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Mean field theory of competing orders in metals with antiferromagnetic exchange interactions

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It has long been known that two-dimensional metals with antiferromagnetic exchange interactions have a weak-coupling instability to the superconductivity of spin-singlet, d -wave electron pairs. We examine additional possible instabilities in the spin-singlet particle-hole channel, and study their interplay with superconductivity. We perform an unrestricted Hartree-Fock-BCS analysis of bond order parameters in a single band model on the square lattice with nearest-neighbor exchange and repulsion, while neglecting on-site interactions. The dominant particle-hole instability is found to be an incommensurate, bi-directional, bond density wave with wavevectors along the $(1, 1)$ and $(1, -1)$ directions, and an internal d -wave symmetry. The magnitude of the ordering wavevector is close to the separation between points on the Fermi surface which intersect the antiferromagnetic Brillouin zone boundary. The temperature dependence of the superconducting and bond order parameters demonstrates their mutual competition. We also obtain the spatial dependence of the two orders in a vortex lattice induced by an applied magnetic field: “halos” of the bond order appear around the cores of the vortices.

PACS numbers:

I. INTRODUCTION

All of the quasi-two dimensional higher temperature superconductors are proximate to metals with strong local antiferromagnetic exchange interactions¹. In some cases, there is even an antiferromagnetic quantum critical point, with a diverging spin correlation length, in the region of the highest critical temperatures for superconductivity^{2,3}. However, in the materials with highest critical temperatures, the hole-doped cuprates, the regions with the strongest superconductivity are well separated from the antiferromagnetic quantum critical point⁴. Interestingly, it is in these same materials that the ‘pseudogap’ regime is best defined, along with the presence of competing charge density wave orders⁵⁻⁹.

In the context of a weak-coupling treatment of the antiferromagnetic exchange interactions¹⁰⁻¹⁵, it has long been known that unconventional spin-singlet superconductivity can appear, with a gap function which changes sign between regions of the Fermi surface connected by the antiferromagnetic ordering wavevector (this corresponds to d -wave pairing, in the context of the cuprate Fermi surface). Recently, quantum Monte Carlo simulations have shown¹⁶ that this mechanism of superconductivity via exchange of antiferromagnetic fluctuations survives in the strongly-coupled regime across the quantum critical point.

Field-theoretical studies¹⁷⁻¹⁹ of the vicinity of the antiferromagnetic quantum critical point in a two-dimensional metal have also found strong evidence for the dominance of a d -wave superconducting instability. These studies¹⁸⁻²⁰ also noted that an instability to a particular type of charge order, an incommensurate d -wave

bond order, was nearly degenerate with the superconducting instability. These results suggest that a combination of fluctuating superconducting and charge orders could describe the pseudogap regime of the hole-doped cuprate superconductors; Ref. 9 has shown that a theory of these fluctuating orders describes the X-ray scattering data⁵⁻⁷ well. However, to establish such a proposal theoretically, we need to understand the evolution of these instabilities in a metal which is well separated from the antiferromagnetic quantum critical point.

A linear stability analysis of a two-dimensional metal with short-range antiferromagnetic interactions, but away from the antiferromagnetic quantum critical point, was carried out recently in Ref. 21 (related studies are in Refs. 22-28). Ref. 21 found that the leading instability upon cooling down from high temperatures was to a d -wave superconductor. However, if one ignored this instability, and looked for the leading instability in the particle-hole channel, it was found to be an incommensurate charge density wave with a d -wave form factor, and wavevectors along the $(1, \pm 1)$ directions of the square lattice. Moreover, the optimum wavevectors of the instability, $(H, \pm H)$ were very close to the separation $(H_0, \pm H_0)$ between certain “hot spots” on the Fermi surface (see Fig. 1); leading subdominant saddle points were also found close to the wavevectors $(\pm H_0, 0)$, $(0, \pm H_0)$ which are observed in the X-ray scattering. The hot spots are special points on the Fermi surface which are separated from one other hot spot by the antiferromagnetic wavevector $\mathbf{K} = (\pi, \pi)$. The wavevector magnitude H_0 appeared in the results,^{21,22} even though they were not treated as special Fermi surface points in the computation, and the antiferromagnetic correlations were short-

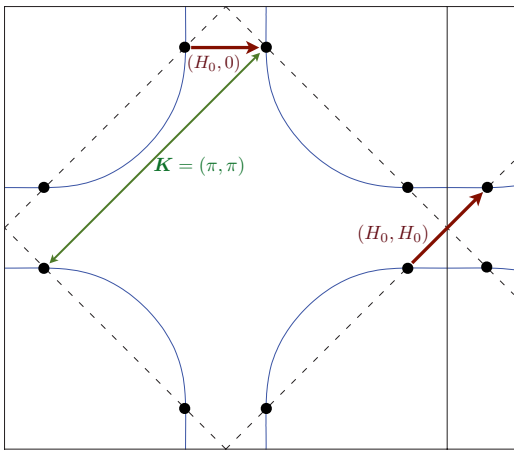


FIG. 1: Fermi surface in the square lattice Brillouin zone, showing the hot spots (filled circles), and defining the value of H_0 .

ranged. But \mathbf{K} can nevertheless be expected to play a role because the Fourier transform of the antiferromagnetic exchange interaction has an extremum at or near \mathbf{K} ; in Ref. 22, the ordering wavevectors were related to the crossing points of $2k_F$ singularities. These results were interpreted as evidence for the applicability of the theory of competing and nearly degenerate superconducting and charge-density wave orders away from the antiferromagnetic quantum critical point.

In this paper, we will extend the earlier computation²¹ beyond the regime of linear instability at high temperature, to a complete determination of the optimal state at low temperature, with co-existing superconducting and charge-density-wave order parameters. This study is the analog of that in Ref. 29 for the case of competition of superconductivity with Ising-nematic order at zero wavevector. We will also study the solution in the presence of an applied magnetic field and a vortex lattice.

We begin in Section II by setting up the Hartree-Fock-BCS equations for the square lattice model with nearest-neighbor exchange interactions (J) and a nearest-neighbor Coulomb repulsion (V). All the variational parameters of the mean-field theory will lie on the nearest-neighbor links: these include a spin-singlet electron pairing amplitude, Q_{ij} , and a spin-singlet particle-hole pairing amplitude, P_{ij} . We will allow for arbitrary spatial dependencies in the P_{ij} and Q_{ij} , including the possibility of time-reversal symmetry breaking solutions with non-zero currents on the links. However, our analysis does not include on-site interactions or on-site variational parameters: we discuss shortcomings in experimental applications possibly due to this omission in Section V.

Our main results on the numerical solutions of the mean-field equations appear in Section III. We always find that the dominant instability in the particle-hole channel is a bi-directional bond density wave with wavevectors very close to the diagonal values $(\pm H_0, \pm H_0)$

determined by the intersections between the Fermi surface and antiferromagnetic Brillouin zone boundary (Fig 1. The bond density wave can co-exist with d -wave superconductivity, and we obtain results on the temperature dependence of the two orders. We also present a solution in the presence of an applied magnetic field, displaying vortices in the superconducting order surrounded by “halos” of bond order, similar to the initial observations by Hoffman *et al.*³⁰ We note that there have been earlier Hartree-Fock-BCS studies of competing orders around vortex cores^{31,32}, but they had local antiferromagnetic order as the driving mechanism.

In Section IV we introduce a simplified momentum space model which has instabilities similar to those obtained in the full lattice model in Section III. This provides a simple and useful physical picture of the structure of the phase diagram. However, it is not possible to extend this model to the spatially inhomogeneous case that arises in the presence of an applied magnetic field.

Section V will discuss missing ingredients in our model computations which could possibly yield charge order at the observed wavevectors $(\pm H_0, 0)$, $(0, \pm H_0)$.

We note that a similar Hartree-Fock-BCS computation on a t - J model has been carried out recently by Laughlin²⁷, and he finds a dominant instability in the particle-hole channel of a state with staggered orbital currents^{27,33–36}. However, his computation does not consider Fermi surfaces with hot spots as in Fig. 1. Our computations do include the staggered orbital current state as a possible saddle point, and for our chosen parameters, the bond density waves described below have a lower energy. Similarly, we also allowed for states with uniform orbital currents,³⁷ and did not find them.

