hamiltonian is:

\[
H = \sum_{i,\eta} \epsilon_{i\eta} a_{i\eta}^\dagger a_{i\eta} + \sum_{i,\eta} \epsilon_{i\eta} c_{i\eta}^\dagger c_{i\eta} + \sum_{i,\eta} \epsilon_{i\eta} b_{i\eta}^\dagger b_{i\eta}
\]

\[
+ g \sum_{i,\eta} \left[ \left( b_{i\eta}^\dagger b_{i\eta} + 2 \right) a_{i\eta}^\dagger a_{i\eta} + h.c \right] + \left( b_{i\eta}^\dagger b_{i\eta} + 2 \right) c_{i\eta}^\dagger c_{i\eta} + h.c \right],
\]

where \( g \) is the interaction constant, \( \epsilon_a \), \( \epsilon_b \) and \( \epsilon_c \) are on-site energies defined with respect to the chemical potential \( \mu \), which we set equal to zero, index \( i \) labels unit cells depicted in Fig. 2, and indices \( \eta \), \( \alpha \), and \( \zeta \) label the plaquettes within the unit cell as illustrated in Fig. 2. Following Ref. 20, whenever the specific value of subscripts \( \eta \) or \( \zeta \) is fixed, as is the case in the interaction term of Hamiltonian (1), we use subscript “e” for \( \eta = 1 \) or “o” for \( \eta = -1 \) referring to the corresponding plaquet as “even” and subscript “o” for \( \eta = -1 \) or “e” referring to the corresponding plaquet as “odd”. Double-subscripts notations such as \( a_{je[i,\alpha]} \) imply that \( a \)-states labeled as \( \{je\} \) must be adjacent to the \( b \)-states labeled as \( \{i,\alpha\} \).

If all terms containing \( c \)-states are removed from Hamiltonian (1), the result would be exactly equivalent to the Hamiltonian considered in Ref. 20. Since \( c \)-states do not directly couple to \( a \)-states, and since \( c \)-states have the same connectivity with the \( b \)-states as \( a \)-states (but shifted), the mean-field solutions of the two models are very similar with the only difference being that \( b \)-states now experience mean field from both \( a \)-states and \( c \)-states, which, in turn, makes that mean field two times larger, and, as a result, the value of the superconducting transition temperature becomes modified.

Since the entire derivation has nearly the same structure and logic as that of Ref. 20 below we only include the formal structure of the derivation and the results, leaving the justification mostly to Ref. 20.

### III. BOGOLIUBOV TRANSFORMATIONS

In the model considered, each of the fermionic states couples to relatively few other states, which makes a mean-field solution only very approximate. We nevertheless proceed with finding a mean-field solution, assuming that gives at least the right qualitative picture of model’s behavior. The first step of this solution is to introduce the Bogoliubov transformation for \( b \)-states within the same plaquette:

\[
b_{i\alpha}^\dagger = s B_{i\alpha} + w e^{-i\phi_\alpha} B_{i\alpha}^\dagger,
\]

\[
b_{i\alpha} = s B_{i\alpha}^\dagger - w e^{-i\phi_\alpha} B_{i\alpha}^\dagger,
\]

where \( s \) and \( w \) are positive real numbers satisfying a constraint arising from canonical fermionic anticommutation relations

\[
s^2 + w^2 = 1,
\]

and \( \phi_\alpha \) are the transformation phases, which are to be determined later by minimizing system’s energy.

Substituting Bogoliubov transformation for \( b \)-states (2) in (1) and keeping only the thermal averages of terms that do not change the occupations of \( B \)-states, we obtain partially averaged Hamiltonian,

\[
H_a = 8 \epsilon_b N \left[ s^2 n_B + w^2 (1 - n_B) \right]
\]

\[
+ \epsilon_a \sum_{i,\eta} a_{i\eta}^\dagger a_{i\eta} + \epsilon_c \sum_{i,\eta} c_{i\eta}^\dagger c_{i\eta}
\]

\[
+ gsw \left( 1 - 2n_B \right) \sum_{\alpha} \left[ \left( e^{-i\phi_\alpha} \sum_{ij} a_{ij}^\dagger c_{ij} + h.c \right) + \left( e^{-i\phi_\alpha} \sum_{ij} c_{ij}^\dagger a_{ij} + h.c \right) \right],
\]

where \( \epsilon_B \) is the energy of \( B \)-quasiparticles and

\[
n_B = \frac{1}{e^{\frac{\epsilon_B}{T}} + 1},
\]

is their occupation number.

