

## Critical temperature enhancement of topological superconductors: A dynamical mean-field study

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We show that a critical temperature  $T_c$  for spin-singlet two-dimensional superconductivity is enhanced by a cooperation between the Zeeman magnetic field and the Rashba spin-orbit coupling, where a superconductivity becomes topologically nontrivial below  $T_c$ . The dynamical mean-field theory with the segment-based hybridization-expansion continuous-time quantum Monte Carlo impurity solver is used for accurately evaluating a critical temperature, without any fermion sign problem. A strong-coupling approach shows that spin-flip-driven local pair hopping leads to part of this enhancement, especially effects of the magnetic field. We propose physical settings suitable for verifying the present calculations, a one-atom-layer system on Si(111) and ionic-liquid-based electric double-layer transistors.

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Interesting materials properties are produced by the interplay between different internal degrees of freedom, such as spin and orbital, leading to the design of devices with useful characteristics [1,2]. Manipulating spins in position or momentum space allows us to address exotic order in low-temperature physics. The application of Zeeman magnetic fields induces a spin imbalance in a system. Spin-orbit couplings (SOCs) create a spin rotation depending on the electron's motion. These effects lead to notable many-body ground states, such as the Fulde-Ferrel-Larkin-Ovchinnikov states [3–5], pair-density wave [6], and topological superfluidity/superconductivity [7–9].

The quest for high- $T_c$  topological superconductors is a compelling issue in materials science. To reveal a way of enhancing  $T_c$  with keeping topological characteristics enables us to not only study topological order in a wide range of temperatures, but also increase the feasibility of implementing topological quantum computing. The superconducting topological insulator  $\text{Cu}_x\text{Bi}_2\text{Se}_3$  shows superconductivity at  $T_c \sim 3.8$  K [10], and is a candidate for bulk topological superconductors [10,11]. Interestingly, its critical temperature is two orders of magnitude larger than a theoretical estimation with electron-phonon couplings [12]. Therefore, using a concrete theoretical method beyond the weak-coupling mean-field theory, clarifying the relevance of the key features of this compounds to  $T_c$  would lead to a clue of designing useful topological materials.

The presence of strong SOC is one of the crucial characteristics in  $\text{Cu}_x\text{Bi}_2\text{Se}_3$ , since the quasiparticle wave function has a strong momentum dependence due to the SOC so that the bulk state has a nontrivial topology [11]. This feature is common with other topological superconducting systems, such as ultracold atomic gases and artificial semiconductor-superconductor heterostructures [13]. Thus, it is interesting how spin degrees of freedom contribute to the critical temperature of topological superconductors.

An attractive idea of producing topological superconductors is to use two-dimensional (2D)  $s$ -wave superconductors with spin manipulations [14]. Mean-field calculations predict that spin-singlet Cooper pairs have unconventional and topological characteristics in the presence of Rashba SOC and Zeeman magnetic fields [14–16]. This setting is suitable for assessing the connection between SOC and  $T_c$ , from two points of view. First, an intrinsic pair breaking (Pauli depairing) effect is involved, owing to the presence of Zeeman magnetic fields. Thus, one may understand how the contributions from SOC overcome the Pauli depairing effects. Second, a topologically nontrivial  $s$ -wave superconducting state is produced by an on-site attractive density-density interaction [14]. It indicates that an arbitrary range of interaction strength can be systematically studied by a reliable theoretical method, the dynamical mean-field theory (DMFT) [17] combined with a numerically exact continuous-time quantum Monte Carlo method [18,19]. Utilizing this theoretical approach, one can take all kinds of local Feynman diagrams.