II. MODEL AND MEAN FIELD EQUATIONS

We will examine the t - J - V on the square lattice, with the dispersion chosen to ensure that there are hot spots on the Fermi surface:

$$\begin{aligned} H &= H_t + H_{JV} \\ H_t &= \sum_{\mathbf{k}, \alpha} \varepsilon(\mathbf{k}) c_{\mathbf{k}, \alpha}^\dagger c_{\mathbf{k}, \alpha} \\ H_{JV} &= \sum_{i < j} \left[\frac{J_{ij}}{4} \sigma_{\alpha\beta}^a \sigma_{\gamma\delta}^a c_{i\alpha}^\dagger c_{i\beta} c_{j\gamma}^\dagger c_{j\delta} \right. \\ &\quad \left. + V_{ij} c_{i\alpha}^\dagger c_{i\alpha} c_{j\beta}^\dagger c_{j\beta} \right]. \end{aligned} \quad (2.1)$$

The dispersion is that in Ref. 21, with

$$\begin{aligned} \varepsilon(\mathbf{k}) &= -2t_1 (\cos(k_x) + \cos(k_y)) - 4t_2 \cos(k_x) \cos(k_y) \\ &\quad - 2t_3 (\cos(2k_x) + \cos(2k_y)) - \mu \end{aligned} \quad (2.2)$$

where $t_1 = 1$, $t_2 = -0.32$, and $t_3 = -0.5t_2$.

It is useful to set up the Hartree-Fock-BCS mean field equations by working in real space. We will work with

the hypothesis that competing orders are controlled by the bond expectation values³⁹, and neglect on-site factorizations of the 4 fermion terms. Then, for each pair of sites, i, j , for which the J_{ij} or V_{ij} are non-zero, we have a pair of complex numbers which will serve as the variational parameters of our mean-field theory; we define these by We define the bond expectation values

$$\begin{aligned}\langle c_{i\alpha}^\dagger c_{j\beta}^\dagger \rangle &= Q_{ij} \varepsilon_{\alpha\beta} \\ \langle c_{i\alpha} c_{j\beta} \rangle &= -Q_{ij}^* \varepsilon_{\alpha\beta} \\ \langle c_{i\alpha}^\dagger c_{j\beta} \rangle &= P_{ij} \delta_{\alpha\beta}\end{aligned}\quad (2.3)$$

with $Q_{ij} = Q_{ji}$ and $P_{ji} = P_{ij}^*$. With these definitions, the Hartree-Fock-BCS factorization of H is

$$H_{HF} = \sum_{i,j} (c_{i\uparrow}^\dagger, c_{i\downarrow}) \begin{pmatrix} A_{ij} & B_{ij} \\ B_{ij}^* & -A_{ji} \end{pmatrix} \begin{pmatrix} c_{j\uparrow}^\dagger \\ c_{j\downarrow}^\dagger \end{pmatrix} \quad (2.4)$$

where

$$\begin{aligned}A_{ij} &= -t_{ij} - (3J_{ij}/4 + V_{ij}) P_{ij}^* - \delta_{ij}\mu \\ B_{ij} &= - (3J_{ij}/4 - V_{ij}) Q_{ij}^*\end{aligned}\quad (2.5)$$

H_{HF} has eigenvalues which occur in pairs, $\omega_\mu, -\omega_\mu$ ($\omega_\mu > 0$), and we write the corresponding eigenvectors as

$$\begin{pmatrix} \mathcal{U}_{i\mu} \\ \mathcal{V}_{i\mu} \end{pmatrix}, \begin{pmatrix} -\mathcal{V}_{i\mu}^* \\ \mathcal{U}_{i\mu}^* \end{pmatrix}. \quad (2.6)$$

Orbital effects of the magnetic field can be introduced by minimal substitution into the hopping parameters as

$$t_{ij} = t_{ij}^{(0)} e^{ia_{ij}}, \quad (2.7)$$

where $t_{ij}^{(0)}$ are hoppings in the absence of a magnetic field and $a_{ij} = \int_{\mathbf{r}_i}^{\mathbf{r}_j} d^3\mathbf{r} \cdot \mathbf{a}(\mathbf{r})$ are Aharonov-Bohm phases resulting from the vector potential $\mathbf{a}(\mathbf{r})$ generated by the magnetic field. While the magnetic field does not break translation invariance in the strict sense, H_{HF} can be translationally invariant in a specific gauge only in a magnetic unit cell, which encloses a full electron (and therefore two superconducting) flux quantum(quantum). In order to maintain spatial translational invariance of the vector potential we insert a pair of superconducting flux quanta (i.e. containing flux $h/2e$) in a pair of plaquettes of the square lattice to compensate the flux of the uniform magnetic field. At the same time we introduce a π phase-shift branch cut for the electrons joining the two plaquettes. The magnetic field leads the superconducting order parameter Q_{ij} to develop a vortex lattice structure. The specific profile for the vector potential described, whose precise description is provided in Appendix A, is chosen so as to simplify the numerical stability of the self-consistency procedure, following previous work⁴⁴. Specifically, in this gauge the phase of the self-consistent order parameter is expected to be nearly

constant so that the initial guess of a constant order parameter would have a phase profile close to the final answer. One would still have a non-vanishing supercurrent proportional to the non-vanishing vector potential \mathbf{a} i.e. $\mathbf{a}|Q|^2$ term in the current density. In our calculations, the vortex cores, which appear as dips in the SC order parameter, are found to exist near the superconducting flux quanta. The details of the calculation of the vector potential \mathbf{a} is given in Appendix A.

Introducing the Bogoliubov operators $\gamma_{\mu\alpha}$ we then have

$$H_{HF} = \sum_{\mu} \omega_{\mu} (\gamma_{\mu\alpha}^\dagger \gamma_{\mu\alpha} - 1) \quad (2.8)$$

where the unitary transformation to the Bogoliubov operators is

$$c_{i\alpha} = \sum_{\mu} \left(\mathcal{U}_{i\mu} \gamma_{\mu\alpha} - \mathcal{V}_{i\mu}^* \varepsilon_{\alpha\beta} \gamma_{\mu\beta}^\dagger \right). \quad (2.9)$$

So we have the expectation values

$$\begin{aligned}\langle c_{i\alpha}^\dagger c_{j\beta}^\dagger \rangle_{HF} &= \tilde{Q}_{ij} \varepsilon_{\alpha\beta} \\ &= -\varepsilon_{\alpha\beta} \sum_{\mu} (\mathcal{U}_{i\mu}^* \mathcal{V}_{j\mu} + \mathcal{U}_{j\mu}^* \mathcal{V}_{i\mu}) \frac{1}{2} \tanh\left(\frac{\omega_{\mu}}{2T}\right) \\ \langle c_{i\alpha} c_{j\beta} \rangle_{HF} &= -\tilde{Q}_{ij}^* \varepsilon_{\alpha\beta} \\ \langle c_{i\alpha}^\dagger c_{j\beta} \rangle_{HF} &= \tilde{P}_{ij} \delta_{\alpha\beta} \\ &= -\delta_{\alpha\beta} \sum_{\mu} (\mathcal{U}_{i\mu}^* \mathcal{U}_{j\mu} - \mathcal{V}_{j\mu}^* \mathcal{V}_{i\mu}) \frac{1}{2} \tanh\left(\frac{\omega_{\mu}}{2T}\right),\end{aligned}\quad (2.10)$$

which defines the complex numbers \tilde{Q}_{ij} and \tilde{P}_{ij} as functions of the Q_{ij} and P_{ij} . Above, we used the orthogonal relations

$$\begin{aligned}\sum_{\mu} (\mathcal{U}_{i\mu}^* \mathcal{U}_{j\mu} + \mathcal{V}_{j\mu}^* \mathcal{V}_{i\mu}) &= \delta_{ij} \\ \sum_{\mu} (\mathcal{U}_{i\mu}^* \mathcal{V}_{j\mu} - \mathcal{U}_{j\mu}^* \mathcal{V}_{i\mu}) &= 0.\end{aligned}\quad (2.11)$$

Finally, the variational estimate for the free energy is

$$\begin{aligned}F &= F_{HF} + \langle H - H_{HF} \rangle \\ &= \sum_{\mu} \left(-\omega_{\mu} - 2T \ln(1 + e^{-\omega_{\mu}/T}) \right) \\ &\quad + \sum_{i < j} \left[2 \left(\frac{3J_{ij}}{4} - V_{ij} \right) \left[-|\tilde{Q}_{ij}|^2 + Q_{ij} \tilde{Q}_{ij}^* + Q_{ij}^* \tilde{Q}_{ij} \right] \right. \\ &\quad \left. + 2 \left(\frac{3J_{ij}}{4} + V_{ij} \right) \left[-|\tilde{P}_{ij}|^2 + P_{ij} \tilde{P}_{ij}^* + P_{ij}^* \tilde{P}_{ij} \right] \right].\end{aligned}\quad (2.12)$$

Our task is to minimize this free energy as a function of the Q_{ij} and P_{ij} . At the saddle points we expect to find $Q_{ij} = \tilde{Q}_{ij}$ and $P_{ij} = \tilde{P}_{ij}$. However, F serves as a

variational estimate even away from the saddle points.