As explained in Ref. 20, in order to assure proper fermionic anticommutation relations for the Bogoliubov counterparts of \( a \)- and \( c \)-states, the Bogoliubov transformation for these states should be made in the quasimomentum space. Therefore, we need to rewrite the Hamiltonian in terms of the real-space Fourier transforms for \( a \) and \( c \) operators. To do the Fourier transforms we first shift the \( c \)-states and \( a \)-states at \( r_e \) and \( r_o \) by vector \( \mathbf{R}_a \) originated from an even \( a \)-state. Now, we define the position of each unit cell by the position \( r_e \) of an even \( a \)-state within this cell. Therefore, \( a \)-states are located at a set of positions \( \{r_e\} \), odd \( a \)-states at \( \{r_e + \mathbf{R}_1\} \), even \( c \)-states at \( \{r_e + \mathbf{L}\} \), and odd \( c \)-states at \( \{r_e + \mathbf{L} + \mathbf{R}_1\} \). Finally we rewrite the Hamiltonian (1) as

\[
H_a = \sum_{r_e} \sum_{\alpha,\beta} \left[ \left( s^2 n_B + w^2 (1 - n_B) \right) \right]
\]

\[
+ \epsilon_a \sum_{r_e,\eta} a_{r_e \eta}^\dagger a_{r_e \eta} + \epsilon_c \sum_{r_e,\eta} c_{r_e \eta}^\dagger c_{r_e \eta}
\]

\[
+ gsw \left( 1 - 2n_B \right) \sum_{\alpha} \left[ \left( e^{-i\phi_\alpha} \sum_{ij} a_{r_e + \mathbf{L},ij}^\dagger c_{r_e + \mathbf{L},ij} + h.c \right) + \left( e^{-i\phi_\alpha} \sum_{ij} c_{r_e + \mathbf{L},ij}^\dagger a_{r_e + \mathbf{L},ij} + h.c \right) \right],
\]

where \( \epsilon_B \) is the energy of \( B \)-quasiparticles and

\[
n_B = \frac{1}{e^{\frac{\epsilon_B}{T}} + 1},
\]

is their occupation number.
We now explicitly write separate Fourier transforms for even and odd \( a\) and \( c\) states as follows:

\[
\begin{align*}
a_e(k) &= \sqrt{\frac{1}{N}} \sum_\mathbf{r} a(\mathbf{r}_e) e^{-ik\mathbf{r}_e}, \\
a_o(k) &= \sqrt{\frac{1}{N}} \sum_\mathbf{r} a(\mathbf{r}_e + \mathbf{R}_1) e^{-ik(\mathbf{r}_e + \mathbf{R}_1)}, \\
c_e(k) &= \sqrt{\frac{1}{N}} \sum_\mathbf{r} c(\mathbf{r}_e + \mathbf{L}) e^{-ik(\mathbf{r}_e + \mathbf{L})}, \\
c_o(k) &= \sqrt{\frac{1}{N}} \sum_\mathbf{r} c(\mathbf{r}_e + \mathbf{L} + \mathbf{R}_1) e^{-ik(\mathbf{r}_e + \mathbf{L} + \mathbf{R}_1)}. 
\end{align*}
\]

Since the superlattice periods for each of the above four kinds of states are the same, the sets of wave vectors \( \{k\} \) are also the same for all four transformations, even though the corresponding states are shifted with respect to each other in real space. Substituting these transformations to (8) we obtain

\[
H_a = 8\epsilon_b N \left[ s^2 n_B + w^2 (1 - n_B) \right] + \sum_\mathbf{r} \left\{ \epsilon_a a^\dagger(\mathbf{r}_e) a(\mathbf{r}_e) + \epsilon_c c^\dagger(\mathbf{r}_e + \mathbf{R}_1) a(\mathbf{r}_e + \mathbf{R}_1) \\
+ \epsilon_a c^\dagger(\mathbf{r}_e + \mathbf{L}) c(\mathbf{r}_e + \mathbf{L}) + \epsilon_c c^\dagger(\mathbf{r}_e + \mathbf{L} + \mathbf{R}_1) c(\mathbf{r}_e + \mathbf{L} + \mathbf{R}_1) \right\} \\
+ g sw (1 - 2n_B) \sum_\alpha \left[ (e^{-i\varphi_\alpha} \sum_\mathbf{r} a(\mathbf{r}_e) a(\mathbf{r}_e + \mathbf{R}_\alpha) + h.c) \\
+ \left( e^{-i\varphi_\alpha} \sum_\mathbf{r} c(\mathbf{r}_e + \mathbf{L}) c(\mathbf{r}_e + \mathbf{L} + \mathbf{R}_5 - \alpha) + h.c \right) \right], \quad (8)
\]

and,

\[
\tilde{V}(k) = \sum_\alpha \exp^{-i\varphi_\alpha - ikR_\alpha - 1} \\
= 2 \exp \left[ -i\frac{\varphi_1 + \varphi_3}{2} \right] \cos \left[ k\mathbf{R}_1 + \frac{\varphi_1 - \varphi_3}{2} \right] \\
+ 2 \exp \left[ -i\frac{\varphi_2 + \varphi_4}{2} \right] \cos \left[ k\mathbf{R}_2 + \frac{\varphi_2 - \varphi_4}{2} \right]. \quad (15)
\]