In this Rapid Communication, we show that a 2D attractive Hubbard model with Rashba SOC possesses  $T_c$  enhancement even though the Zeeman magnetic field is applied. To treat an arbitrary strength of on-site  $U$ , we adopt the DMFT combined with a numerically exact continuous-time quantum Monte Carlo method. We point out that this approach accurately estimates  $T_c$  even in the present spin-active many-body system since a symmetric property of the many-body Hamiltonian in spin and  $k$  space ensures the absence of the fermion negative sign problem [19]. Our main results are shown in Figs. 1 and 2. The critical temperature on a certain filling changes with a nonmonotonic manner, varying the magnitude of the Zeeman field and the Rashba SOC. A cooperation between the Zeeman field and SOC is a key of the  $T_c$  enhancement. A strong-coupling approach shows that the part of the enhancement (i.e., the magnetic field dependence) is explained by local pair hopping [20], due to a spin-flip process. The rest of the enhancement (i.e., the SOC dependence) is still elusive. We speculate that the enhancement is related to a change of a winding number on the normal-electron Fermi surfaces. Moreover, we propose physical settings suitable for verifying the present calculations, one-atom-layer TI-Pb

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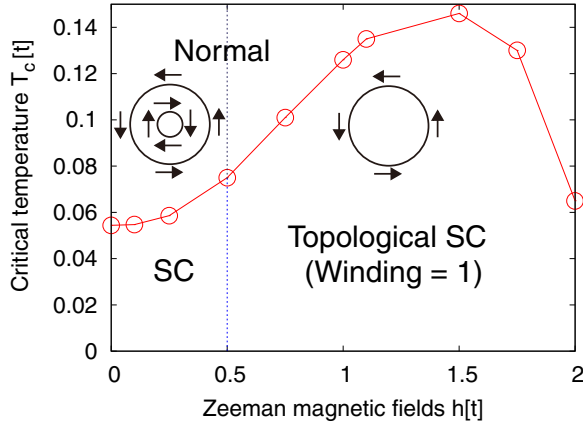


FIG. 1. Zeeman-magnetic-field dependence of a critical temperature, with attractive on-site coupling  $U = -3t$ , spin-orbit coupling  $\alpha = 1t$ , and filling  $\nu = 1/8$ . The dashed-dotted line shows that in a noninteracting case ( $U = 0$ ) a winding number on the Fermi surfaces changes.

on Si(111) [21] and ionic-liquid-based electric double-layer transistors (EDLTs) [22].

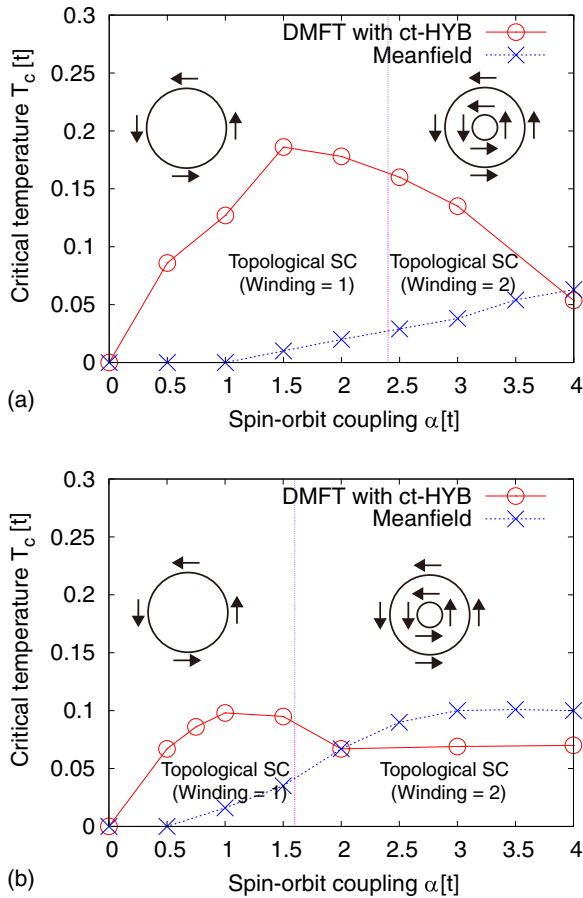


FIG. 2. Spin-orbit coupling dependence of a critical temperature, with (a) Zeeman magnetic field  $h = t$  and filling  $\nu = 1/8$  and (b)  $h = 0.5t$  and  $\nu = 1/16$ . The attractive on-site coupling,  $U = -3t$ , is common. Each vertical dashed-dotted line has the same meaning as that in Fig. 1.

