

Enhancement of superconducting T_c due to the spin-orbit interaction

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We calculate the superconducting T_c for a system which experiences Rashba spin-orbit interactions. Contrary to the usual case where the electron-electron interaction is assumed to be wave vector independent, where superconductivity is suppressed by the spin-orbit interaction (except for a small region at low electron or hole densities), we find an enhancement of the superconducting transition temperature when we include a correlated hopping interaction between electrons. This interaction originates in the expansion of atomic orbitals due to electron-electron repulsion and gives rise to superconductivity only at high electron (low hole) densities. When superconductivity results from this interaction it is enhanced by spin-orbit coupling, in spite of a suppression of the density of states. The degree of electron-hole asymmetry about the Fermi surface is also enhanced.

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I. INTRODUCTION

Spin-orbit coupling is prevalent in condensed matter systems and can have a profound impact on the properties of metals and insulators [1,2], not just at surfaces, but in the bulk. For superconductivity, the spin-orbit interaction was invoked immediately following BCS [3], mainly to address discrepancies in the Knight shift measurements [4,5] and the predictions from BCS theory [6–10].

More recently, as more superconductors with a crystal structure that lacked a center of inversion symmetry were becoming common, this discussion was revived [11,12], utilizing the Rashba model of spin-orbit coupling [13,14], and once again focusing attention on the nonzero Knight shift at low temperature. These papers also explicitly identified the novel feature in these superconductors: a mixed singlet-triplet state, which was implicit all along since spin had been identified in the early work as *not* a good quantum number. The impact on thermodynamic properties (including the superconducting critical temperature, T_c) was not really considered. Indeed, in Anderson's initial treatment of this problem [9], he essentially repeated the arguments made in his more famous “Dirty Superconductors” paper [15], but now for spin-orbit coupling, with the implication that for weak spin-orbit coupling T_c would be unaffected.

A few years later it was pointed out that in principle a large enhancement in T_c could occur because of an enhancement in the electronic density of states in the low-density region, due to an effective “dimensionality reduction” [16]. However, as we further demonstrate below, this enhancement is confined to a rather narrow electron density window, and the overall scale of T_c is low for a weakly coupled system.

An interesting general question remains, which is the impact of the Rashba spin-orbit interaction on superconducting T_c in the presence of different types of pairing interactions. Some calculations have been recently performed in Ref. [17] for the extended Hubbard model. The generic short-range attractive interaction (e.g., the attractive Hubbard model) already results in a mixed singlet-triplet state due to the spin-orbit interaction.

However, as we will show (and also found in Ref. [17]), in that case the spin-orbit interaction suppresses superconductivity. In this paper we include a specific off-diagonal term in the interaction, previously considered by two of us [18], in the context of cuprate superconductivity. This interaction is noteworthy in that it has the form of an off-diagonal matrix element of the Coulomb interaction between electrons in Wannier orbitals, rather than a diagonal matrix element representing a density-density repulsion or attraction. As explained at length previously [19–21], the so-called “correlated hopping” interaction arises inevitably because the many-body electron wave functions make significant adjustments to minimize the energy associated with Coulombic repulsions.

In the following section we will introduce the model and briefly discuss some important one-electron properties. These determine the appropriate basis with which we consider the pairing interaction, the so-called Rashba basis. We follow the usual BCS description for the pairing state; this leads to a simple parametrization of the wave-vector dependence of the order parameter, in the presence of spin-orbit coupling. We then present results for T_c as a function of the various interaction strengths and as a function of the electron density. In general, with the correlated hopping interaction present, spin-orbit coupling leads to a significant enhancement of superconducting T_c . We then end with a summary.

II. TIGHT-BINDING HAMILTONIAN, INCLUDING CORRELATED HOPPING AND SPIN-ORBIT COUPLING

As described in earlier work [18,22], a tight-binding model that includes both the on-site Hubbard “ U ” interaction and the correlated hopping term Δt is

$$H_{\text{Mod}} = -t \sum_{\langle ij \rangle} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) + U \sum_i n_{i\uparrow} n_{i\downarrow} \quad (1)$$

$$+ \Delta t \sum_{\langle ij \rangle} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) (n_{i-\sigma} + n_{j-\sigma}). \quad (2)$$

Here, $c_{i\sigma}^\dagger$ creates an electron on site i with spin $\sigma = \uparrow, \downarrow$, and $\langle ij \rangle$ means that we only consider hopping between nearest-neighbor sites i, j . In what follows we will assume a square lattice. The tight-binding parameters are the hopping integral t , the on-site repulsion U , and the correlated hopping parameter Δt , described in detail in [18]. Briefly, this term represents the fact that electrons will hop with an altered hopping parameter when other electrons are nearby. It was considered by Hubbard in his original publication on the Hubbard model [23] and then dropped as he focused on the on-site interaction alone.

We add to this Hamiltonian a Rashba spin-orbit coupling term [13]. Such a term is generic for systems that either lack inversion symmetry [24] or experience some Fermi surface instability [25] while maintaining time-reversal symmetry as well as a uniaxial symmetry. For a square lattice, the most generic spin-dependent quadratic hopping term, restricted to nearest neighbors, is

$$H_{SO} = \sum_{i\alpha\beta} (c_{i\alpha}^\dagger \vec{a} \cdot \vec{\sigma}^{\alpha\beta} c_{i+\hat{x},\beta} + c_{i\alpha}^\dagger \vec{b} \cdot \vec{\sigma}^{\alpha\beta} c_{i+\hat{y},\beta} + \text{H.c.}). \quad (3)$$

The uniaxial symmetry to be enforced is a rotation by $\pi/2$ about the $\hat{z}$ axis through each site i . Applying such a rotation to this term using $R_\phi c_{j\alpha} R_\phi^{-1} = e^{-i\alpha\phi} c_{R_\phi^{-1}j,\alpha}$ gives

$$H_{SO} = \sum_{i\alpha\beta} e^{i(\alpha-\beta)\pi/4} (c_{i+\hat{y},\alpha}^\dagger \vec{a} \cdot \vec{\sigma}^{\alpha\beta} c_{i,\beta} + c_{i\alpha}^\dagger \vec{b} \cdot \vec{\sigma}^{\alpha\beta} c_{i+\hat{x},\beta}) + \text{H.c.} \quad (4)$$