We close this section by expressing the Q_{ij} and P_{ij} in terms of the momentum-space order parameters used in Ref. 21. For the superconducting order, we have

$$Q_{ij} = \frac{1}{V} \sum_{\mathbf{k}} e^{i\mathbf{k} \cdot (\mathbf{r}_i - \mathbf{r}_j)} \Delta_S(\mathbf{k}), \quad (2.13)$$

where V is the system volume. The d -wave superconductor corresponds to $\Delta_S(\mathbf{k}) = 2\Delta_0(\cos(k_x) - \cos(k_y))$, which implies

$$\begin{aligned} Q_{i,i+\hat{x}} &= \Delta_0 \\ Q_{i,i+\hat{y}} &= -\Delta_0 \end{aligned} \quad (2.14)$$

with Δ_S real (without loss of generality).

For the charge order, we have a set of orders $\Delta_{\mathbf{H}}(\mathbf{k})$ for ordering wavevectors \mathbf{H} , and these are related to the P_{ij} via

$$P_{ij} = \sum_{\mathbf{H}} \left[\frac{1}{V} \sum_{\mathbf{k}} e^{i\mathbf{k} \cdot (\mathbf{r}_i - \mathbf{r}_j)} \Delta_{\mathbf{H}}(\mathbf{k}) \right] e^{i\mathbf{H} \cdot (\mathbf{r}_i + \mathbf{r}_j)/2}. \quad (2.15)$$

The momentum space charge orders must obey $\Delta_{-\mathbf{H}}(\mathbf{k}) = \Delta_{\mathbf{H}}^*(\mathbf{k})$. And solutions which preserve time-reversal symmetry have $\Delta_{\mathbf{H}}(\mathbf{k}) = \Delta_{\mathbf{H}}(-\mathbf{k})$. In our models with bond order parameters only along nearest neighbor links, we must have

$$\begin{aligned} \Delta_{\mathbf{H}}(\mathbf{k}) &= \\ C_1 \cos(k_x) + C_2 \cos(k_y) + C_3 \sin(k_x) + C_4 \sin(k_y) \end{aligned} \quad (2.16)$$

where C_{1-4} are \mathbf{H} -dependent complex numbers. For the optimum incommensurate charge density wave state of Ref. 21 at wavevector $\mathbf{H} \approx (H_0, H_0)$, we have $C_2 = -C_1$ and $C_3 = C_4 = 0$. Similarly, for the ‘staggered-flux’ state of Refs. 27,33–36 we have $\mathbf{H} = (\pi, \pi)$, $C_4 = -C_3$ and $C_1 = C_2 = 0$. And the current-carrying states of Ref. 37 have $\mathbf{H} = (0, 0)$, $C_1 = C_2 = 0$, and $C_3 \neq 0$, $C_4 \neq 0$.

III. NUMERICAL SOLUTIONS

The mean-field ground state of the Hamiltonian in Eq. 2.1 can be obtained by minimizing the free-energy $F[P, Q]$ defined in Eq. 2.12 relative to the mean-field BDW potentials P_{ij} and the SC pair potentials Q_{ij} . As described in Appendix B, the first derivatives of F in the potentials P_{ij} and Q_{ij} i.e. $\partial_{P_{ij}} F$ and $\partial_{Q_{ij}} F$, can be computed using perturbation theory. Local minima of the free-energy $F[P_{ij}, Q_{ij}]$ in the variables P_{ij} and Q_{ij} , which are then solutions of the set of equations $\partial_P F = \partial_Q F = 0$, are obtained by solving the minimization problem using the Quasi-Newton method as implemented in the `fminunc` routine in MATLAB. The Quasi-Newton iterations are continued until the derivatives of

the free-energy F fall below 10^{-5} . We verify that the obtained solution is the global minimum by choosing the initial values of P and Q that we start the minimization from. For a true global minima, general values of the initial perturbations P_{ij} and Q_{ij} lead to the same final ground state solution at the end of the iterations. It is possible to constrain the symmetry of the solution obtained by constraining the initial values of P_{ij} and Q_{ij} . Therefore, if we choose $P = Q = 0$ in the initial state, the final solution will continue to respect translational, 4-fold rotational and $U(1)$ symmetry and will not develop either BDW or SC order. It however can develop a uniform value $P_{ij} = P^{(0)}$ proportional to the nearest neighbor repulsion V . Since the final solution will continue to obey time-reversal symmetry, $P^{(0)}$ is found to be real. The hopping parameter t_1 in the microscopic Hamiltonian in Eq. 2.1 is a phenomenological parameter, which is chosen to reproduce the bandwidth of the electron dispersion that is measured in experiment. We therefore subtract $P^{(0)}$ from the bare hopping so that $t_1 + P^{(0)}$ becomes equal to the measured hopping parameter.

For our calculations we choose an $N \times N$ lattice site unit cell with $N = 24$ so that any translation symmetry breaking that we obtain as a result of interaction must be commensurate with the 24×24 unit cell. We find our results to be qualitatively similar for larger values of N . While the Hamiltonian is periodic with the N lattice sites in each direction, the electronic eigenvectors $\Psi(\mathbf{r})$ (where \mathbf{r} are positions on the lattice sites) described in Eq. 2.6 of the mean-field Hamiltonian obey phase twisted periodic boundary conditions $\Psi_{\mathbf{q}}(\mathbf{r} + \mathbf{R}) = e^{i\mathbf{q} \cdot \mathbf{R}} \Psi_{\mathbf{q}}(\mathbf{r})$, where \mathbf{q} is a Bloch wave-vector and \mathbf{R} is either $\mathbf{R} = N\hat{x}$ or $\mathbf{R} = N\hat{y}$. Thus eigenstates in our periodic lattice are indexed by the Bloch wave-vector $\mathbf{q} = 2\pi(n_x\hat{x} + n_y\hat{y})/M$, where n_x and n_y are integers from 0 to $M - 1$. For our calculation we choose $M = 4$, so that the electronic states effectively correspond to periodic boundary conditions on a supercell which is $NM = 96$ lattice sites in each direction. The value of M is chosen not only to converge the final answer obtained, but also to suppress translational symmetry breaking within the unit cell that is induced by the magnetic field. While the magnetic field, in the absence of superconductivity does not break translational invariance, the finite size effects resulting from a finite grid of Bloch vectors lead to a translational symmetry breaking similar to the way a uniform magnetic flux on a torus breaks translational invariance. Our choice of $M = 4$ produces a negligible translational symmetry breaking effect even in the presence of a magnetic flux.

Following previous work²¹ we observe that the free-energy F at infinitesimal strength of symmetry breaking in the BDW and SC sectors can be analyzed by expanding the free-energy $F[P_{ij}, Q_{ij}, J_{ij}, V_{ij}]$ to quadratic order in P and Q . For a critical strengths of the interaction parameters J_{ij} and V_{ij} , the state with $P_{ij} = Q_{ij} = 0$ is unstable towards a symmetry broken state with either BDW order (i.e. $P_{ij} \neq 0$) or SC order (i.e. with $Q_{ij} \neq 0$).

In this limit F can be decomposed as

$$F[P_{ij}, Q_{ij}, J_{ij}, V_{ij}] = F_{BDW}[P_{ij}, J_{ij}^{BDW}] + F_{SC}[Q_{ij}, J_{ij}^{SC}], \quad (3.1)$$

where

$$J_{ij}^{BDW} = J_{ij} + 4V_{ij}/3 \quad (3.2)$$

parametrizes the instability to symmetry breaking in the BDW channel and

$$J_{ij}^{SC} = J_{ij} - 4V_{ij}/3 \quad (3.3)$$

parameterizes the instability in the SC channel.