The single-orbital attractive Hubbard Hamiltonian with the Rashba SOC and the Zeeman magnetic field on 2D square lattice is [13,14]

$$\mathcal{H} = \sum_{k\sigma\sigma'} \hat{h}_0^{\sigma\sigma'}(\mathbf{k}) c_{k\sigma}^\dagger c_{k\sigma'} + U \sum_i n_{i\uparrow} n_{i\downarrow}, \quad (1)$$

where  $\hat{h}_0(\mathbf{k}) = -\mu - 2t(\cos k_x + \cos k_y) + \alpha\mathcal{L}(\mathbf{k}) - h\hat{\sigma}_3$  and  $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$  ( $\sigma = \uparrow, \downarrow$ ). The hopping parameter  $t$  is positive, whereas the coupling constant of the on-site interaction  $U$  is negative. Throughout this Rapid Communication, we use the unit system with  $\hbar = k_B = 1$ . The unit of energy is  $t$ . The electron annihilation (creation) operator with spin  $\sigma$  is  $c_{i\sigma}$  ( $c_{i\sigma}^\dagger$ ) on spatial site  $i$ . In the momentum representation they are  $c_{k\sigma}$  and  $c_{k\sigma}^\dagger$ . The symbol  $\hat{\sigma}_j$  is the  $j$ th component of the  $2 \times 2$  Pauli matrices ( $j = 1, 2, 3$ ). The Rashba SOC term is described by  $\alpha\mathcal{L}(\mathbf{k}) = \alpha(\hat{\sigma}_1 \sin k_y - \hat{\sigma}_2 \sin k_x)$ , with positive  $\alpha$ . The strength of the Zeeman magnetic field is  $h$ . In our calculations, the chemical potential,  $\mu$  is tuned, with fixed filling  $\nu$ .

Let us summarize the topological properties of a superconducting state in this model within the weak-coupling Bardeen-Cooper-Schrieffer (BCS) theory [14]. The topological number is the Thouless-Kohmoto-Nightingale-Nijs invariant [23,24] on a 2D torus in momentum space. According to this invariant, the criteria of topological superconductivity are derived by Sato *et al.* (Table I in Ref. [14]). We focus on the case just below  $T_c$ ; the amplitude of the superconducting order parameter vanishes (i.e.,  $|\Delta| \rightarrow 0+$ ). Then, we find that the criteria in Ref. [14] are regarded as the changes of a winding number on the Fermi surfaces, where the winding number is defined as an  $xy$ -plane spin rotation on the Fermi surfaces. Note that this characterization requires only the knowledge on the normal-state Fermi surfaces. The occurrence of a topological superconducting state just below  $T_c$  is associated with a nonzero winding number on the Fermi surfaces. Hence, although here we only consider the normal states just above  $T_c$ , we can obtain a connection of normal-state instability with topological superconductivity.

We show our calculation method. To calculate one- and two-particle Green's functions, we utilize the DMFT with the segment-based hybridization-expansion continuous-time quantum Monte Carlo impurity solver (ct-HYB) [18,25,26]. The segment-based algorithm is the fastest update method of ct-HYB solvers, and is applicable to our system if (i) the interaction terms of the Hamiltonian conserve spin and (ii) in the effective Anderson impurity model the one-body local Hamiltonian does so. The first condition is satisfied since the system has only a density-density interaction. Let us consider the second one. The one-body local Hamiltonian matrix  $\hat{H}_f$  is related to  $\hat{h}_0(\mathbf{k})$  via [27]

$$\hat{H}_f = \sum_{\mathbf{k}} \hat{h}_0(\mathbf{k}) = -\mu - h\hat{\sigma}_3. \quad (2)$$

Since  $\hat{H}_f$  is diagonal in the spin space, the second condition is fulfilled. Moreover, we point out that there is no fermion sign problem when self-energy is diagonal in the spin space [19]. Since  $\mathcal{H}$  is invariant under the transformation  $c_{k\sigma} \rightarrow \sum_{\sigma'} (\hat{\sigma}_3)_{\sigma\sigma'} c_{-k\sigma'}$ , we find that the off-diagonal elements of self-energy in the spin space are zero in the present system [28]. Accordingly, the evaluation of  $T_c$  is accurately performed by

the DMFT with ct-HYB. Here, the effective impurity problem is solved by an open-source program package, IQIST [29].