Matching this to (3) restricts the values of $\vec{a}$ and $\vec{b}$ to be

$$a_x = 0 = b_y, \quad (5)$$

$$a_y \equiv -iV_{SO} = -b_x. \quad (6)$$

Thus the Rashba hopping term on the direct lattice is

$$H_{SO} = V_{SO} \sum_{i\alpha\beta} (ic_{i\alpha}^\dagger \sigma_x^{\alpha\beta} c_{i+\hat{y},\beta} - ic_{i\alpha}^\dagger \sigma_y^{\alpha\beta} c_{i+\hat{x},\beta}) + \text{H.c.}, \quad (7)$$

where V_{SO} parameterizes the Rashba spin-orbit coupling. In general, this parameter depends on the atomic spin-orbit coupling and on the details of the band structure, and should be determined from experiment or *ab initio* studies [1,26]. The largest values of V_{SO} typically occur at surfaces or interfaces (e.g., BiTeI has $V_{SO}/t \approx 0.8$ [27]). It is important to recognize that in the tight-binding picture, a Rashba term should be present whenever there is inversion asymmetry in the site point group (with some preserved uniaxial symmetry) [28]. This means that even quasi-two-dimensional materials whose crystal structure is centrosymmetric can have bulk Rashba spin splitting if there is polarity in any given plane. This is true, for example, in YBCO, where the yttrium and barium ions on opposite sides of the copper oxide planes produce a local electric dipole moment. For the cuprates, the Rashba parameter has been estimated to be $V_{SO}/t \approx 0.008$ [29]. Larger spin splittings ($V_{SO}/t \approx 0.04$) can be found in the $\text{LaAlO}_3/\text{SrTiO}_3$ interface, which supports a superconducting 2D electron gas, though the magnitude of this splitting is still under debate [30,31].

In a single-band model where the correlated hopping interaction Δt arises simply from an off-diagonal matrix element of the Coulomb interaction between neighboring Wannier orbitals, as discussed by Hubbard [23] and others [22,32], the spin-orbit interaction would not be expected to modify the interaction terms in the Hamiltonian. Instead, within the “dynamic Hubbard model” [19] the interaction Δt arises from the modification of the on-site electron wave function when another electron occupies the site, due to Coulomb repulsion. This effect is modeled by the site Hamiltonian [19],

$$H_i = \omega a_i^\dagger a_i + [U + g\omega(a_i^\dagger + a_i)]n_{i\uparrow}n_{i\downarrow}, \quad (8)$$

where the boson creation and annihilation operators $a_i^\dagger, a_i$ describe the electronic excitations of an electron when a second electron is added to the orbital. A generalized Lang-Firsov transformation [19,33]

$$c_{i\sigma} = e^{g(a_i^\dagger - a_i)\tilde{n}_{i,-\sigma}} \tilde{c}_{i\sigma} \equiv X_{i\sigma} \tilde{c}_{i\sigma} \quad (9)$$

relates the original fermion operators $c_{i\sigma}$ to new fermion quasiparticle operators $\tilde{c}_{i\sigma}$ that both destroy the electron at the site and change the state of the boson so that the boson field follows the fermion motion. Since $X_{i\sigma}^\dagger = X_{i\sigma}^{-1}$, the transformation preserves fermion anticommutation relations. To obtain a low-energy effective Hamiltonian we consider only ground-state to ground-state transitions of the boson field, and in this approximation the relation Eq. (19) becomes [19]

$$c_{i\sigma}^\dagger = [1 - (1 - S)\tilde{n}_{i,-\sigma}] \tilde{c}_{i\sigma}^\dagger, \quad (10)$$

where $S = e^{-g^2/2}$. The on-site repulsion U is lowered to $U_{eff} = U - \omega g^2$, and bilinear terms in fermion operators at different sites transform as follows:

$$c_{i\sigma}^\dagger c_{j\sigma'} = \tilde{c}_{i\sigma}^\dagger \tilde{c}_{j\sigma'} [1 - (1 - S)(\tilde{n}_{i,-\sigma} + \tilde{n}_{j,-\sigma'}) + (1 - S)^2 \tilde{n}_{i,-\sigma} \tilde{n}_{j,-\sigma'}]. \quad (11)$$

We will be interested in the regime where the band is close to full. The coefficient in the parenthesis of Eq. (21) when the occupations are such that $\tilde{n}_{i,-\sigma} + \tilde{n}_{j,-\sigma'} = 1$ is S , and when $\tilde{n}_{i,-\sigma} + \tilde{n}_{j,-\sigma'} = 2$ is S^2 . Their difference is

$$S - S^2 = S(1 - S) \equiv \frac{\Delta t}{t}, \quad (12)$$

which defines the correlated hopping Δt in this model. The term involving Δt in Eq. (2) then results from replacing the bare operators $c_{i\sigma}$ by the quasiparticle operators $\tilde{c}_{i\sigma}$ in the hopping term (and renaming the quasiparticle operators $\tilde{c}_{i\sigma} \rightarrow c_{i\sigma}$), and discarding terms involving six fermion operators that will be unimportant for low hole concentrations [20]. Similarly, the spin-orbit interaction term (7) is modified to

$$H_{SO} = iV_{SO} \sum_{i,\alpha\beta} \left(c_{i,\alpha}^\dagger \sigma_x^{\alpha\beta} c_{i+\hat{y},\beta} \left[1 - \frac{\Delta t}{t} (n_{i,\beta} + n_{i+\hat{y},\alpha}) \right] - c_{i,\alpha}^\dagger \sigma_y^{\alpha\beta} c_{i+\hat{x},\beta} \left[1 - \frac{\Delta t}{t} (n_{i,\beta} + n_{i+\hat{x},\alpha}) \right] \right) + \text{H.c.}, \quad (13)$$

so that the full Hamiltonian of our model is $H_{\text{Mod}} + H_{SO} - \mu \sum_{i,\sigma} n_{i\sigma}$, where μ is the chemical potential.