By minimizing the free-energy for the value $J^{SC} = 0$ for different values of J^{BDW} , we find that the non-interacting ground state is unstable towards the formation of a BDW of the form shown in Fig. 2 for $J^{BDW} \geq 2.4$ at a temperature $T = 0.1$. Alternatively, it is possible to study the formation of the BDW state without breaking the superconducting $U(1)$ symmetry by setting the initial value of $Q = 0$. Note that the ordered state is essentially that found in the quadratic instability computation of Ref. 21: it is a bond-ordered state with bi-directional order at the wavevectors $\approx (\pm H_0, \pm H_0)$ and an internal d -wave angular momentum for the particle-hole pair. Next, we introduce a magnetic field, as mentioned previously, with one electronic flux quantum per the 24×24 lattice: this corresponds to a relatively large field of $\sim 14T$. As described at the end of Sec. II and Appendix A, the magnetic field is introduced by adding a complex phase to the hopping parameters in Eq. 2.1 that corresponds to the vector potential from the magnetic field. Even at this relatively large field we find a negligible effect of the magnetic field on the wave-vector of the BDW order parameter.

On introducing a finite value for the superconducting coupling constant $J^{SC} \neq 0$ in the absence of a magnetic field one expects a finite value of the superconducting order parameter. Since the BDW does not gap the entire Fermi surface and the superconducting instability is guaranteed to occur for attractive interactions at sufficiently low temperatures, one expects to find SC coinciding with BDW at small J^{SC} at low temperatures. The presence of the BDW reduces the superconducting transition temperature and the order parameter, but does not eliminate the SC state completely. This indicates a competition between the two phases.

The competition between BDW and SC is seen clearly from Fig. 3. At sufficiently high $T > 0.11$, the SC order parameter vanishes even though in the range of T considered here, the BDW order parameter with a structure similar to that shown in Fig. 2 exists. As one lowers the temperature, in the presence of BDW, one sees the onset of a SC order parameter below $T < 0.11$. As expected from the exchange interaction J_{ij} the superconductivity is of d -wave symmetry as is manifest from the difference between the signs of the order parameters on the horizontal and vertical bonds in Fig. 4(a). In the intermediate

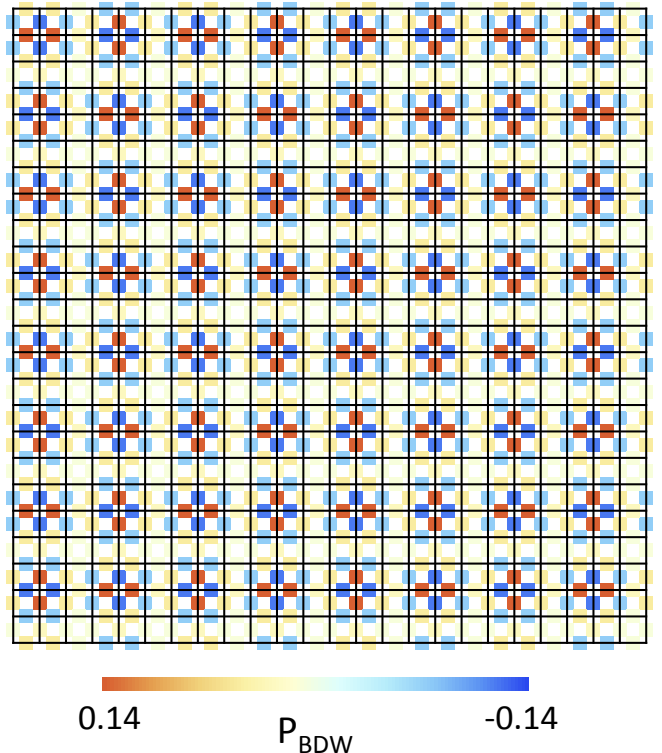


FIG. 2: BDW order parameter plotted on the 24×24 unit cell at $J^{SC} = 0$ and $J^{BDW} = 2.4$ (defined in the text) in the absence of a B-field. The lines intersect on the lattice (Cu) sites, while the colored squares on the bonds (O sites) represent the values of P_{ij} on each bond. By Fourier transforming, we find that the BDW contains Fourier components at both $(\pi/3, \pm\pi/3)$, whose magnitude and direction essentially coincide with those found in previous work²¹. Our calculation shows that the checker-board pattern with both wave-vectors co-existing is the energetically favored result. Repeating the calculation at a finite magnetic field with one electronic flux quantum per unit cell does not significantly alter this pattern.

regime of temperature $0.085 < T < 0.11$, for the parameters in Fig. 3, one finds coexistence between BDW and SC order parameters. On the other hand as T is reduced further below $T < 0.085$ the SC amplitude increases sufficiently so that it dominates over the BDW order. At this point, the coexistent state between the SC and BDW becomes energetically unfavorable compared to the pure SC state and the BDW order parameter jumps to zero in a transition that is first order within mean-field theory. At the same temperature $T \sim 0.085$ the SC also increases discontinuously.

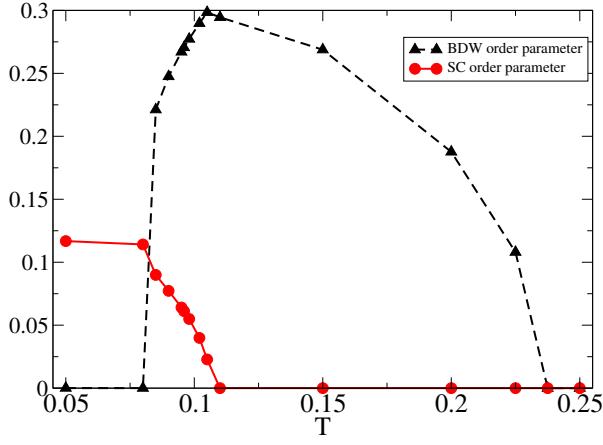


FIG. 3: BDW and SC order parameter as a function of temperature T (in units where $t_1 = 1$) demonstrates coexistence and competition between the order parameters. For this plot we choose $J^{SC} = 1.8$ and $J^{BDW} = 2.8$.