Bogoliubov transformations for \( a \) and \( c \) states can now be defined as,

\[
\begin{align*}
a_o(k) &= u(k) A_o(k) + v(k) e^{i\phi_o(A)} A^\dagger_o(-k), \\
c_o(k) &= p(k) C_o(k) + q(k) e^{i\phi_o(C)} C^\dagger_o(-k),
\end{align*}
\]

where \( u(k) \), \( v(k) \), and \( p(k) \) are the real-valued coefficients for \( a \) and \( c \) states respectively, subjected to a constraint arising from the fermionic canonical commutation relations for \( A \) and \( C \) operators:

\[
\begin{align*}
|u(k)|^2 + |v(k)|^2 &= 1, \\
|p(k)|^2 + |q(k)|^2 &= 1,
\end{align*}
\]

and \( \phi_o \) and \( \phi_c \) are complex phases — all to be found by the energy minimization.

We now complete the following steps: (i) we substitute the above canonical transformation for \( a \) and \( c \) states into Hamiltonian (13), then (ii) obtain the energy of the system by summing over the thermal averages of the diagonal terms — the result is given in Appendix (14), and then (iii) minimize the resulting energy with respect to the choice of phases \( \phi_o(k) \) and \( \phi_c(k) \), which, as explained in Appendix A gives conditions:

\[
\begin{align*}
\cos[\phi_V(k) + \phi_o(k)] &= 1, \\
\cos[\phi_V(k) + \phi_c(k)] &= 1,
\end{align*}
\]

were \( \phi_V(k) \) and \( \phi_0(k) \) are the complex phases of \( V(k) \) and \( V(k) \) respectively, which, in turn, depend on phases \( \{\varphi_\alpha\} \). (The actual values of phases \( \phi_o(k) \) and \( \phi_c(k) \) do not need to be obtained explicitly, because they will not enter any quantity further computed in this paper.) With the above conditions, the expression for the energy of the system becomes:

\[
\begin{align*}
E &= 8\epsilon_b N \left[ s^2 n_B + w^2 (1 - n_B) \right] \\
+ 2\epsilon_a \sum_\mathbf{k} \left\{ u^2(k)n_A(k) + v^2(k)[1 - n_A(k)] \right\} \\
+ 2\epsilon_c \sum_\mathbf{k} \left\{ p^2(k)n_C(k) + q^2(k)[1 - n_C(k)] \right\} \\
+ 2 g sw (1 - 2n_B) \sum_\mathbf{k} \left\{ u(k)v(k)[1 - n_A(k)]|V(k)| \\
+ p(k)q(k)[1 - n_C(k)]|\tilde{V}(k)| \right\}, \quad (24)
\end{align*}
\]
where,
\[ n_A(k) = \frac{1}{\exp(\epsilon_A(k)/T) + 1}, \quad \text{(25)} \]
\[ n_C(k) = \frac{1}{\exp(\epsilon_C(k)/T) + 1}, \quad \text{(26)} \]
are the Bogoliubov quasiparticle occupation number and \( \epsilon_A(k), \epsilon_C(k) \) are their energies, to be given in the next section.

**IV. RESULTS**

As argued in Ref.\(^\text{[20]}\), the chemical potential of the system is likely to coincide with either \( \epsilon_b \) or \( \epsilon_a \) (same as \( \epsilon_c \)), which, given our convention \( \mu = 0 \), means that either \( \epsilon_b = 0 \) or \( \epsilon_a = \epsilon_c = 0 \). Below, we treat these two cases separately, referring to them as “Case I” and “Case II” respectively, and also refer to the case of \( \epsilon_a = \epsilon_b = \epsilon_c = 0 \) as the “critical case”.

The coefficients of the Bogoliubov transformations for both Cases I and II are obtained in Appendices\([B] and [C]\) respectively by minimizing the total energy \([24]\) at fixed quasiparticle occupation numbers. We then substitute those coefficients back to Eq.\([24]\) and obtain the energy of a Bogoliubov quasiparticle by taking derivative of the total energy \([24]\) with respect to the quasiparticle occupation numbers \( n_A(k), n_C(k) \) or \( n_B \).