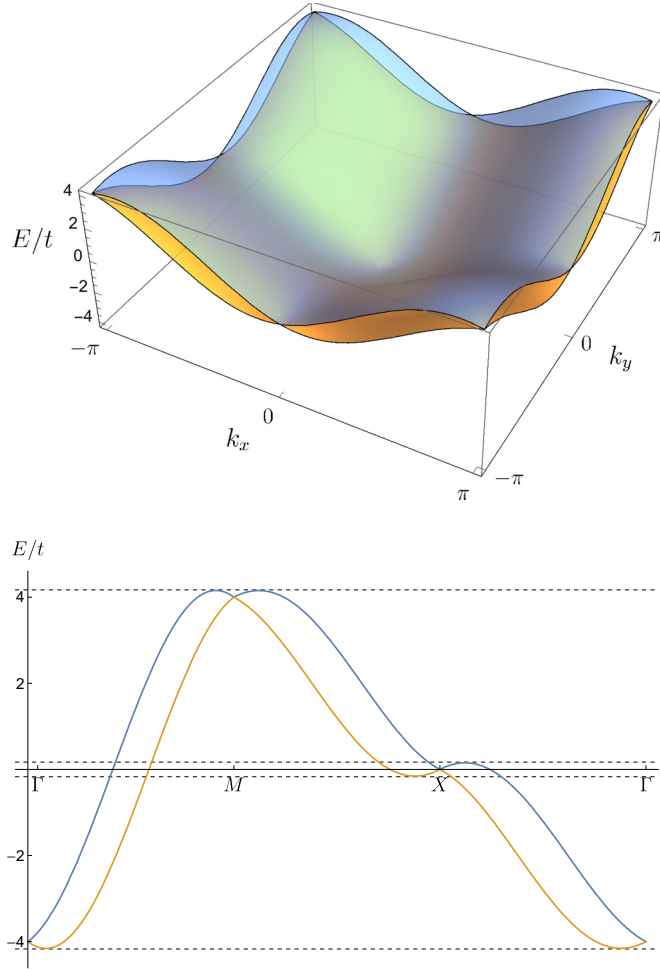


FIG. 1. Free particle Rashba spectrum on a square lattice with $V_{SO} = 0.4t$. The blue and orange bands represent the $s = -1$ and $s = +1$ helicity bands, respectively. The dashed lines in the bottom figure show the locations of Van Hove singularities.

In the usual BCS fashion, we Fourier transform this Hamiltonian and eliminate interactions between pairs with finite momentum to obtain a reduced Hamiltonian

$$\begin{aligned}
 H = & \sum_{\mathbf{k}, \sigma} (\epsilon_{\mathbf{k}} - \mu) c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} - 2V_{SO} \sum_{\mathbf{k}} (\sin k_y (c_{\mathbf{k}\uparrow}^\dagger c_{\mathbf{k}\downarrow} + c_{\mathbf{k}\downarrow}^\dagger c_{\mathbf{k}\uparrow})) \\
 & + i \sin k_x (c_{\mathbf{k}\uparrow}^\dagger c_{\mathbf{k}\downarrow} - c_{\mathbf{k}\downarrow}^\dagger c_{\mathbf{k}\uparrow}) \\
 & + \frac{1}{N} \sum_{\mathbf{k}} V^0(\mathbf{k}, \mathbf{k}') c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger c_{-\mathbf{k}'\downarrow} c_{\mathbf{k}'\uparrow} \\
 & + \frac{1}{N} \sum_{\mathbf{k}\mathbf{k}'} \sum_{\alpha\beta} (V_{\alpha\beta}^R(\mathbf{k}') c_{\mathbf{k}\alpha}^\dagger c_{-\mathbf{k}\beta}^\dagger c_{\mathbf{k}'\alpha} c_{-\mathbf{k}'\beta} \\
 & + V_{\alpha\beta}^R(\mathbf{k}) c_{\mathbf{k}\beta}^\dagger c_{-\mathbf{k}\beta}^\dagger c_{\mathbf{k}'\beta} c_{-\mathbf{k}'\alpha}),
 \end{aligned} \quad (14)$$

where $\epsilon_{\mathbf{k}} \equiv -2t(\cos k_x + \cos k_y)$ and $V^0(\mathbf{k}, \mathbf{k}') \equiv U - 2\frac{\Delta t}{t}(\epsilon_{\mathbf{k}} + \epsilon_{\mathbf{k}'})$ are the dispersion and interaction in the absence of spin-orbit coupling. The correlated hopping and Rashba terms are coupled via the interaction $V_{\alpha\beta}^R(\mathbf{k}) \equiv 2V_{SO}\frac{\Delta t}{t}(\sin k_x \sigma_{\alpha\beta}^y + \sin k_y \sigma_{\alpha\beta}^x)$. Throughout this paper, we work in units where the lattice parameter is unity.

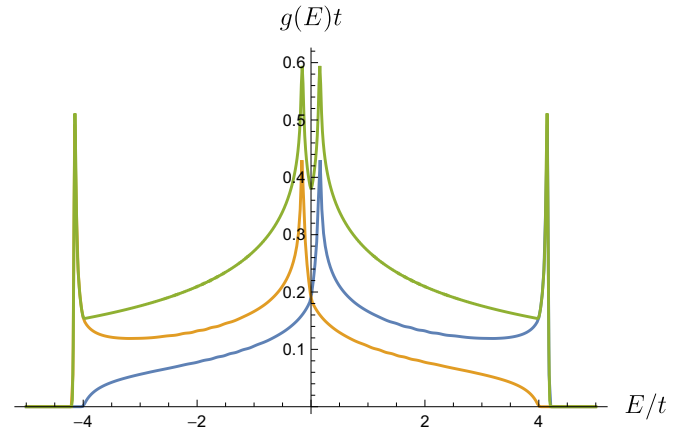


FIG. 2. Noninteracting single-particle Rashba density of states on a square lattice for the lower helicity band (orange), upper helicity band (blue), and the two combined (green). Here we have set $V_{SO} = 0.4t$.

