Edge superconducting correlation in the attractive-U Kane-Mele-Hubbard model

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The two-dimensional Kane-Mele model with attractive Hubbard interaction U is studied by using a self-consistent mean-field theory. At $U = 0$, the ground state is a topological insulator. At U larger than a critical value U_c, the ground state is a bulk superconductor. At $0 < U < U_c$, the bulk remains insulating while the edge state shows superconducting correlation. The effective model for the edge superconducting state is discussed.

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A topological insulator (TI) is insulating in the bulk but has gapless edge states protected by time-reversal invariance.[1–3] The topological insulating state results from its nontrivial band topology induced by spin-orbit interaction, and is characterized by a Z_2 topological invariant. Recent predictions and discoveries of two-dimensional (2D) and three-dimensional (3D) TI in a variety of materials have greatly promoted the field.[4–7] It is interesting to note that the TIs may be candidates for the possible realization of Majorana fermion[8,9] and for new types of spintronic or magnetoelectric devices.[10–12] The effect of strong correlation in TIs is also a challenging issue.[13–24]

One type of the problems concerning strong correlation effect in TIs is about the electron-electron interaction induced topological insulating state,[13–15] and the other type is about the novel phase transition between the topological insulating state and other quantum states.[16–24] The Kane-Mele-Hubbard model is a simple 2D model for a TI with electron-electron interaction.[17–24] It is a Hubbard model on a honeycomb lattice with spin-orbit coupling. The Kane-Mele model,[25] i.e., a tight-binding model on a honeycomb lattice with spin-orbit coupling, describes a 2D topological insulating state, which is also called the quantum spin Hall (QSH) state due to the analogy to the quantum Hall effect. Note that the QSH state has been proposed to be realized in various materials.[26–28] One of the interesting problems in the Kane-Mele-Hubbard model is the interplay between the spin-orbit coupling and electron-electron interaction. Recently, several proposals have been reported for the phase diagram of the model.[17–24]

Superconductivity in TIs is also a research focus. It has been predicted that a Majorana fermion may be realized on a TI surface via inducing superconductivity by proximity effect. In experiment, a 3D TI can be tuned into a superconductor through doping with copper[29,30] or by applying high pressure.[31,32] There have been several theoretical works to examine the possible superconductivity in a 3D TI.[33–36] It is predicted that the superconductivity may occur at sufficient strong pairing. Though some works about the superconductivity on the surface of a 3D topological insulator have been reported,[35–38] there have not been many theoretical studies on the superconductivity in a 2D TI.

In this paper, we study the attractive Kane-Mele-Hubbard model in two dimensions by using a self-consistent mean-field method. As the attractive U increases from zero, the ground state of the 2D bulk remains to be insulating, but the edge states become superconducting due to the gapless edge states, which causes mean-field superconducting instability. The bulk superconductivity occurs only at U larger than a critical value U_c due to the gapness of the TI. We discuss an effective model for the edge superconducting state (ESS) and interpret the mean-field ESS as a superconducting correlation in one dimension.

The attractive U Kane-Mele-Hubbard model is defined as $H = H_0 + H_U$, where H_0 is the Kane-Mele model for the QSH system and H_U describes the attractive Hubbard U term. We have

$$H_0 = -t \sum_{\langle ij\rangle\sigma} c^\dagger_{i\sigma} c_{j\sigma} + i\lambda_{\rm so} \sum_{\langle\langle ij\rangle\rangle\sigma\sigma'} \upsilon_{ij} c^\dagger_{i\sigma} \tau^z_{\sigma\sigma'} c_{j\sigma'} - \mu \sum_{i\sigma} c^\dagger_{i\sigma} c_{i\sigma}, \quad (1)$$