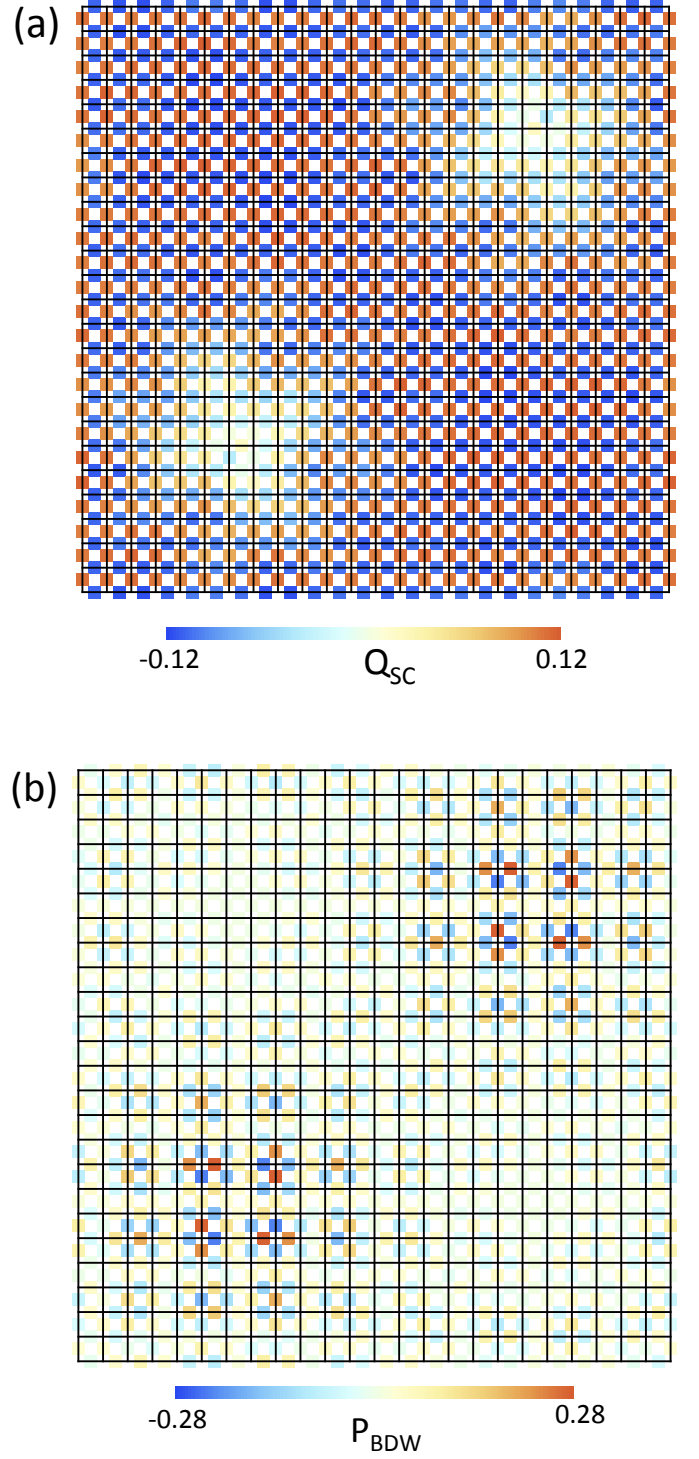


FIG. 4: (a) Real part of superconducting order parameter in the presence of a magnetic field. The SC order parameter shows the d -wave symmetry as a difference of signs between horizontal and vertical bonds. The SC order parameter is suppressed near the vortex core. (b) The suppression of the SC order parameter allows the nucleation of a BDW halo near the vortex core. For this plot we have chosen $J^{SC} = 1.9$ and $J^{BDW} = 2.8$ and $T = 0.09$, which is near the coexistence region.

The application of a magnetic field leads to interesting behavior in the vicinity of the coexistence region of the BDW and SC order parameters. The magnetic field is introduced using a vector potential, as discussed at the end of Sec. II, and leads to a pair of vortex cores per unit cell where the SC order parameter is suppressed as seen in Fig. 4(a). As seen in Fig. 4(b), the suppression of the SC order parameter near the vortex core favors the nucleation of a BDW halo near the vortex core. This is expected from Fig. 3 where we see that a large SC order parameter destabilizes the BDW order parameter at low temperatures. Similarly, one might expect that the large SC order parameter far from the vortex core might destabilize the BDW state.

IV. HOT SPOT MODEL

Our solution of the full lattice model in Section III only found stable charge order at the wavevectors $(H_0, \pm H_0)$ defined from the hot spots in Fig. 1. This suggests that we may be able extract similar physics in a model which focuses only on the vicinity of the hotspots. We will propose such a model here, and show that it allows rapid computation of the equilibrium phase diagram; the model has similarities to the structure of earlier studies of the competition between commensurate spin density wave order and superconductivity³⁸. However, our model cannot be extended to spatially inhomogeneous situations, as it is defined in momentum space, and introduces an artificial sharp cutoff at the end of Fermi arcs.

We introduce 4 species of fermions $\Psi_{a\alpha}$, $a = 1 \dots 4$, $\alpha = \uparrow, \downarrow$ which reside in the vicinities of 4 of the hot spots, as shown in Fig. 5. Their dispersions are defined by the momentum space theory

$$H_0 = \sum_{\mathbf{k}} \left[\epsilon_1(\mathbf{k}) \Psi_{1\alpha}^\dagger(\mathbf{k}) \Psi_{1\alpha}(\mathbf{k}) + \epsilon_2(\mathbf{k}) \Psi_{2\alpha}^\dagger(\mathbf{k}) \Psi_{2\alpha}(\mathbf{k}) + \epsilon_1(-\mathbf{k}) \Psi_{3\alpha}^\dagger(\mathbf{k}) \Psi_{3\alpha}(\mathbf{k}) + \epsilon_2(-\mathbf{k}) \Psi_{4\alpha}^\dagger(\mathbf{k}) \Psi_{4\alpha}(\mathbf{k}) \right]. \quad (4.1)$$

We take the origin of momentum space at the hot spots, and orient the x -axis orthogonal to the Fermi surface for the $\Psi_{1,3}$ fermions; so we can write

$$\epsilon_1(\mathbf{k}) = k_x + \gamma k_y^2. \quad (4.2)$$

We have taken the Fermi velocity to be unit, while γ measures the curvature of the Fermi surface. The dispersion $\epsilon_2(\mathbf{k})$ has the form obtained by rotating $\epsilon_1(\mathbf{k})$ so that the direction orthogonal to the Fermi surfaces of the $\Psi_{2,4}$ has a linear dispersion; we will not need its explicit form and so do not write it out. We chose the convenient momentum space cutoffs $-\Lambda < k_x, k_y < \Lambda$, and $\sum_{\mathbf{k}} \equiv \int d^2k/\Lambda^2$, and the value $\gamma = 1/\Lambda$. Here $\Lambda \ll \pi$ in the units of the underlying lattice, so that we are only accounting for the immediate vicinities of the hot spots.

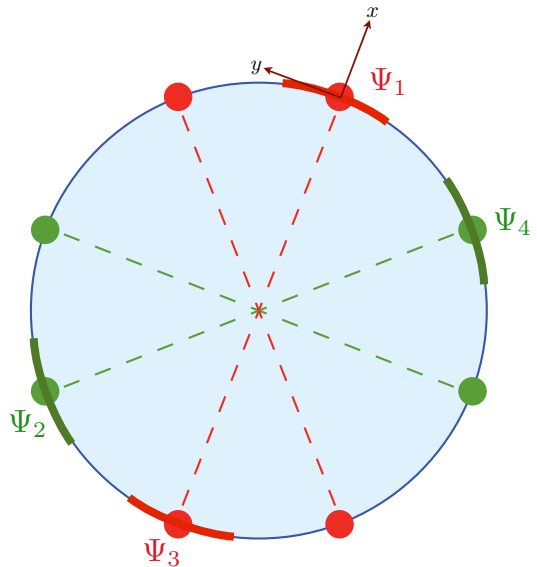


FIG. 5: Definitions of the $\Psi_{1,2,3,4}$ fermions around the Fermi surface. Each fermion resides around a curved patch of the Fermi surface shown by the thick lines. The Fermi surface is centered at the corners of the Brillouin zone shown in Fig. 1. The red (green) hot spots are where the superconducting and bond density wave orders are positive (negative).

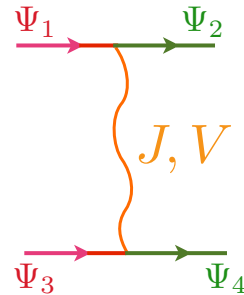


FIG. 6: Interactions between the $\Psi_{1,2,3,4}$ fermions.

However, by rescaling momenta and all the couplings in our continuum model we can change the value Λ , and we use units in which $\Lambda = \pi$.

Next, we add interactions between these fermions. For this, we simply include the J and V terms of the lattice model, and project out the terms which lead to scattering between the hotspots, as illustrated in Fig. 6. This gives us

$$H_1 = \int d^2x \left[-J \left(\Psi_{1\alpha}^\dagger \vec{\sigma}_{\alpha\beta} \Psi_{2\beta} + \Psi_{2\alpha}^\dagger \vec{\sigma}_{\alpha\beta} \Psi_{1\beta} \right) \cdot \left(\Psi_{3\gamma}^\dagger \vec{\sigma}_{\gamma\delta} \Psi_{4\delta} + \Psi_{4\gamma}^\dagger \vec{\sigma}_{\gamma\delta} \Psi_{3\delta} \right) - V \left(\Psi_{1\alpha}^\dagger \Psi_{2\alpha} + \Psi_{2\alpha}^\dagger \Psi_{1\alpha} \right) \left(\Psi_{3\beta}^\dagger \Psi_{4\beta} + \Psi_{4\beta}^\dagger \Psi_{3\beta} \right) \right] \quad (4.3)$$

The full Hamiltonian $H_0 + H_1$ has an exact

$SU(2) \times SU(2)$ pseudospin rotation symmetry¹⁸ when $\gamma = 0$ (so that there is no Fermi surface curvature) and $V = 0$.