The first two lines above constitute the noninteracting Hamiltonian, which is diagonalized in the Rashba basis to produce a spectrum

$$\epsilon_{ks} = \epsilon_k - 2sV_{SO}\sqrt{\sin^2 k_x + \sin^2 k_y}, \quad (15)$$

where $s = \pm 1$ represents two helicity branches, with corresponding eigenvectors

$$c_{\mathbf{k}s}^\dagger = \frac{1}{\sqrt{2}}(c_{\mathbf{k}\uparrow}^\dagger + s e^{i\theta(\mathbf{k})} c_{\mathbf{k}\downarrow}^\dagger). \quad (16)$$

Here we have defined the phase factor

$$e^{i\theta(\mathbf{k})} \equiv \frac{\sin k_y - i \sin k_x}{\sqrt{\sin^2 k_x + \sin^2 k_y}}, \quad (17)$$

which governs the mixing of spin-up and spin-down components for eigenstates of the noninteracting Hamiltonian. This mixing ensures that pairs are always formed in a mixed singlet-triplet state. An example of the noninteracting spectrum as well as the density of states is shown in Figs. 1 and 2, respectively. The density of states is determined by numerically integrating

$$\begin{aligned}
 g(E) &= 4 \sum_s \int_0^\pi \frac{dk_x}{2\pi} \int_0^\pi \frac{dk_y}{2\pi} \delta(E - \epsilon_{ks}) \\
 &= \lim_{\sigma \rightarrow 0} \frac{1}{\pi^{3/2} \sigma t} \sum_s \int_0^\pi dk_x \int_0^\pi dk_y e^{-(E/t - \epsilon_{ks}/t)^2 / \sigma^2}.
 \end{aligned} \quad (18)$$

Potentially important details concerning van Hove singularities, etc., are carefully derived in Refs. [34] and [35]. In particular, while a one-dimensional-like square-root singularity arises at the bottom of the band for parabolic dispersion [16], in a tight-binding model the density of states is a constant at the bottom of the band and has a singularity very close to the bottom of the band where there is a saddle point. Reference [34] makes it clear that for weak values of V_{SO} the saddle-point energy, $E_{\text{sad}} = -2t[1 + \sqrt{1 + (V_{SO}/t)^2}]$, is very close to the

minimum energy, $E_{\min} = -4t[1 + \sqrt{V_{\text{SO}}^2/(2t^2)}]$. Hence, this small separation is not even visible in Fig. 2.

In the conventional BCS program, the next step would be to restrict the Hamiltonian (14) to interactions between singlet pairs. In view of the Rashba spin-mixing, however, it is clear that this would not capture the right pairing physics and that it is natural to consider pairs within the same helicity band at zero total momentum. Allowing for interband pairing in the absence of a magnetic field would be akin to considering FFLO states where pairs have finite total momentum. At zero field, the pairing is expected to be intraband [36,37]. Indeed, if one follows the prescription of time-reversed pairing due to Anderson [9], then $c_{\mathbf{k}s}$ should be matched with its time-reversed partner $-se^{i\theta(\mathbf{k})}c_{-\mathbf{k}s}$. Upon transforming (14) to the helicity basis and retaining only interaction terms involving intraband pairs, we are left with the effective Hamiltonian

$$H = \sum_{\mathbf{k}s} (\epsilon_{\mathbf{k}s} - \mu) c_{\mathbf{k}s}^\dagger c_{\mathbf{k}s} + \frac{1}{4N} \sum_{\mathbf{k}\mathbf{k}'} \sum_{ss'} V_{ss'}(\mathbf{k}, \mathbf{k}') c_{\mathbf{k}s}^\dagger c_{-\mathbf{k}s}^\dagger c_{-\mathbf{k}'s'} c_{\mathbf{k}'s'}, \quad (19)$$

where

$$V_{ss'}(\mathbf{k}, \mathbf{k}') = s' e^{i\theta(\mathbf{k}')} s e^{-i\theta(\mathbf{k})} \left(U + 8\Delta t(s_k + s_{k'}) + 4V_{\text{SO}} \frac{\Delta t}{t} \left[s' \sqrt{\sin^2 k'_x + \sin^2 k'_y} + s \sqrt{\sin^2 k_x + \sin^2 k_y} \right] \right). \quad (20)$$

Here we have defined $s_k \equiv \frac{1}{2}(\cos k_x + \cos k_y)$.

III. MEAN-FIELD THEORY

We now study the effective Hamiltonian within mean-field theory. We choose a pairing mean field of time-reversed electron pairs. As discussed above, this is represented in the helicity basis as $b_{\mathbf{k}s} \equiv se^{i\theta(\mathbf{k})} \langle c_{-\mathbf{k}s} c_{\mathbf{k}s} \rangle$. Writing $c_{-\mathbf{k}s} c_{\mathbf{k}s} = se^{-i\theta(\mathbf{k})} b_{\mathbf{k}s} + \delta c_{\mathbf{k}s}$ and neglecting terms of order $(\delta c_{\mathbf{k}s})^2$, we get the mean-field Hamiltonian

$$H_{\text{MF}} = \sum_{\mathbf{k}s} (\epsilon_{\mathbf{k}s} - \mu) c_{\mathbf{k}s}^\dagger c_{\mathbf{k}s} - \frac{1}{2} \sum_{\mathbf{k}s} \Delta_{\mathbf{k}s}^* c_{-\mathbf{k}s} c_{\mathbf{k}s} - \frac{1}{2} \sum_{\mathbf{k}s} \Delta_{\mathbf{k}s} c_{\mathbf{k}s}^\dagger c_{-\mathbf{k}s}^\dagger + \frac{1}{2} \sum_{\mathbf{k}s} \Delta_{\mathbf{k}s} s e^{i\theta(\mathbf{k})} b_{\mathbf{k}s}^*, \quad (21)$$

where we have defined the gap parameter as

$$\Delta_{\mathbf{k}s} \equiv -\frac{1}{2N} \sum_{\mathbf{k}'s'} V_{ss'}(\mathbf{k}, \mathbf{k}') s' e^{-i\theta(\mathbf{k}')} b_{\mathbf{k}'s'}. \quad (22)$$

Note that this gap function may be written as $\Delta_{\mathbf{k}s} = se^{-i\theta_k} \bar{\Delta}_{\mathbf{k}s}$, where $\bar{\Delta}_{\mathbf{k}s}$ transforms under an irreducible representation of the lattice point group (in this model the trivial representation of the dihedral group D_8). The unusual phase factor $se^{-i\theta_k}$ that is local in k space is a feature of spin-orbit coupling and is discussed in Ref. [38].