where the sums over $\langle ij\rangle$ and $\langle\langle ij\rangle\rangle$ run over the nearest neighbor (NN) and next-nearest neighbor, respectively. σ denotes spin-up or spin-down, t is the hopping amplitude, and μ is the chemical potential. The second term is the spin-orbit interaction, with $\lambda_{\rm so}$ the spin-orbit coupling constant. τ is the Pauli matrix. $\upsilon_{ij} = \pm 1$, depending on the relative orientation of the two bonds connecting sites i and j.[25] Since the honeycomb lattice is a bipartite lattice, it is convenient to divide the lattice into two sublattices, A and B, and denote $a_{i\sigma}$ ($b_{i\sigma}$) to be an annihilation operator of an electron on sublattice A (B). The Hubbard U term is $H_U = -U\sum_i n_{i\uparrow} n_{i\downarrow}$ with $U > 0$, which will be treated within a mean-field approximation. To have a better understanding of the superconducting state, we first study the bulk properties in a periodic boundary condition in both x and y directions. We then consider the zigzag ribbon structure and study the edge states.

The Hamiltonian Eq. (1) can be expressed in momentum space. The first term with the NN hopping becomes

$$H_{\rm NN} = -t \sum_{k\sigma} (\gamma_k a^\dagger_{k\sigma} b_{k\sigma} + \gamma^*_k b^\dagger_{k\sigma} a_{k\sigma}),$$

where $\gamma_k \equiv \gamma(k) = \sum_{\delta_i} e^{ik\delta_i}$. $\delta_{i=1,2,3}$ are the three NN vectors on the honeycomb lattice [see Fig. 1(a)], $\delta_1 = a_0(\frac{1}{2},\frac{\sqrt{3}}{2})$, $\delta_2 = a_0(\frac{1}{2},-\frac{\sqrt{3}}{2})$, and $\delta_3 = a_0(-1,0)$. Here a_0 is the lattice constant.

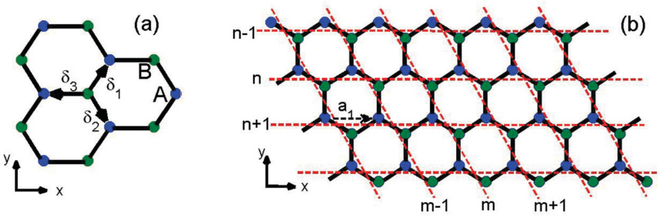

FIG. 1. (Color online) Schematic illustration of the (a) honeycomb lattice and (b) zigzag ribbon structure of the quantum Hall system.

The spin-orbit coupling term in Eq. (1) becomes

$$H_{\rm so} = \sum_k \lambda_k [a^\dagger_{k\uparrow}a_{k\uparrow} - a^\dagger_{k\downarrow}a_{k\downarrow} - b^\dagger_{k\uparrow}b_{k\uparrow} + b^\dagger_{k\downarrow}b_{k\downarrow}],$$

where

$$\lambda_k = 2\lambda_{\rm so}\left[-\sin(\sqrt{3}a_0k_y) + 2\cos\left(\frac{3}{2}a_0k_x\right)\sin\left(\frac{\sqrt{3}}{2}a_0k_y\right)\right].$$

Within the mean-field approximation, the attractive Hubbard U term becomes

$$H_U \approx -\sum_k [\Delta_A a^\dagger_{k\uparrow}a^\dagger_{-k\downarrow} + \Delta^*_A a_{-k\downarrow}a_{k\uparrow} + \Delta_B b^\dagger_{k\uparrow}b^\dagger_{-k\downarrow} + \Delta^*_B b_{-k\downarrow}b_{k\uparrow}],$$

with $\Delta_A = \frac{U}{N_s}\sum_k\langle a_{-k\downarrow}a_{k\uparrow}\rangle$. Since the sublattices A and B are equivalent, we consider $\Delta_A = \Delta_B = \Delta$. In the Nambu spinor representation $\Phi^+_k = (a^+_{k\uparrow}, b^+_{k\uparrow}, a_{-k\downarrow}, b_{-k\downarrow})$, we have

$$H = \sum_k \Phi^+_k H_k \Phi_k,$$

with

$$H_k = \begin{pmatrix} \lambda_k - \mu & -t\gamma_k & -\Delta & 0 \\ -t\gamma^*_k & -\lambda_k - \mu & 0 & -\Delta \\ -\Delta^* & 0 & -\lambda_k + \mu & t\gamma_k \\ 0 & -\Delta^* & t\gamma^*_k & \lambda_k + \mu \end{pmatrix}.$$