We now proceed with the Hartree-Fock-BCS theory of the hotspot model $H_0 + H_1$. This is now straightforward because it is easy to identify the bond density wave order parameter as the particle-hole pair condensate of fermions on antipodal points of the Fermi surface. We therefore introduce the condensates

$$\begin{aligned}\Delta_1(\mathbf{k}) &= \langle \varepsilon_{\alpha\beta} \Psi_{1\alpha}^\dagger(\mathbf{k}) \Psi_{3\beta}^\dagger(-\mathbf{k}) \rangle \quad ; \quad \Delta_1 \equiv \sum_{\mathbf{k}} \Delta_1(\mathbf{k}) \\ \Delta_2(\mathbf{k}) &= \langle \varepsilon_{\alpha\beta} \Psi_{2\alpha}^\dagger(\mathbf{k}) \Psi_{4\beta}^\dagger(-\mathbf{k}) \rangle \quad ; \quad \Delta_2 \equiv \sum_{\mathbf{k}} \Delta_2(\mathbf{k}) \\ \Pi_1(\mathbf{k}) &= \langle \Psi_{1\alpha}^\dagger(\mathbf{k}) \Psi_{3\alpha}(\mathbf{k}) \rangle \quad ; \quad \Pi_1 \equiv \sum_{\mathbf{k}} \Pi_1(\mathbf{k}) \\ \Pi_2(\mathbf{k}) &= \langle \Psi_{2\alpha}^\dagger(\mathbf{k}) \Psi_{4\alpha}(\mathbf{k}) \rangle \quad ; \quad \Pi_2 \equiv \sum_{\mathbf{k}} \Pi_2(\mathbf{k})\end{aligned}\quad (4.4)$$

The superconducting order parameters are $\Delta_{1,2}$, while the bond density wave order parameters are $\Pi_{1,2}$. We will find that optimal state has a d -wave signature for both the superconducting and bond orders, with $\Delta_1 = -\Delta_2$ and $\Pi_1 = -\Pi_2$. With the above orders, the mean field Hamiltonian is

$$\begin{aligned}H_{MF} &= H_0 + \frac{(3J - V)}{2} \left(-\Delta_1 \varepsilon_{\alpha\beta} \Psi_{2\alpha}(\mathbf{k}) \Psi_{4\beta}(-\mathbf{k}) \right. \\ &\quad + \Delta_2^* \varepsilon_{\alpha\beta} \Psi_{1\alpha}^\dagger(\mathbf{k}) \Psi_{3\beta}^\dagger(-\mathbf{k}) - \Delta_2 \varepsilon_{\alpha\beta} \Psi_{1\alpha}(\mathbf{k}) \Psi_{3\beta}(-\mathbf{k}) \\ &\quad \left. + \Delta_1^* \varepsilon_{\alpha\beta} \Psi_{2\alpha}^\dagger(\mathbf{k}) \Psi_{4\beta}^\dagger(-\mathbf{k}) \right) \\ &\quad + \frac{(3J + V)}{2} \left(\Pi_1 \Psi_{4\alpha}^\dagger(\mathbf{k}) \Psi_{2\alpha}(\mathbf{k}) + \Pi_2^* \Psi_{1\alpha}^\dagger(\mathbf{k}) \Psi_{3\alpha}(\mathbf{k}) \right. \\ &\quad \left. + \Pi_2 \Psi_{3\alpha}^\dagger(\mathbf{k}) \Psi_{1\alpha}(\mathbf{k}) + \Pi_1^* \Psi_{2\alpha}^\dagger(\mathbf{k}) \Psi_{4\alpha}(\mathbf{k}) \right).\end{aligned}\quad (4.5)$$

We diagonalize this Hamiltonian by writing the Hamiltonian for $\Psi_{1,3}$ as

$$\begin{aligned}H_{MF} &= \sum_{\mathbf{k}} \left(\Psi_{1\uparrow}^\dagger(\mathbf{k}), \Psi_{3\uparrow}^\dagger(\mathbf{k}), \Psi_{1\downarrow}(-\mathbf{k}), \Psi_{3\downarrow}(-\mathbf{k}) \right) M(\mathbf{k}) \\ &\quad \times \begin{pmatrix} \Psi_{1\uparrow}(\mathbf{k}) \\ \Psi_{3\uparrow}(\mathbf{k}) \\ \Psi_{1\downarrow}^\dagger(-\mathbf{k}) \\ \Psi_{3\downarrow}^\dagger(-\mathbf{k}) \end{pmatrix} + \sum_{\mathbf{k}} (\epsilon_1(-\mathbf{k}) + \epsilon_1(\mathbf{k})),\end{aligned}\quad (4.6)$$

where the 4×4 matrix $M(\mathbf{k})$ is

$$M(\mathbf{k}) = \begin{pmatrix} \epsilon_1(\mathbf{k}) & (3J + V)\Pi_2^*/2 & 0 & 0 \\ (3J + V)\Pi_2/2 & \epsilon_1(-\mathbf{k}) & (3J - V)\Delta_2/2 & 0 \\ 0 & (3J - V)\Delta_2/2 & 0 & (3J - V)\Delta_2^*/2 \\ (3J - V)\Delta_2^*/2 & 0 & -\epsilon_1(-\mathbf{k}) & -(3J + V)\Pi_2/2 \\ -\epsilon_1(-\mathbf{k}) & -(3J + V)\Pi_2/2 & 0 & -\epsilon_1(\mathbf{k}) \end{pmatrix} \quad (4.7)$$

Let $U(\mathbf{k})$ be the unitary matrix which diagonalizes $M(\mathbf{k})$:

$$U^\dagger(\mathbf{k}) M(\mathbf{k}) U(\mathbf{k}) = \Lambda(\mathbf{k}) \quad (4.8)$$

where $\Lambda(\mathbf{k})$ is a diagonal matrix with entries $\lambda_i(\mathbf{k})$. Then

$$\begin{aligned}\sum_{\mathbf{k}} \langle \Psi_{1\uparrow}^\dagger(\mathbf{k}) \Psi_{3\uparrow}(\mathbf{k}) \rangle &= \sum_{\mathbf{k}} \sum_i U_{1i}^*(\mathbf{k}) U_{2i}(\mathbf{k}) f(\lambda_i(\mathbf{k})) \\ &\equiv \tilde{\Pi}_1/2 \\ \sum_{\mathbf{k}} \langle \Psi_{1\downarrow}^\dagger(-\mathbf{k}) \Psi_{3\downarrow}(-\mathbf{k}) \rangle &= -\sum_{\mathbf{k}} \sum_i U_{3i}(\mathbf{k}) U_{4i}^*(\mathbf{k}) f(\lambda_i(\mathbf{k})) \\ &\equiv \tilde{\Pi}_1/2 \\ \sum_{\mathbf{k}} \langle \Psi_{1\uparrow}^\dagger(\mathbf{k}) \Psi_{3\downarrow}^\dagger(-\mathbf{k}) \rangle &= \sum_{\mathbf{k}} \sum_i U_{1i}^*(\mathbf{k}) U_{4i}(\mathbf{k}) f(\lambda_i(\mathbf{k})) \\ &\equiv \tilde{\Delta}_1/2 \\ \sum_{\mathbf{k}} \langle \Psi_{1\downarrow}^\dagger(-\mathbf{k}) \Psi_{3\uparrow}^\dagger(\mathbf{k}) \rangle &= -\sum_{\mathbf{k}} \sum_i U_{3i}(\mathbf{k}) U_{2i}^*(\mathbf{k}) f(\lambda_i(\mathbf{k})) \\ &\equiv -\tilde{\Delta}_1/2\end{aligned}\quad (4.9)$$

Assuming the state with $\Delta_1 = -\Delta_2$ and $\Pi_1 = -\Pi_2$, the free energy is

$$\begin{aligned}\frac{F}{2} &= F_{MF} + \left\langle \frac{H}{2} - H_{MF} \right\rangle_{MF} \\ &= \sum_{\mathbf{k}} (\epsilon_1(-\mathbf{k}) + \epsilon_1(\mathbf{k})) - T \sum_{\mathbf{k}} \sum_i \ln \left(1 + e^{-\lambda_i(\mathbf{k})/T} \right) \\ &\quad + \frac{(3J - V)}{2} \left(-\tilde{\Delta}_1^* \tilde{\Delta}_1 + \tilde{\Delta}_1^* \tilde{\Delta}_1 + \tilde{\Delta}_1^* \tilde{\Delta}_1 \right) \\ &\quad + \frac{(3J + V)}{2} \left(-\tilde{\Pi}_1^* \tilde{\Pi}_1 + \tilde{\Pi}_1^* \tilde{\Pi}_1 + \tilde{\Pi}_1^* \tilde{\Pi}_1 \right).\end{aligned}\quad (4.10)$$