The mean-field Hamiltonian may be diagonalized by means of the Bogoliubov transformation

$$c_{\mathbf{k}s} = u_{\mathbf{k}s}^* \hat{\alpha}_{\mathbf{k}s} - s e^{-i\theta(\mathbf{k})} v_{\mathbf{k}s} \hat{\alpha}_{-\mathbf{k}s}^\dagger, \quad (23)$$

where the coefficients $u_{\mathbf{k}s}, v_{\mathbf{k}s}$ are chosen to satisfy $u_{\mathbf{k}s} = u_{-\mathbf{k}s}$, $v_{\mathbf{k}s} = v_{-\mathbf{k}s}$, and $|u_{\mathbf{k}s}|^2 + |v_{\mathbf{k}s}|^2 = 1$. It is readily found that the values of these parameters that diagonalize the Hamiltonian are given by the equations

$$|v_{\mathbf{k}s}|^2 = \frac{1}{2} [1 - (\epsilon_{\mathbf{k}s} - \mu)/E_{\mathbf{k}s}], \quad (24)$$

$$|u_{\mathbf{k}s}|^2 = \frac{1}{2} [1 + (\epsilon_{\mathbf{k}s} - \mu)/E_{\mathbf{k}s}], \quad (25)$$

$$u_{\mathbf{k}s} v_{\mathbf{k}s}^* = -\frac{\bar{\Delta}_{\mathbf{k}s}^*}{2E_{\mathbf{k}s}}, \quad (26)$$

where $E_{\mathbf{k}s} \equiv \sqrt{(\epsilon_{\mathbf{k}s} - \mu)^2 + |\Delta_{\mathbf{k}s}|^2}$. The final mean-field Hamiltonian then reads

$$H_{\text{MF}} = \sum_{\mathbf{k}s} E_{\mathbf{k}s} \hat{\alpha}_{\mathbf{k}s}^\dagger \hat{\alpha}_{\mathbf{k}s} + E_g, \quad (27)$$

where the ground-state energy is given by

$$E_g = \frac{1}{2} \sum_{\mathbf{k}s} [(\epsilon_{\mathbf{k}s} - \mu) - E_{\mathbf{k}s} + \bar{\Delta}_{\mathbf{k}s} b_{\mathbf{k}s}^*]. \quad (28)$$

In terms of the new fermionic quasiparticle operators, we have

$$b_{\mathbf{k}s} = u_{\mathbf{k}s}^* v_{\mathbf{k}s} (2\langle \hat{\alpha}_{\mathbf{k}s}^\dagger \hat{\alpha}_{\mathbf{k}s} \rangle - 1), \quad (29)$$

which means the gap function must satisfy the finite-temperature self-consistency condition

$$\Delta_{\mathbf{k}s} = -\frac{1}{2N} \sum_{\mathbf{k}'s'} V_{ss'}(\mathbf{k}, \mathbf{k}') \frac{\Delta_{\mathbf{k}'s'}}{2E_{\mathbf{k}'s'}} [1 - 2f(E_{\mathbf{k}'s'})], \quad (30)$$

where $f(E)$ is the Fermi function.

IV. GAPEQUATIONS

The self-consistency condition determines the ansatz for $\bar{\Delta}_{\mathbf{k}s}$:

$$\bar{\Delta}_{\mathbf{k}s} = \Delta^0 + \Delta^s s_k + \Delta^{x-y} s \sqrt{\sin^2 k_x + \sin^2 k_y}. \quad (31)$$

Note that while the gap parameter definitively has the (extended) s -wave symmetry of the lattice, it will always be mixed singlet-triplet, unlike in conventional BCS theory. With this ansatz, the self-consistency condition yields three coupled equations:

$$\Delta^0 = -\frac{1}{2N} \sum_{\mathbf{k}'s'} \left(U + 8\Delta t s_{k'} + 4\frac{\Delta t}{t} V_{\text{SO}} s' \sqrt{\sin^2 k'_x + \sin^2 k'_y} \right) g(E_{\mathbf{k}'s'}) \bar{\Delta}_{\mathbf{k}'s'}, \quad (32)$$

$$\Delta^s = -\frac{1}{2N} \sum_{\mathbf{k}'s'} 8\Delta t g(E_{\mathbf{k}'s'}) \bar{\Delta}_{\mathbf{k}'s'}, \quad (33)$$

$$\Delta^{x-y} = -\frac{1}{2N} \sum_{\mathbf{k}'s'} 4\frac{\Delta t}{t} V_{\text{SO}} g(E_{\mathbf{k}'s'}) \bar{\Delta}_{\mathbf{k}'s'}, \quad (34)$$