**A. Case I: \( \epsilon_b = 0 \)**

In Case I, the above procedure gives the following quasiparticle energies:
\[ \epsilon_A(k) = \sqrt{\epsilon_a^2 + \frac{1}{4}g^2(1 - 2n_B)^2|V(k)|^2}, \quad \text{(27)} \]
\[ \epsilon_C(k) = \sqrt{\epsilon_c^2 + \frac{1}{4}g^2(1 - 2n_B)^2|\tilde{V}(k)|^2}, \quad \text{(28)} \]
\[ \epsilon_B = \frac{g^2}{16N(1 - 2n_B)} \sum_k \left[ \frac{(1 - 2n_A(k))}{\epsilon_A(k)}|V(k)|^2 \right. \]
\[ + \left. \frac{(1 - 2n_C(k))}{\epsilon_C(k)}|\tilde{V}(k)|^2 \right]. \quad \text{(29)} \]

The mean-field approach now requires finding a non-trivial solution for \( n_A(k), n_C(k), n_B, \epsilon_A(k), \epsilon_C(k) \), and \( \epsilon_B \) from Eqs.\([5, 25, 26, 27, 28, 29]\). In general, it can only be done numerically, but one can also obtain a closed analytical equation for the critical temperature \( T_c \) using the fact that, near the transition, the superconducting state is close to the normal states, which allows one to use the limits
\[ \epsilon_A(k) \to \epsilon_a, \quad \epsilon_C(k) \to \epsilon_c, \quad (1 - 2n_B) \to \frac{\epsilon_a}{2T_c}. \]

Detailed calculations can be found in Appendix B. This gives
\[ T_c = \frac{g^2}{8} \left( \frac{\exp(|\epsilon_a|/T_c) - 1}{\exp(|\epsilon_a|/T_c) + 1} \frac{1}{|\epsilon_a|} \right), \quad \text{(30)} \]
from which, the mean-field \( T_c \) can be obtained numerically.

As explained in Ref.\([20]\), the density of A- and C- states has a Van Hove singularity located at the value corresponding to \( |V(k)| = 2 \) and \( |\tilde{V}(k)| = 2 \). We identify this singularity with the superconducting gap, which we, therefore, give by formula
\[ \Delta = \sqrt{\epsilon_a^2 + g^2(1 - 2n_B)^2}, \quad \text{(31)} \]
As \( T \to T_c \), it approaches not to zero but to \( |\epsilon_a| \), which we associate with the pseudogap.

**B. Case II: \( \epsilon_a = \epsilon_c = 0 \)**

Following the same procedure as for Case I, we obtain:
\[ \epsilon_B = \sqrt{\epsilon_b^2 + \frac{g^2}{64}C^2}, \quad \text{(32)} \]
\[ \epsilon_A(k) = \frac{g^2(1 - 2n_B)\tilde{C}|V(k)|}{16\epsilon_b}, \quad \text{(33)} \]
\[ \epsilon_C(k) = \frac{g^2(1 - 2n_B)\tilde{C}|\tilde{V}(k)|}{16\epsilon_b}, \quad \text{(34)} \]
where
\[ \tilde{C} = C_a + C_c, \quad \text{(35)} \]
\[ C_a = \frac{1}{N} \sum_k (1 - 2n_A(k))|V(k)|, \quad \text{(36)} \]
\[ C_c = \frac{1}{N} \sum_k (1 - 2n_C(k))|\tilde{V}(k)|. \quad \text{(37)} \]

Detailed calculations can be found in Appendix C. The same approach as in Case I now gives the critical temperature
\[ T_c = \frac{g^2}{4|\epsilon_b|} \left( \frac{\exp(|\epsilon_b|/T_c) - 1}{\exp(|\epsilon_b|/T_c) + 1} \right), \quad \text{(38)} \]
The superconducting gap parameter
\[ \Delta = \frac{g^2(1 - 2n_B)\tilde{C}}{8\epsilon_B}, \tag{39} \]
associated with Van Hove singularity for A- and B- states located at \( |V(k)| = |\tilde{V}(k)| = 2 \).

C. Temperature evolution of the superconducting gap

In Fig. 3, we present numerically computed temperature dependencies of the superconducting gaps for Cases I and II given by Eqs. (31) and (39) respectively.

The families of plots for Cases I and II are connected through the critical case \( \epsilon_a = \epsilon_b = \epsilon_c = 0 \), which is represented by the thick red line. This case corresponds to the ratio \( \Delta(0)/T_c = 2\sqrt{2} \). Solid lines above the thick line represent Case I and below the thick line Case II. The dashed line shows the standard result of the Bardeen-Cooper-Schrieffer theory.