The main target in our calculations is the pair susceptibility with respect to a spin-singlet  $s$ -wave state at temperature  $T$  [30],

$$\chi = \frac{1}{N} \int_0^{1/T} \langle O(\tau)O^\dagger \rangle d\tau = T \sum_{nn'} \chi_{\uparrow\downarrow\uparrow\uparrow}(i\omega_n, i\omega_{n'}; 0), \quad (3)$$

with  $O = \sum_i c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger$ . The total number of lattice sites is  $N$ . The fermionic Matsubara frequency is  $\omega_n = \pi T(2n + 1)$ , with  $n \in \mathbb{Z}$ . Here,  $\chi_{abcd}(i\omega_n, i\omega_{n'}; 0)$  is a two-particle lattice Green's function with a zero Bosonic Matsubara frequency. A divergence in  $\chi$  (or equivalently a sign change in  $1/\chi$ ) indicates a possible transition into a superconducting phase. In the effective impurity model, one- and two-particle local Green's functions,  $G_{ab}^{\text{loc}}(i\omega_n)$  and  $\chi_{abcd}^{\text{loc}}(i\omega_n, i\omega_{n'}; 0)$ , respectively, are calculated by the Gardena component of the IQIST package. One-particle Green's function in the original lattice model is  $\hat{G}(\mathbf{k}, i\omega_n) \equiv [i\omega_n - \hat{h}_0(\mathbf{k}) - \hat{\Sigma}(i\omega_n)]^{-1}$ , with self-energy  $\hat{\Sigma}(i\omega_n)$ . Two-particle lattice Green's functions are obtained by simultaneously solving two Bethe-Salpeter equations with a common vertex function  $\underline{\Gamma}$  [30,31],

$$\underline{\underline{\chi}}^{\text{loc}} = \underline{\underline{\chi}}^{\text{loc},0} + \underline{\underline{\chi}}^{\text{loc},0} \underline{\underline{\Gamma}} \underline{\underline{\chi}}^{\text{loc}}, \quad (4a)$$

$$\underline{\underline{\chi}} = \underline{\underline{\chi}}^0 + \underline{\underline{\chi}}^0 \underline{\underline{\Gamma}} \underline{\underline{\chi}}. \quad (4b)$$