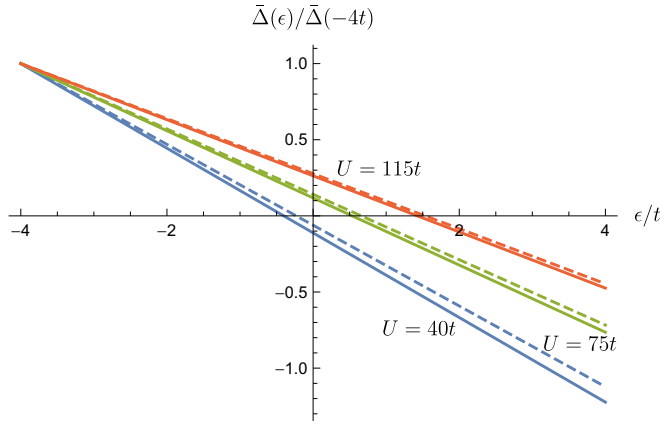


FIG. 3. Low-temperature gap dependence on kinetic energy for various values of U . Here we have set $\Delta t = 4.5t$, $n = 1.875$, $k_B T = 0.01t$. The solid lines correspond to $V_{SO} = 0.5$. The dashed lines show the result for $V_{SO} = 0$. A slightly larger value for the absolute value of the slope indicates that V_{SO} increases the asymmetry around the Fermi level.

where we have defined $g(E) \equiv \frac{1}{2E}[1 - 2f(E)]$. Equations (33) and (34) reveal that there are in fact only two independent parameters, since

$$\Delta^{x-y} = \frac{V_{SO}}{2t} \Delta^s. \quad (35)$$

This also means that the gap function is a linear function of the kinetic energy, since

$$\bar{\Delta}_{ks} = \Delta^0 + \Delta^s \left(s_k + \frac{s V_{SO}}{2t} \sqrt{\sin^2 k_x + \sin^2 k_y} \right) \quad (36)$$

$$= \Delta^0 - \Delta^s \epsilon_{ks}/(4t). \quad (37)$$

This energy dependence is in stark contrast with that of the constant gap used in conventional BCS theory. In the context of electron tunneling, it will cause an energy dependence in the conductance, independent of the density of states. This is seen as an asymmetry in the tunneling current for bias voltages of different sign [18,39]. This asymmetry is slightly enhanced by spin-orbit coupling, though the enhancement diminishes with increasing U , as seen in Fig. 3.

The linearized version of the self-consistency equations is a 3×3 determinant equation that determines the critical temperature. Note that in the limit of no spin-orbit coupling, Δ^{x-y} vanishes, and this reduces to two coupled equations which have been solved in Ref. [18]. Due to the presence of the chemical potential in the Fermi function we must simultaneously solve the number equation

$$n = 1 - \frac{1}{2N} \sum_{k's'} \frac{(\epsilon_{k's'} - \mu)}{E_{k's'}} \tanh(\beta E_{k's'}/2). \quad (38)$$

The determinant and number equations are solved together iteratively. That is, we iterate over temperatures until the determinant equation is satisfied, and for each temperature, the chemical potential is found from the number equation. The same strategy is used to solve for the gap function below T_c .

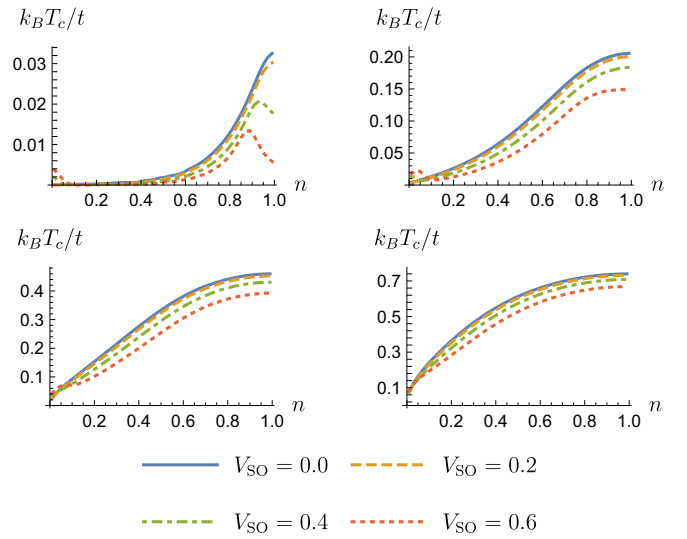


FIG. 4. Critical temperature as a function of electron density for various values of the spin-orbit coupling with $\Delta t = 0$: $U = -t$ (top left), $U = -2t$ (top right), $U = -3t$ (bottom left), and $U = -4t$ (bottom right). By particle-hole symmetry, the plot above half filling is a reflection of this plot, i.e., $T_c(2-n) = T_c(n)$ for $0 < n < 1$.

V. RESULTS

Figure 4 shows the critical temperature T_c as a function of electron density for the attractive Hubbard model with correlated hopping turned off ($U < 0$, $\Delta t = 0$). We see that except at very low ($n \rightarrow 0$) and high ($n \rightarrow 2$) densities, increasing the spin-orbit coupling has the effect of decreasing the critical temperature. This is understood by noting that the available phase space for intraband pairs is reduced by the presence of spin-orbit coupling, except at the bottom and top of the band where all states are of the same helicity and the density of states becomes singular. Recall that the density of states is lower for the $s = +$ ($s = -$) band in the electron (hole) doped part of the band. Indeed, half-filling, which would have the highest T_c in the absence of spin-orbit coupling, shows a dip due to the minimum (see Fig. 2) in the density of states.

Figures 5 and 6 show a very different effect. Here correlated hopping has been turned on ($U > 0$, $\Delta t \neq 0$). This breaks particle-hole symmetry, and we see that the Rashba spin-orbit

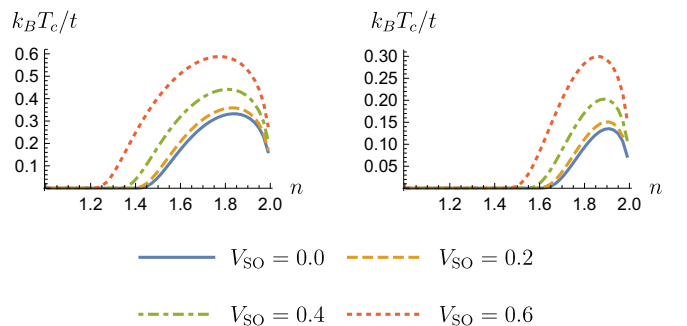


FIG. 5. Critical temperature as a function of electron density for various values of the spin-orbit coupling with $\Delta t = 4.5t$: $U = 90t$ (left), $U = 115t$ (right).