Thus, if the assumptions of the present model are valid, the critical-case ratio \( \Delta(0)/T_c = 2\sqrt{2} \) signifies the transition from the conventional behavior \( \Delta(T_c) = 0 \) for \( \Delta(0)/T_c < 2\sqrt{2} \) to unconventional behavior \( \Delta(T_c) \neq 0 \) for \( \Delta(0)/T_c > 2\sqrt{2} \). The value of \( \Delta(0)/T_c = 2\sqrt{2} \) for the critical case makes important quantitative difference from the critical case result \( \Delta(0)/T_c = 4 \) for the grid-based model of Refs. 30–33, which involved only a- and b-states. Such a difference was to be expected, because the coupling between b- and c-states in the present model leads to additional energy advantage for the superconducting state and hence higher superconducting transition temperature for the same value of the coupling constant \( g \).

V. COMPARISON WITH EXPERIMENT

In Fig. 4, we show how the predictions of the present model for the temperature dependence of the superconducting gap compare with the available experimental results for break junctions (BJ) 37–39 and the interlayer tunneling (ILT) 40–41 in bismuth families of cuprates. This is the same set of experimental data as the one used in Ref. 30 for testing the grid-based model. The predictions of the grid-based model are also plotted in Fig. 4.

The model predictions, when limited to Cases I or II only, require two input parameters \( \Delta(0) \) and \( T_c \), which help us to determine \( g \) and \( |\epsilon_a| \) for Case I, or \( |\epsilon_b| \) for Case II. The choice between Cases I and II is made on the basis of the ratio \( \Delta(0)/T_c \) being larger or smaller than \( 2\sqrt{2} \).

All plots in Fig. 4 demonstrate either very good or satisfactory agreement between the predictions of the present model and the experiment. In comparison with the predictions of the grid-based model, the agreement with experiment has improved overall. Specifically, it became better in frames (a, b, c, d, e, f, g, o, q, r, s), remained about the same in frames (k, l, m, p), and became worse in frames (h, i, j). It should be remarked here that the experimental data themselves are subject to a number of uncertainties, including, in particular, the overheating effect for the ILT measurements.

We further remark that, despite the significant experimental difficulty of measuring \( \Delta(T) \) close to \( T = T_c \), the very notion of the existence of the critical ratio \( \Delta(0)/T_c \) which separates the dependencies ending with \( \Delta(T_c) = 0 \) from those ending with \( \Delta(T_c) \neq 0 \) appears to be reasonably supported by experiments, and, moreover, the value \( 2\sqrt{2} \) for such a critical ratio obtained in this work leads to more consistent predictions than the critical value 4 obtained in Ref. 30 for the grid-based model.

VI. CONCLUSIONS

In the present paper, we generalized the superconductivity model proposed in Ref. 30 for the grid background to the background formed by the checkerboard of spin vortices. The technical difference is that the former involves two kinds of fermionic states, while the later involves three, even though two of the three are similar. We have shown that the qualitative predictions of the grid-based model largely remain intact, which means that the detailed analysis of the grid-based model of Ref. 30 can also be extended to the spin-vortices-based model. Therefore, we did not find it necessary to repeat it here. The most important difference between the spin-vortices-based model and the grid-based model turns out to be the critical ratio \( \Delta(0)/T_c \) above which the temperature
dependence of the superconducting gap ends at the value $\Delta(T_c) \neq 0$, which, in turn, is probably related to the pseudogap. For spin vortices, this critical value is $2\sqrt{2}$, while, for grid, it is 4. We have demonstrated that the predictions for the temperature evolution of the superconducting gap for the spin-vortices-based model exhibits good agreement with experiments, and moreover, this agreement is somewhat better than for the grid-based model.

In the broader context of cuprate superconductivity, the model considered in this work is still rather oversimplified. However, one can use it to develop intuition about more realistic settings that must involve the fluctuations of the spin background, as well as other interactions between fermions.

### Appendix A: Total energy of the system

In this Appendix, we elaborate on the derivation steps (ii) and (iii) mentioned after Eq. (20).

Substituting the canonical transformation for $a$ and $c$:...
states \((16)\) in \((13)\), we obtain

\[
E = 8\epsilon_bN \left[ s^2n_B + w^2(1 - n_B) \right] \\
+ 2\epsilon_c \sum_k \left\{ u^2(k)n_A(k) + v^2(k)[1 - n_A(k)] \right\} \\
+ 2\epsilon_c \sum_k \left\{ p^2(k)n_C(k) + q^2(k)[1 - n_C(k)] \right\} \\
+ 2gs w(1 - 2n_B) \sum_k \\
\left[ u(k)v(k)(1 - 2n_A(k))[V(k)]\cos[\phi_V(k) + \phi_a(k)] \\
+ p(k)q(k)(1 - 2n_C(k))[\tilde{V}(k)]\cos[\phi_V(k) + \phi_c(k)] \right],
\]

where all variables are defined in Section (III).