We determined the phase diagrams by solving the above mean-field equations for $J_1 = 1.2$, and the phase diagrams as a function of V are in Fig. 7. Note the similar-

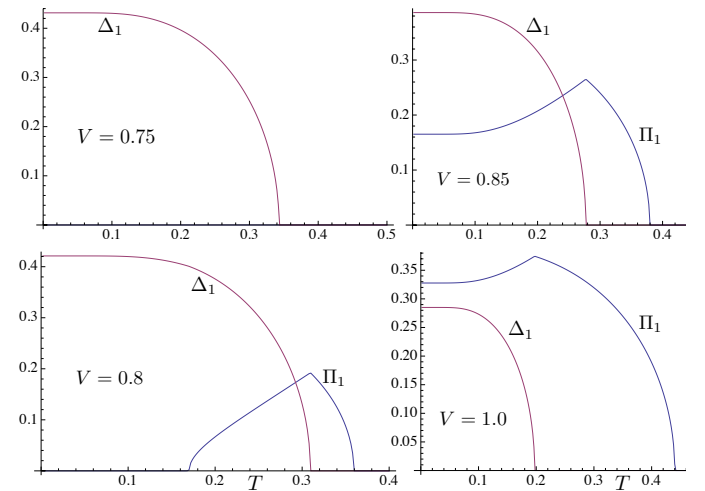


FIG. 7: Superconducting (Δ_1) and bond (Π_1) orders in the hot spot model as a function of T and V for $J = 1.2$.

ity of the T evolution in the region of co-existing orders to that obtained in the solution of the full lattice model earlier in Fig. 3.

The basic features of Figs. 7 can be understood by interplay between the two terms which break the pseudospin symmetry: the Fermi surface curvature γ (which prefers superconductivity) and the nearest-neighbor Coulomb repulsion, V (which prefers bond order). When $\gamma = V = 0$, the two orders are degenerate, and the free energy can be shown to depend only upon $|\Delta_1|^2 + |\Pi_1|^2$. This is a consequence of the pseudospin symmetry, and any co-existence state with the same overall magnitude is also degenerate. When we turn on only γ , but keep $V = 0$, superconductivity appears first upon lowering T ; this gaps out the Fermi surface completely (in the present hotspot model), and bond order never appears down to the lowest T . The same situation remains when a small $V > 0$ is turned on, and indeed as long as superconductivity is the first instability upon lowering T . On the other hand, when V is large enough and positive, the first instability upon lowering T is to bond order. At its initial onset, the bond order only gaps out the Fermi surface in the immediate vicinity of the hot spots, but a reconstructed Fermi surface does appear; see Fig. 8.

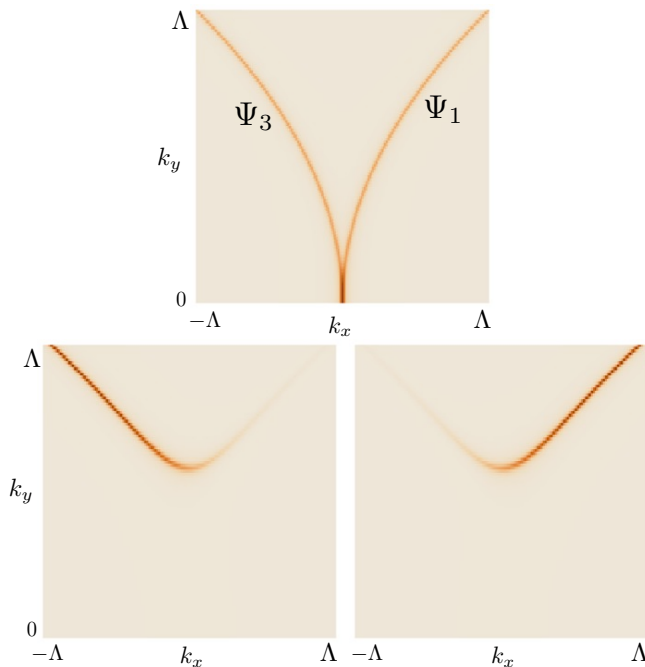


FIG. 8: Spectral density of the Ψ_1 and Ψ_3 fermions at zero frequency. The top figure shows both fermions in the metal with no ordering, and so plots $\epsilon_1(\pm\mathbf{k})$ from Eq. (4.2). These Fermi surfaces are those in Fig. 5, but shifted in momentum space so that their hotspots coincide. The displayed momenta are in a small vicinity of the hotspots, with momentum cutoffs are $\pm\Lambda$. The bottom figures show the spectral densities of $\Psi_{1,3}$ respectively in the presence of bond density wave order, $\Pi_1 \neq 0$. Note that this opens up a gap near $\mathbf{k} = 0$, but reconstructed Fermi surfaces remain.

At lower T , this reconstructed Fermi surface undergoes a BCS instability, yielding a state with co-existing superconductivity and bond order. And as we lower T further, the superconductivity continues to increase in strength at the expense of the bond order: this is because the superconductivity has the Cooper-logarithm in its susceptibility irrespective of the Fermi surface curvature, while the bond order is suppressed by the Fermi surface curvature.

V. CONCLUSIONS

A shortcoming in the experimental applications of the present mean-field computations of the t - J - V model is that they have consistently preferred an incommensurate d -wave charge density wave order along the $(1, \pm 1)$ directions. This is in contrast to previous treatments^{40–43} of the t - J - V model at $T = 0$ in the superconducting state, which also imposed an on-site $U = \infty$ constraint in a particular large N limit; the latter computations found commensurate d -wave bond order, but oriented along the $(1, 0)$, $(0, 1)$ directions, as in the experimental observations.^{5–7} On the other hand, in these $U = \infty$ computations, the Fermi surface structure appeared to play no role in determining the magnitude of the ordering wavevector. This suggests to us that it would be worthwhile to examine the instabilities of the t - J - V model in the high temperature normal state, while also imposing the $U = \infty$ constraint: such a computation could determine the mechanism of the orientation of the ordering wavevector, while also displaying the role of the Fermi surface and the hot spots.

Our present results, along with the recent results of Ref. 9, also suggest a recipe for obtaining higher critical temperatures for superconductivity. The point made in Ref. 9 is that it is the combined instabilities of the high temperature metal to superconductivity and charge order which lead to a large regime of fluctuations in the pseudogap regime. So we need to suppress the charge ordering instability, while preserving superconductivity. The model of Section IV showed this can be achieved by increasing the Fermi surface curvature. At the same time, we need a large J to maintain the pairing instability. We note that large Fermi surface curvatures are found in the pnictides, which have so far not shown any charge-ordering instabilities, as expected in our approach; on the other hand, the larger J 's are in the cuprates. It would therefore be worthwhile to search for quasi-two-dimensional compounds which combine these desirable features of the existing high temperature superconductors.

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Appendix A: Magnetic field BDW/SC

In this section we discuss how we choose the lattice vector potential for the Hamiltonian following Wang and Vafeek⁴⁴. The magnetic field enters Eq. (2.7) through the phase a_{ij} . We note that the gauge transformation in the Hamiltonian takes the form

$$\begin{aligned} c_{i,\sigma}^\dagger &\rightarrow c_{i,\sigma}^\dagger e^{i\Lambda_i} \\ a_{ij} &\rightarrow a_{ij} - (\Lambda_i - \Lambda_j). \end{aligned} \quad (\text{A1})$$

Neither the orders P, Q defined in the previous sections are invariant under the gauge transformation. However

$$\mathcal{P}_{ij} = e^{-ia_{ij}} \langle c_{i,\sigma}^\dagger c_{j,\sigma} \rangle. \quad (\text{A2})$$

Similarly $\tilde{\rho}_{P,i,j} = e^{-ia_{ij}} \rho_{P,i,j}$ is a gauge-invariant version of ρ_P . The superconducting order parameter Q breaks gauge invariance and there is no gauge invariant form of Q .