The double underline indicates that an object is a matrix on a vector space including two spin indices and the Matsubara frequency;  $\chi_{abcd}(i\omega_n, i\omega_{n'})$  is embedded into  $(\underline{\underline{\chi}})^{ll'}$  with  $l = (a, b, n)$  and  $l' = (d, c, n')$ , for example. We take all the processes of the DMFT framework, regardless of spin conservation or not. In the Bethe-Salpeter equations the matrix objects with superscript 0 contain bare two-particle Green's functions produced by one-particle Green's functions. In the effective impurity model, we have  $\chi_{abcd}^{\text{loc},0}(i\omega_n, i\omega_{n'}) = \chi_{dacb}^{\text{loc},gg}(i\omega_n)\delta_{n,n'}$  and  $\tilde{\chi}_{abcd}^{\text{loc},0}(i\omega_n, i\omega_{n'}) = \chi_{abcd}^{\text{loc},0}(i\omega_n, i\omega_{n'}) - \chi_{cabd}^{\text{loc},gg}(i\omega_n)\delta_{n,-n'-1}$ , with  $\chi_{abcd}^{\text{loc},gg}(i\omega_n) = G_{ab}^{\text{loc}}(i\omega_n)G_{cd}^{\text{loc}}(-i\omega_n)$ . In a similar manner we define bare two-particle Green's functions in the lattice model; all local one-particle Green's functions are replaced with lattice one-particle Green's functions, and  $\chi_{abcd}^{\text{gg}}(i\omega_n)$  is defined as  $\chi_{abcd}^{\text{gg}}(i\omega_n) = \sum_{\mathbf{k}} G_{ab}(\mathbf{k}, i\omega_n)G_{cd}(-\mathbf{k}, -i\omega_n)$ . In the calculation of the two-particle Green's functions, the  $\mathbf{k}$ -mesh size and the  $n$ -mesh size are  $192 \times 192$  and  $64$ , respectively. The numerical calculations on  $\underline{\underline{\chi}}$  are performed by an equation not explicitly including  $\underline{\underline{\Gamma}}$ :  $\underline{\underline{\chi}} = \underline{\underline{\chi}}^{\text{loc}}(1 - \underline{\underline{A}})^{-1}\underline{\underline{B}}$  with  $\underline{\underline{A}} \equiv ([\underline{\underline{\chi}}^{\text{loc},0}]^{-1} - [\underline{\underline{\chi}}^0]^{-1})\underline{\underline{\chi}}^{\text{loc}} + 1 - \underline{\underline{B}}^{\text{loc}}$ ,  $\underline{\underline{B}} \equiv [\underline{\underline{\chi}}^0]^{-1}\underline{\underline{\chi}}^0$ , and  $\underline{\underline{B}}^{\text{loc}} \equiv [\underline{\underline{\chi}}^{\text{loc},0}]^{-1}\underline{\underline{\chi}}^{\text{loc},0}$  (for details, see Ref. [32]).

Figure 1 shows  $T_c$  with respect to the change of the Zeeman magnetic field when  $\alpha = t$ ,  $U = -3t$ , and  $\nu = 1/8$ . The critical temperature increases with increasing  $h$ , and takes a peak around  $h = 1.5t$ . Then, the decrease of  $T_c$  occurs in a stronger magnetic field; this reduction corresponds to the Pauli depairing effect. We mention that the weak-coupling mean-field calculations indicate the complete suppression of  $T_c$  even in the weak magnetic field  $h = 1t$  [see, e.g., Fig. 2(a) at  $\alpha =$

$1t$ ]. We note that a weak-coupling approach in the presence of spatial phase fluctuations [33,34] predicts the decrease of  $T_c$  with increasing Zeeman magnetic fields. We infer from Fig. 1 a relation between the  $T_c$  enhancement and the change of the winding number on the Fermi surfaces from 0 (conventional, nontopological,  $s$  wave) to 1 (topological  $s$  wave). To study this point more closely, we consider a different way of changing the winding number. We focus on a region of parameter sets in which the winding number transits from 1 to 2, increasing  $\alpha$  with fixed  $\nu$  and  $h$ . Figure 2 shows the behaviors of  $T_c$  in the DMFT calculations (red circle), as well as the results obtained by the weak-coupling mean-field calculations (blue cross). We find in the DMFT calculations that the behavior of  $T_c$  is nonmonotonic as  $\alpha$ . In contrast, the weak-coupling mean-field critical temperature monotonically grows up as  $\alpha$  since the in-plane Rashba SOC may suppress the Pauli depairing effect induced by the Zeeman magnetic field along the  $z$  axis [35]. In the DMFT calculations, an optimal value of  $\alpha$  in the enhancement of  $T_c$  locates at the region of the winding number to be 1. Thus, our calculations suggest that the parameter region in which the winding number is 1 is suitable for realizing a topological superconducting state at a high temperature. We stress that these results occur at different parameter sets, as shown in Figs. 2(a) and 2(b). It is important to note that calculating a topological invariant in interacting systems is desirable for finding the genuine topological transition point. The renormalized Zeeman magnetic field and the chemical potential due to the self-energy at the zero energy [36] would shift the lines of winding-number changes in Figs. 1 and 2.