Two interaction terms in the above expression have phase-dependent factors \(\cos[\phi_V(k) + \phi_a(k)]\) and \(\cos[\phi_V(k) + \phi_c(k)]\). Eventually, the variational ground-state energy obtained by finding \(u(k), v(k), p(k)\) and \(q(k)\) will monotonically decrease with the increasing absolute value of these terms. This implies that the variational energy will be minimized for \(|\cos[\phi_V(k) + \phi_a(k)]| = 1\) and \(|\cos[\phi_V(k) + \phi_c(k)]| = 1\). Choosing the sign of cosines in these relations is just a matter of sign convention for the Bogoliubov transformation coefficients later converting into the sign of the products \(swu(k)v(k)\) and \(swp(k)q(k)\).

**Appendix B: Case I**

For \(\epsilon_b = 0\), the Bogoliubov transformation parameters \(s\) and \(w\) enter the energy \((24)\) only as a term proportional to \(sw\). For such a case, given the constraint \(s^2 + w^2 = 1\), the minimization of energy \((24)\) gives, \(s = \sqrt{\frac{1}{2}}, w = -\sqrt{\frac{1}{2}}\). The relative negative sign of \(s\) and \(w\) implies later the positive relative sign for the pairs of transformation parameters \(\{u(k), v(k)\}\) and \(\{p(k), q(k)\}\). The minimization of energy \((24)\) with respect to \(u(k), v(k), p(k), q(k)\), finally, gives

\[
u(k) = \sqrt{\frac{1}{2} + \frac{1}{2} \sqrt{1 + \frac{T_2^2(k)}{Q_2^2(k)}}},
\]

\[
v(k) = \sqrt{\frac{1}{2} - \frac{1}{2} \sqrt{1 + \frac{T_2^2(k)}{Q_2^2(k)}}},
\]

\[
p(k) = \sqrt{\frac{1}{2} + \frac{1}{2} \sqrt{1 + \frac{T_2^2(k)}{Q_2^2(k)}}},
\]

\[
q(k) = \sqrt{\frac{1}{2} - \frac{1}{2} \sqrt{1 + \frac{T_2^2(k)}{Q_2^2(k)}}},
\]

where,

\[
T_a(k) = g(1 - 2n_B)(1 - 2n_A(k))[V(k)],
\]

\[
Q_a(k) = 2\epsilon_c(1 - 2n_A(k)),
\]

\[
T_c(k) = g(1 - 2n_B)(1 - 2n_c(k))[\tilde{V}(k)],
\]

\[
Q_c(k) = 2\epsilon_c(1 - 2n_A(k)).
\]

The total energy \(E\) of the system in this case can be expressed as

\[
E = -\sum_k \left[ (1 - 2n_A(k)) \epsilon_A(k) \\
+ (1 - 2n_C(k)) \epsilon_C(k) - \epsilon_a - \epsilon_c \right],
\]

which is an implicit function of \([V(k)]\) and \([\tilde{V}(k)]\). Both \([V(k)]\) and \([\tilde{V}(k)]\) are a function of four phases \(\varphi_1, \varphi_2, \varphi_3\) and \(\varphi_4\) entering Eqs. \((14)\) [15]. Therefore the energy equation should be further minimized with respect to the values of these phases. Such minimization imposes only one constraint

\[
\frac{\varphi_2 + \varphi_4 - \varphi_1 - \varphi_3}{2} = \frac{\pi}{2} + \pi n.
\]

**Appendix C: Case II**

In this case, \(\epsilon_a = \epsilon_c = 0\) in Eq. \((24)\) and, as a result, the minimization of energy gives \(u(k) = v(k) = p(k) = q(k) = 1/\sqrt{2}\). The minimization with respect to \(s\) subject to condition \((3)\) now gives

\[
s^4 - s^2 + \frac{\tilde{T}^2}{4(Q^2 + \tilde{T}^2)} = 0
\]

where we introduced the following parameters:

\[
Q \equiv 8\epsilon_b N(2n_B - 1),
\]

\[
\tilde{T} = T_a + T_c,
\]

\[
T_a = g(1 - 2n_B)C_a N,
\]

\[
T_c = g(1 - 2n_B)C_c N.
\]

The parameters \(C_a\) and \(C_c\) are defined by Eqs. \((36)\) [37]. Solving the bi-quadratic equation \((C1)\), we obtain

\[
s = \sqrt{\frac{1}{2} + \frac{1}{2} \sqrt{1 + \frac{\tilde{T}^2}{Q^2}}},
\]

\[
w = -\sqrt{\frac{1}{2} - \frac{1}{2} \sqrt{1 + \frac{\tilde{T}^2}{Q^2}}},
\]
We obtain $\epsilon_B$ by varying energy $[24]$ with respect to $n_B$:
\[
\epsilon_B = \frac{1}{8N} \frac{dE}{dn_B} = \epsilon_b[s^2 - w^2] + 2gw(-2) \sum_k \{u(k)v(k)(1 - 2n_A(k))|V(k)| + p(k)q(k)(1 - 2n_C(k))(k)|\hat{V}(k)|\}.
\]
By substituting the parameters defined by Eqs. $[C3]$ and $[C2]$, we obtain
\[
\epsilon_B = \epsilon_b\sqrt{\frac{Q^2}{Q^2 + T^2}} - 2\frac{T}{2\sqrt{Q^2 + T^2}}\frac{1}{1 - 2n_B}T,
\]
which, after some manipulations gives Eq.$[32]$.