A choice of a_{ij} formally breaks translation invariance since if \mathbf{A} were periodic in some unit cell its integral around the boundary would have to vanish forcing the flux in the unit cell to be zero. However, translation invariance can be recovered in a lattice system by performing a "singular" gauge transformation where one threads one quantum of flux Φ_0 through a single plaquette of the lattice. Since this has no effect on lattice electrons, we can choose \mathbf{A} to be periodic and satisfy

$$\nabla \times \mathbf{A} = (B - \Phi_0 \delta(\mathbf{r})) \hat{z}. \quad (\text{A3})$$

For a lattice system we use the discrete curl to state this as

$$A_v(\mathbf{r}) - A_h(\mathbf{r}) + A_h(\mathbf{r} + \hat{y}) - A_v(\mathbf{r} + \hat{x}) = \Phi(\mathbf{r}), \quad (\text{A4})$$

where $A_{v,h}(\mathbf{r})$ are the phases associated with the bonds connecting $\mathbf{r} \rightarrow \mathbf{r} + \hat{y}$ and $\mathbf{r} \rightarrow \mathbf{r} + \hat{x}$ respectively. The flux $\Phi(\mathbf{r})$ is contained in the plaquette surrounded by the lattice sites $\mathbf{r}, \mathbf{r} + \hat{y}, \mathbf{r} + \hat{x} + \hat{y}, \mathbf{r} + \hat{x}$ i.e. it is the plaquette containing \mathbf{r} at its bottom left corner.

The vector potential $A(\mathbf{r})$ is gauge dependent. For the purpose of representing vortices, we choose the gauge which minimizes the magnitude of A i.e. $F = \int d\mathbf{r} |\nabla A|^2$. This gauge has vanishing discrete divergence

$$A_v(\mathbf{r} + \hat{y}) - A_v(\mathbf{r}) + A_h(\mathbf{r} + \hat{y}) - A_h(\mathbf{r} + \hat{y} - \hat{x}) = 0. \quad (\text{A5})$$

The above divergenceless condition is solved by defining A in terms of plaquette variables $\psi(\mathbf{r})$ (defined similar to

$\Phi(\mathbf{r})$) so that we define

$$\begin{aligned} A_v(\mathbf{r} + \hat{x}) &= \psi(\mathbf{r} + \hat{x}) - \psi(\mathbf{r}) \\ A_h(\mathbf{r} + \hat{y}) &= -\psi(\mathbf{r} + \hat{y}) + \psi(\mathbf{r}) \\ A_v(\mathbf{r} + \hat{y}) - A_v(\mathbf{r}) + A_h(\mathbf{r} + \hat{y}) - A_h(\mathbf{r} + \hat{y} - \hat{x}) \\ &= \psi(\mathbf{r} + \hat{y}) - \psi(\mathbf{r} + \hat{y} - \hat{x}) - \psi(\mathbf{r}) + \psi(\mathbf{r} - \hat{x}) \\ &\quad - \psi(\mathbf{r} + \hat{y}) + \psi(\mathbf{r}) + \psi(\mathbf{r} + \hat{y} - \hat{x}) - \psi(\mathbf{r} - \hat{x}) = 0, \end{aligned} \quad (\text{A6})$$

which is now manifestly divergenceless.

Substituting into the curl equation we get

$$A_v(\mathbf{r}) - A_h(\mathbf{r}) + A_h(\mathbf{r} + \hat{y}) - A_v(\mathbf{r} + \hat{x}) \quad (\text{A7})$$

$$\begin{aligned} &= 4\psi(\mathbf{r}) - \psi(\mathbf{r} - \hat{x}) - \psi(\mathbf{r} + \hat{x}) - \psi(\mathbf{r} + \hat{y}) - \psi(\mathbf{r} - \hat{y}) \\ &= \Phi(\mathbf{r}). \end{aligned} \quad (\text{A8})$$

The above lattice system is easily solved by Fourier transforms by substituting

$$\begin{aligned} \psi(\mathbf{r}) &= \sum_{\mathbf{G}} \psi_{\mathbf{G}} e^{i\mathbf{G} \cdot \mathbf{r}} \\ \Phi(\mathbf{r}) &= 4 \sum_{\mathbf{G}} \psi_{\mathbf{G}} (\sin^2 G_x/2 + \sin^2 G_y/2) e^{i\mathbf{G} \cdot \mathbf{r}} \\ \Phi(\mathbf{r}) &= \Phi_0 [\delta(\mathbf{r} - \mathbf{r}_1) + \delta(\mathbf{r} - \mathbf{r}_2)] - \frac{2\Phi_0}{N_{lat}} \\ &= \sum_{\mathbf{G}} \Phi_{\mathbf{G}} e^{i\mathbf{G} \cdot \mathbf{r}} \\ \Phi_{\mathbf{G}} &= \frac{1}{N_{lat}} \sum_{\mathbf{r}} \Phi(\mathbf{r}) e^{-i\mathbf{G} \cdot \mathbf{r}} \\ &= \frac{\Phi_0}{N_{lat}} [e^{i\mathbf{G} \cdot \mathbf{r}_1} + e^{i\mathbf{G} \cdot \mathbf{r}_2} - 2\delta_{\mathbf{G}=0}] \\ \psi_{\mathbf{G} \neq 0} &= \frac{\Phi_0}{4N_{lat}(\sin^2 G_x/2 + \sin^2 G_y/2)} [e^{i\mathbf{G} \cdot \mathbf{r}_1} + e^{i\mathbf{G} \cdot \mathbf{r}_2}], \end{aligned} \quad (\text{A9})$$

where $\Phi_0 = 2\pi$.

To minimize the supercurrent, we want to consider a gauge with two spatially separated vortices. This is obtained by placing Φ_0 flux in one of the vortices on the diagonal of a square unit cell and having a diagonal branch-cut connecting the vortex to the other vortex on the diagonal. The sign of the hopping $t_{jj'}$ is flipped along the diagonal branch-cut. While this gauge is arbitrary, the phase of the superconducting order parameter is expected to be close to uniform in this gauge.

Appendix B: Evaluating gradients of free-energy F

For the minimization of the free-energy we need to compute the gradient of the free-energy F in Eq. (2.12). Writing the order parameter operators \tilde{P} and \tilde{Q} as $\langle U_n \rangle$ and the potential amplitudes as λ_n , we can write the

free-energy in Eq. 2.12 in the form

$$\begin{aligned} F[\lambda] &= F_{MF}[\lambda] = \sum_n L_{n,n} \langle U_n \rangle^2 - \lambda_n \langle U_n \rangle + F_{HF} \\ F_{HF} &= -T \text{Tr}[\log(\cosh \beta H_0)] \\ &= -T \sum_n -\epsilon_n + \log(1 + e^{-\beta \epsilon_n(\lambda)}) \end{aligned} \quad (\text{B1})$$

where ϵ_n are eigenvalues of H_0 . Using a Taylor expansion in λ we note that the first derivative of F_{HF} depends only on the diagonal in energy terms of U i.e.

$$\partial_{\lambda_n} F_{HF} = \sum_p \frac{U_{n,p,p}}{1 + e^{\beta \epsilon_p}} = \text{Tr}[U_n (1 + e^{\beta H_0})^{-1}] \quad (\text{B2})$$

$$= \langle U_n \rangle. \quad (\text{B3})$$

Similarly, the second derivative can involve only two states p, q at a time and therefore can be derived by considering a 2×2 matrix to be

$$\begin{aligned} \partial_{\lambda_n, \lambda_m} F_{HF} &= \\ &= - \sum_{p,q} U_{n,p,q} U_{m,q,p} \frac{\tanh(\epsilon_p/2T) - \tanh(\epsilon_q/2T)}{2(\epsilon_p - \epsilon_q)}, \end{aligned} \quad (\text{B4})$$

where one is careful to take the limit $\epsilon_p - \epsilon_q \rightarrow 0$ for the diagonal terms $p = q$. Using these results

$$\partial_{\lambda_p} F_{MF}[\lambda] = \sum_n \partial_{\lambda_p} \langle U_n \rangle (2L_{n,n} \langle U_n \rangle - \lambda_n) \quad (\text{B5})$$

$$= \sum_n (2L_{n,n} \langle U_n \rangle - \lambda_n) \partial_{\lambda_n, \lambda_p} F_{HF}. \quad (\text{B6})$$

Using the definiteness of the derivative $\partial_{\lambda_n, \lambda_p} F_{HF}$, we note that the minimum of the free-energy, which satisfies $\partial_{\lambda} F_{MF} = 0$ also satisfies the mean field equations

$$\lambda_n = 2L_{n,n} \langle U_n \rangle. \quad (\text{B7})$$

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