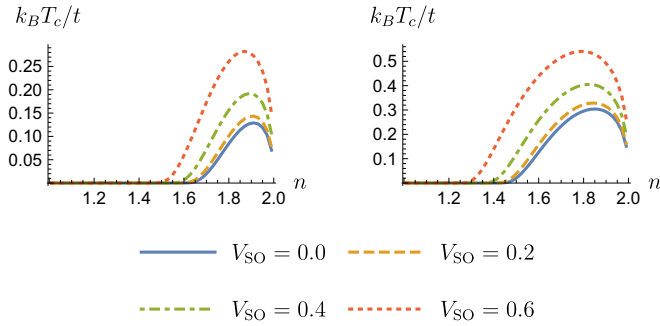


FIG. 6. Critical temperature as a function of electron density for various values of the spin-orbit coupling with $U = 75t$: $\Delta t = 3.5t$ (left), $\Delta t = 4t$ (right).

coupling and correlated hopping cooperate to enhance the critical temperature in the high electron (low hole) density regime. This, too, follows from the single-particle density of states. The spin-orbit coupling and correlated hopping couple to produce an effective interaction whose sign matches the sign of the helicity band [see the last two lines of Eq. (20)]. At high electron densities, the $s = +$ density of states is suppressed, and the $s = -$ density of states increases towards the singularity at the top of the band. Thus, the pair interaction becomes dominantly attractive and its magnitude increases with V_{SO} and Δt . In fact, the maximum value of the critical temperature shows a quadratic dependence on the spin-orbit coupling, as seen in Fig. 7.

The gap and number equations are solved at finite temperature as well. We can check the gap ratio as well, but due to the energy dependence of the gap, it is more appropriate to use the minimum value of the excitation energy. This occurs when

$$\epsilon_{ks} = \frac{\mu + \Delta^0 \frac{\Delta^s}{4t}}{1 + \left(\frac{\Delta^s}{4t}\right)^2}, \quad (39)$$

at which point the excitation energy is

$$E_{\min} = \frac{|\Delta^0 - \mu \frac{\Delta^s}{4t}|}{\sqrt{1 + \left(\frac{\Delta^s}{4t}\right)^2}}. \quad (40)$$

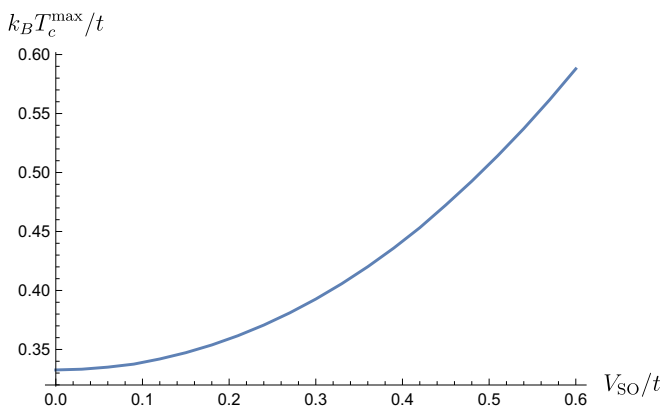


FIG. 7. Maximum critical temperature as a function of spin-orbit coupling with $U = 90t$, $\Delta t = 4.5t$.

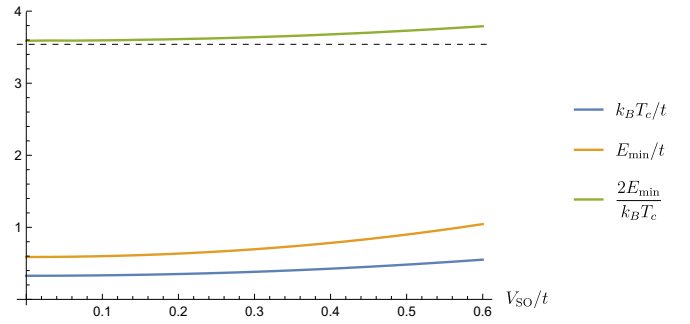


FIG. 8. Critical temperature $E_{\min}$ and the corresponding gap ratio at low temperature as a function of spin-orbit coupling. Here we have set $U = 90t$, $\Delta t = 4.5t$, $n = 1.875$, $k_B T = 0.01t$. The dashed line shows the conventional BCS value.

This value is plotted in Fig. 8 along with the gap ratio. We see that for these parameter values the spin-orbit coupling introduces very little deviation from the BCS value.

VI. CONCLUSION

We have shown that within a 2D tight-binding model on a square lattice, correlated hopping and Rashba spin-orbit coupling work together to enhance the critical temperature of superconductivity, even with significant repulsive on-site interactions. This is in contrast to the Rashba model with attractive on-site interactions and no correlated hopping, where the spin-orbit coupling inhibits superconductivity. The analysis was done within a mean-field treatment of the model assuming Cooper pairs to form within the same helicity band of the noninteracting Rashba spectrum.

The enhancement is strongest in the high-electron-density regime. This is relevant for the cuprates at low hole doping, where the oxygen p band is nearly full. Rashba spin-splitting is expected to be present in many cuprates, though its magnitude is likely much smaller than the values considered in this paper.

The superconducting gap for this model is thermodynamically similar to the gap in conventional BCS theory in many regards, except that the broken particle-hole symmetry of our model will produce a tunneling asymmetry in a metal-superconductor junction [18,39].

It is interesting to look at the symmetry of the gap function as well. The gap in this model has an extended s -wave symmetry, but we should note that if nearest-neighbor repulsion were added to our model, the gap symmetries will be enriched by the presence of two additional d -wave phases. It should be noted that these are not the symmetries of the full gap function but rather the part that transforms under irreducible representations of the lattice point group. In particular, the gap carries an additional complex phase due to the spin-orbit coupling. It would be interesting to see if this phase is observable.