The quasiparticle excitation energies for A- and C-states are calculated in a similar way — as $\epsilon_A(k) = \frac{dE}{dn_A(k)}$ and $\epsilon_C(k) = \frac{dE}{dn_C(k)}$, which gives Eqs.$[33]$ and $[34]$ respectively. The total energy of the system in this case is
\[
E = -2N[(1 - 2n_B)\epsilon_B - \epsilon_b].
\]
In this case, phases $\varphi_n$ also obey the constraint $[B4]$. 

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1. J. M. Tranquada, B. J. Sternlieb, J. D. Axe, Y. Nakamura, and S. Uchida, Nature (London) 375, 561 (1995).
2. K. Yamada, C. H. Lee, K. Kurahashi, J. Wada, S. Wakkimoto, S. Ueki, H. Kimura, Y. Endoh, S. Hosoya, G. Shirane, R. J. Birgeneau, M. Greven, M. A. Kastner, and Y. J. Kim, Phys. Rev. B 57, 6165 (1998).
3. J. E. Hoffman, E. W. Hudson, K. M. Lang, V. Madhavan, H. Eisaki, S. Uchida, J. C. Davis, Science 295, 5554, 466-469 (2002).
4. K. McElroy, R. W. Simmonds, J. E. Hoffman, D.-H. Lee, J. Orenstein, H. Eisaki, S. Uchida, and J. C. Davis, Nature 422, 592-596 (2003).
5. M. Vershinin, Shashank Misra, S. Ono, Y. Abe, Yoichi Ando, Ali Yazdani, Science 303, 5666, 1995-1998 (2004).
6. T. Hanaguri, C. Lupien, Y. Kohsaka, D.-H. Lee, M. Azuma, M. Takano, H. Takagi, and J. C. Davis, Nature 430, 1001-1005 (2004).
7. P. Abbamonte, A. Rusdyi, S. Smadici, G. D. Gu, G. A. Sawatzky, and D. L. Feng, Nature Physics 1, 155-158 (2005).
8. Seiki Komiya, Han-Dong Chen, Shou-Cheng Zhang, and Yoichi Ando, Phys. Rev. Lett. 94, 207004 (2005).
9. K. McElroy, D.-H. Lee, J. E. Hoffman, K. M. Lang, J. Lee, E. W. Hudson, H. Eisaki, S. Uchida, and J. C. Davis, Phys. Rev. Lett. 94, 197005 (2005).
10. W. D. Wise, M. C. Boyer, Kamalesh Chatterjee, Takeshi Kondo, T. Takeuchi, H. Ikuta, Yayu Wang, and E. W. Hudson, Nature Physics 4, 696-699 (2008).
11. Eduarad H. Da Silva Neto, Pegor Aynajian, Alex Frano, Riccardo Comin, Enrico Schierle, Eugen Wescokie, Andras Gyenis, Jinsheng Wen, John Schneeloch, Zhijun Xu, Shimpei Ono, Gends Gu, Mathieu Le Tacon, Ali Yazdani, Science 343, 6169, 393-396 (2014).
12. R. Comin, R. Sutarto, F. He, E. H. da Silva Neto, L. Chauviere, A. Fraha, R. Liang, W. N. Hardy, D. A. Bonn, Y. Yoshida, H. Eisaki, A. J. Achkar, D. G. Hawthorn, B. Keimer, G. A. Sawatzky, and A. Damascelli, Nature Materials 14, 796-800 (2015).
13. J. M. Tranquada, N. Ichikawa, K. Kakurai, and S. Uchida, J. Phys. Chem. Solids 60, 8-9, 1019-1023 (1999).
14. K. Mitsen and O. M. Ivanenko, Phys. Usp. 47, 493 (2004).
15. John A. Robertson, Steven A. Kivelson, Eduardo Fradkin, Alan C. Fang, and Aharon Kapitulnik, Phys. Rev. B 74, 134507 (2006).
16. J. M. Tranquada, Neutron Scattering Studies of Antiferromagnetic correlations in Cuprates, in Handbook of High-Temperature Superconductivity, Editors: J. R. Schrieffer and J. S. Brooks, Springer, (2006).
17. B. V. Fine, Phys. Rev. B 75, 060504(R) (2007).
18. B. V. Fine, J. Supercond. Nov. Magn. 24, 1207 (2011).
19. B. V. Fine, J. Supercond. Nov. Magn. 26, 2621-2626 (2013).
20. B. V. Fine, Phys. Rev. B 70, 224508 (2004).
21. N. B. Christensen, H. M. Ronnow, J. Mesot, R. A. Ewings, N. Momono, M. Oda, M. Ido, M. Enderle, D. F. McMorrow, and A. T. Boothroyd, Phys. Rev. Lett. 98, 197003 (2007).
22. G. Seibold, Phys. Rev. B 58, 15520 (1998).
23. M. Berciu and S. John, Phys. Rev. B 59, 15143 (1999).
24. C. Timm and K. H. Bennemann, Phys. Rev. Lett. 84, 4994 (2000).
25. H. Koizumi, J. Phys. Soc. Jpn. 77, 034712 (2008).
26. J. A. Wilson, J. Phys. Condens. Matter 21, 245702 (2009).
27. M. Azzouz, B W Ramakko, and G Presenza-Pitman, J. Phys. Condens. Matter 22, 345605 (2010).
28. Q. Li, M. H"acker, G. D. Gu, A. M. Tsvelik, and J. M. Tranquada, Phys. Rev. Lett. 99, 067001 (2007).
29. E. Berg, E. Fradkin, E.-A. Kim, S. A. Kivelson, V. Oganesyan, J. M. Tranquada, and S. C. Zhang, Phys. Rev. Lett. 99, 127003 (2007).
30. B. V. Fine, Phys. Rev. Lett. 94, 157005 (2005).
31. J. M. Tranquada, G. D. Gu, M. H"acker, Q. Jie, H.-J. Kang, R. Klingeler, Q. Li, N. Tristam, J. S. Wen, G. Y. Xu, Z. J. Xu, J. Zhou, and M. v. Zimmermann, Phys. Rev. B 78, 174529 (2008).
32. B. V. Fine and T. Egami, Phys. Rev. B 77, 014519 (2008).
33. T. Egami, B. V. Fine, D. Parshall, A. Subedi and D. J. Singh, Adv. Condens. Matter Phys. 2010, 164916 (2010).
34. J. Ranninger and T. Domanski, Phys. Rev. B 81, 014514 (2010).
35. G. Pawlowski, R. Micnas, and S. Robaszkiewicz, Phys. Rev. B 81, 064514 (2010).
36. J. Bardeen, L. N Cooper, and J. R. Schrieffer, Phys. Rev. 108, 1175 (1957).
37. S. I. Venedeev, A. G. M. Jansen, P. Samuely, V. A.
Stepanov, A. A. Tsvetkov, and P. Wyder, Phys. Rev. B 49, 9823 (1994).