Now, we derive a strong-coupling-limit formula of  $T_c$ , to get the picture on the enhancement of  $T_c$  with respect to the changes of  $\alpha$  and  $h$ . In a strong-coupling limit  $|U| \rightarrow \infty$ , the model can be rewritten as a pseudospin ( $S = 1/2$ ) quantum Heisenberg model, whose Hamiltonian is given by  $\mathcal{H}_{\text{eff}} = \sum_{\langle ij \rangle} [-J(S_i^x S_j^x + S_i^y S_j^y) + J S_i^z S_j^z] - H \sum_i S_i^z$ , where  $\sum_{\langle ij \rangle}$  considers nearest neighbors only and the pseudospin up and down states are doubly occupied and unoccupied local states, respectively. The effective coupling constant and the pseudospin field are  $J(t, \alpha, h, U) \equiv 4t^2/|U| + |U|\alpha^2/(|U|^2 - 4h^2)$  and  $H = -2\mu + U$ , respectively. The mean-field analysis in this effective Hamiltonian gives the critical temperature. Thus, we obtain the expression of  $T_c$ ,

$$T_c(\alpha, h) = \frac{(1 - 2\nu)J(t, \alpha, h, U)}{\tanh^{-1}(1 - 2\nu)}. \quad (5)$$

We show that part of the enhancement ( $h$  dependence of  $T_c$ ) is explained by local pair hopping [20] in terms of the strong-coupling approach. We find that, even in the half-filling case ( $\nu = 1/2$ ), the critical temperature enhances with increasing  $h$ , as shown in Fig. 3(a). A key of the enhancement of  $T_c$  is depicted in Fig. 3(b); a pair on the  $i$ th site can hop into the  $(i + 1)$ th site via a virtual spin-flip process coming from nonvanishing  $\alpha$  of second-order perturbation (lower diagram on the middle panel). A strong Zeeman magnetic field splits the energy levels between the spin-flip (lower diagram) and spin-conserved (upper diagram) processes; the presence of the Zeeman field tends to increase the rate of the spin-flip process. Therefore, this spin-flip-driven local pair hopping is responsible for the  $T_c$  enhancement under nonzero  $h$ , although

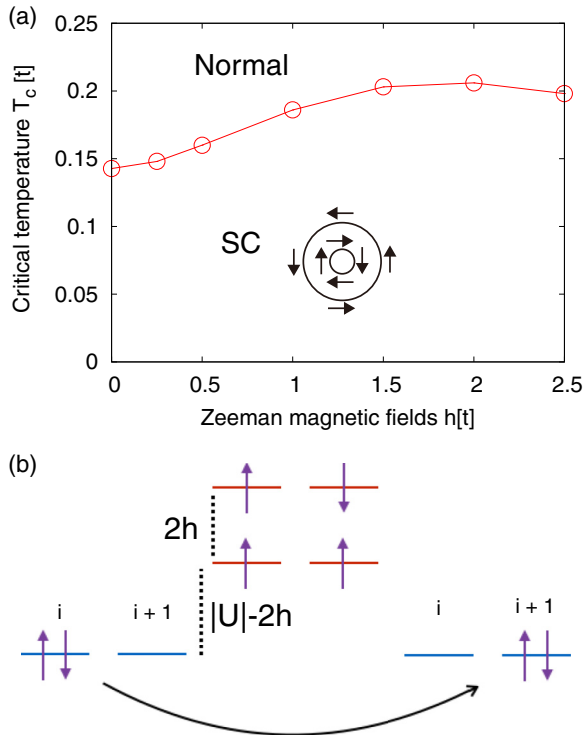


FIG. 3. (a) Zeeman-magnetic-field dependence of a critical temperature at half filling ( $\nu = 1/2$ ). Other settings are equal to those in Fig. 1. (b) Schematic diagram of pair hopping from the  $i$ th to  $(i + 1)$ th sites via either spin-flip (lower panel) or spin-conserved (upper panel) processes.

most of our DMFT calculations are outside the strong-coupling regime since the energy of the singly occupied state is smaller than the energies of the doubly occupied and empty states. In Ref. [32], we also show that the spin-flip processes are important for the  $T_c$  enhancement in the DMFT calculations.