Note added in proof.

Recently, we became aware of several relevant references:

(1) Ref. [17] by Ptok, Rodriguez, and Karpia, referred to in the introduction.

(2) Ref. [40] by Rout, Maniv, and Dagan “Link between the Superconducting Dome and Spin-Orbit Interaction in the (111) $\text{LaAlO}_3/\text{SrTiO}_3$ Interface,” reporting that the strength of

the spin-orbit interaction in that system tracks the magnitude of T_c across the superconducting dome.

(3) Ref. [41] by Stornaiuolo et al. on the same system as Ref. [40] also suggests such a link.

We point out that our work provides a possible explanation for the observations in Refs. [40,41], hence suggests that correlated hopping plays an important role in that system.

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- [1] R. Winkler, *Spin-Orbit Coupling Effects in Two-Dimensional Electron and Hole Systems* (Springer, Berlin, 2003).
 - [2] E. Bauer and M. Sigrist, *Non-Centrosymmetric Superconductors: Introduction and Overview* (Springer Science & Business Media, New York, 2012), Vol. 847.
 - [3] J. Bardeen, L. N. Cooper, and J. R. Schrieffer, *Phys. Rev.* **108**, 1175 (1957).
 - [4] F. Reif, *Phys. Rev.* **106**, 208 (1957).
 - [5] G. M. Androes and W. D. Knight, *Phys. Rev. Lett.* **2**, 386 (1959).
 - [6] R. A. Ferrell, *Phys. Rev. Lett.* **3**, 262 (1959).
 - [7] P. C. Martin and L. P. Kadanoff, *Phys. Rev. Lett.* **3**, 322 (1959).
 - [8] J. R. Schrieffer, *Phys. Rev. Lett.* **3**, 323 (1959).
 - [9] P. W. Anderson, *Phys. Rev. Lett.* **3**, 325 (1959).
 - [10] A. Abrikosov and L. P. Gor'kov, *Sov. Phys. JETP* **15**, 752 (1962).
 - [11] V. Edel'shtein, *Soviet Physics-JETP (English Translation)* **68**, 1244 (1989).
 - [12] L. P. Gor'kov and E. I. Rashba, *Phys. Rev. Lett.* **87**, 037004 (2001).
 - [13] E. I. Rashba and V. I. Sheka, *Fiz. Tverd. Tela: Collected Papers* **2**, 162 (1959).
 - [14] E. I. Rashba, *Sov. Phys. Solid State* **2**, 1109 (1960).
 - [15] P. W. Anderson, *J. Phys. Chem. Solids* **11**, 26 (1959).
 - [16] E. Cappelluti, C. Grimaldi, and F. Marsiglio, *Phys. Rev. Lett.* **98**, 167002 (2007).
 - [17] A. Ptok, K. Rodríguez, and K. J. Kapcia, *Phys. Rev. Materials* **2**, 024801 (2018).
 - [18] J. E. Hirsch and F. Marsiglio, *Phys. Rev. B* **39**, 11515 (1989).
 - [19] J. E. Hirsch, *Phys. Rev. Lett.* **87**, 206402 (2001).
 - [20] J. E. Hirsch, *Phys. Rev. B* **62**, 14498 (2000).
 - [21] J. E. Hirsch, *Phys. Rev. B* **65**, 214510 (2002).
 - [22] R. Micnas, J. Ranninger, and S. Robaszkiewicz, *Rev. Mod. Phys.* **62**, 113 (1990).
 - [23] J. Hubbard, *Proc. R. Soc. London, Ser. A* **276**, 238 (1963).
 - [24] Yu. A. Bychkov and E. I. Rashba, *JETP Lett.* **39**, 78 (1984).
 - [25] C. Wu, K. Sun, E. Fradkin, and S.-C. Zhang, *Phys. Rev. B* **75**, 115103 (2007).
 - [26] L. Petersen and P. Hedegård, *Surf. Sci.* **459**, 49 (2000).
 - [27] H. Fu, *Phys. Rev. B* **87**, 075139 (2013).
 - [28] X. Zhang, Q. Liu, J.-W. Luo, A. J. Freeman, and A. Zunger, *Nat. Phys.* **10**, 387 (2014).
 - [29] V. M. Edelstein, *Phys. Rev. Lett.* **75**, 2004 (1995).
 - [30] M. Ben Shalom, M. Sachs, D. Rakhmilevitch, A. Palevski, and Y. Dagan, *Phys. Rev. Lett.* **104**, 126802 (2010).
 - [31] Z. Zhong, A. Tóth, and K. Held, *Phys. Rev. B* **87**, 161102 (2013).
 - [32] S. Kivelson, W.-P. Su, J. R. Schrieffer, and A. J. Heeger, *Phys. Rev. Lett.* **58**, 1899 (1987).
 - [33] I. Lang and Y. A. Firsov, *Sov. Phys. JETP* **16**, 1301 (1963).
 - [34] Z. Li, L. Covaci, M. Berciu, D. Baillie, and F. Marsiglio, *Phys. Rev. B* **83**, 195104 (2011).
 - [35] Z. Li, L. Covaci, and F. Marsiglio, *Phys. Rev. B* **85**, 205112 (2012).
 - [36] F. Loder, A. P. Kampf, and T. Kopp, *J. Phys.: Condens. Matter* **25**, 362201 (2013).
 - [37] K.-C. Weng and C. Hu, *Sci. Rep.* **6**, 29919 (2016).
 - [38] I. A. Sergienko and S. H. Curnoe, *Phys. Rev. B* **70**, 214510 (2004).
 - [39] F. Marsiglio and J. E. Hirsch, *Physica C: Supercond.* **159**, 157 (1989).
 - [40] P. K. Rout, E. Maniv, and Y. Dagan, *Phys. Rev. Lett.* **119**, 237002 (2017).
 - [41] D. Stornaiuolo, D. Massarotti, R. Di Capua, P. Lucignano, G. P. Pepe, M. Salluzzo, and F. Tafuri, *Phys. Rev. B* **95**, 140502(R) (2017).