38 N. Miyakawa, P. Guptasarma, J. F. Zasadzinski, D. G. Hinks, and K. E. Gray, Phys. Rev. Lett. 80, 157 (1998).

39 A.I. Akimenko, R. Aoki, H. Murakami, V.A. Gudimenko, Physica C (Amsterdam) 319, 59-72 (1999).

40 Minoru Suzuki, Takao Watanabe, and Azusa Matsuda, Phys. Rev. Lett. 82, 5361 (1999).

41 Minoru Suzuki and Takao Watanabe, Phys. Rev. Lett. 85, 4787 (2000).

42 V. M. Krasnov, A. Yurgens, D. Winkler, P. Delsing, and T. Claeson, Phys. Rev. Lett. 84, 5860 (2000).

43 A. Yurgens, D. Winkler, T. Claeson, S. Ono, and Yoichi Ando, Phys. Rev. Lett. 90, 147005 (2003).

44 Yoshiharu Yamada, Kenkichi Anagawa, Takasada Shibauchi, Takenori Fujii, Takao Watanabe, Azusa Matsuda, and Minoru Suzuki, Phys. Rev. B 68, 054533 (2003).

45 V. M. Krasnov, Physica C (Amsterdam) 372-376, 103 (2002).

46 V. M. Krasnov, Phys. Rev. B 65, 140504 (2002).

47 V. M. Krasnov, M. Sandberg, and I. Zogaj, Phys. Rev. Lett. 94, 077003 (2005).

48 A. Yurgens, D. Winkler, T. Claeson, S. Ono, and Yoichi Ando, Phys. Rev. Lett. 92, 259702 (2004).

49 V. N. Zavaritsky, Phys. Rev. Lett. 92, 259701 (2004).

50 V. N. Zavaritsky, Physica C (Amsterdam) 404, 440 (2004).