The local-pair-hopping scenario, however, does not fully explain the behavior of  $T_c$ . Under the fixed Zeeman magnetic field, the dependence of  $T_c$  on  $\alpha$  in the strong-coupling formula is quite different from the DMFT calculations, as shown in Fig. 2; the critical temperature in the DMFT calculations is *not* a monotonic increase function of  $\alpha$ , even though the Pauli depairing effect could be suppressed for large  $\alpha$ . We can find that the DMFT calculations with  $U = -7t$  are consistent with the strong-coupling formula;  $T_c$  monotonically increases within our calculations in  $0 \leq \alpha \leq 4t$ . Thus, explaining the  $\alpha$  dependence of  $T_c$  in an intermediate range of on-site  $U$  would require a different scenario. It is an interesting future issue of unveiling the remaining origin of  $T_c$  enhancement. We speculate that focusing on the change of the winding number might give us an insight on this elusive issue.

Now, we propose two physical systems available for testing our theoretical calculations. The first setup is to apply Zeeman magnetic fields to one-atom-layer Tl-Pb compounds on Si(111). Matetskiy *et al.* [21] observed the occurrence of giant Rashba effects in this setting without the Zeeman field.

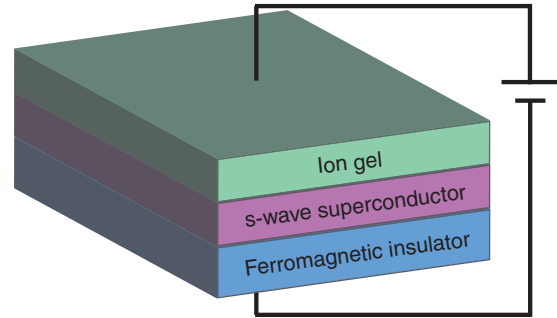


FIG. 4. Schematic figure of ionic-liquid-based electric double-layer transistors (EDLTs).

The second setup is to use EDLT with a layered structure built up by an  $s$ -wave superconductor and a ferromagnetic insulator, as shown in Fig. 4. The idea of fabricating related systems is shown in Fig. 2(a) of Ref. [22]. Tuning electric fields allows us to control the electron's filling and the strength of SOC. This EDLT setup would be a plausible system to design 2D topological superconductors.

Finally, we discuss a link of our calculations with  $\text{Cu}_x\text{Bi}_2\text{Se}_3$ , from the viewpoint of  $T_c$  enhancement. Although the present system is quite different from  $\text{Cu}_x\text{Bi}_2\text{Se}_3$ , we have an interesting correspondence between the two systems. One of the authors (Y.N.) found in the calculations of impurity effects [37] that the presence of orbital imbalance leads to similar effects to those induced by a spin imbalance, even though an external magnetic field is absent. In the present system a strong Zeeman magnetic field induces the coherent hopping of a localized pair via a spin-flip process, leading to the increase of  $T_c$ . Hence, in  $\text{Cu}_x\text{Bi}_2\text{Se}_3$ , a large orbital imbalance might cause an orbital-flip process contributing to the enhancement of  $T_c$ . The DMFT study in the model of  $\text{Cu}_x\text{Bi}_2\text{Se}_3$  is our important future issue.

In summary, we showed that a 2D attractive Hubbard model with Rashba SOC and a Zeeman magnetic field possesses  $T_c$  enhancement, by using the DMFT combined with the numerically exact ct-HYB solver without any fermion sign problem. With the use of a strong-coupling approximation, part of the enhancement (i.e., the magnetic field dependence) was explained by the scenario of a local pair hopping induced by a spin-flip process. The rest of the enhancement (i.e., the SOC dependence) is still in an open issue. We speculated that the enhancement is related to a change of a winding number of the normal-electron Fermi surfaces. Moreover, we proposed that EDLTs are good stages for designing topological superconductivity. Finally, we discussed a high  $T_c$  in  $\text{Cu}_x\text{Bi}_2\text{Se}_3$  with the use of the result in our two-dimensional system.

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