Diagonalizing H_k, the excitation energies of the Bogoliubov quasiparticles are $E_{\nu=\pm}(k) = \sqrt{(\epsilon_k \pm \mu)^2 + \Delta^2}$ with $\epsilon_k = \sqrt{\lambda_k^2 + t^2|\gamma_k|^2}$ and ν is the band index. The gap equation is

$$\frac{1}{U} = \frac{1}{4N_A}\sum_{k\nu}\frac{1}{E_\nu}\tanh\left(\frac{\beta E_\nu}{2}\right). \qquad (2)$$

The average electron density is

$$n_e - 1 = -\frac{1}{N_A}\sum_{k\nu}\left[\frac{\eta_\nu\epsilon_k - \mu}{E_\nu}\tanh\left(\frac{\beta E_\nu}{2}\right)\right], \qquad (3)$$

where $n_e = N_e/2N_A$, N_A is the number of sites on sublattice A, and $\eta_{\nu=\pm} = \pm 1$. Thus, for given n_e and U, Δ and μ can be determined self-consistently with the above equations.[40] Here we calculate the half filling case ($n_e = 1$) at zero temperature. In Fig. 2(a), we show the zero-temperature superconducting gap Δ as a function of U and $\lambda_{\rm so}$. We see that for any $\lambda_{\rm so}$ there exists a critical U_c; Δ becomes nonzero only at $U > U_c$. The finite value of U_c reflects the competition between the Cooper pairing and the gapped

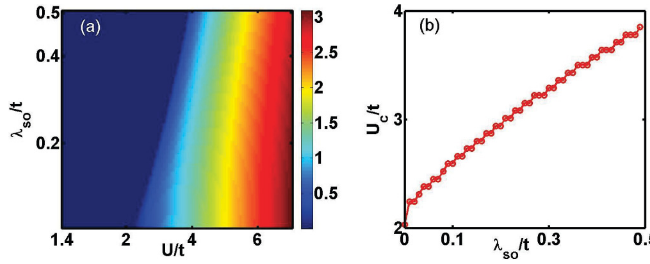

FIG. 2. (Color online) (a) Bulk superconducting gap Δ in parameter space of U/t and $\lambda_{\rm so}$ and (b) critical value of U for bulk superconductivity (U_c) as a function of $\lambda_{\rm so}$, obtained from mean-field theory for the Hamiltonian Eq. (1) at half filled (average one electron per site) at zero temperature.

insulator. Since there is a bulk gap, the attractive U may induce superconductivity only if the pairing energy is sufficiently large. The superconductivity in such a gapped system has been previously discussed in a semiconductor system.[39] The calculated U_c is plotted in Fig. 2(b) as a function of $\lambda_{\rm so}$. $\lambda_{\rm so}$ determines the bulk gap in the Kane-Mele model. We expect U_c to increase with $\lambda_{\rm so}$ since a larger U_c is needed to overcome a larger bulk gap. A special case is $U_c \approx 2.1t$ for $\lambda_{\rm so} = 0$, which indicates that even without the bulk gap there is a finite U_c at the half filling. This property has been noticed in the previous study of the optical lattice systems[41] and is due to zero density of states at the Dirac points.

We now study the edge states of the 2D model. For this purpose, we consider a zigzag ribbon structure as shown in Fig. 1(b). We use a periodic boundary condition in the longitudinal direction (x direction) and a finite width in the transverse direction (y direction). The unit cell of the ribbon structure is labeled by integer indices m and n. The tight-binding Hamiltonian can be written as

$$H_{\rm ribbon} = \int \frac{dk_x}{2\pi}\phi^\dagger(k_x)H_{\rm ribbon}(k_x)\phi(k_x), \qquad (4)$$

where $\phi^\dagger(k_x) = [\ldots, a^\dagger_\uparrow(k_xn), b^\dagger_\uparrow(k_xn), \ldots, a^\dagger_\downarrow(k_xn), b^\dagger_\downarrow(k_xn), \ldots]$ is the basis ($4N$ vector) with $n = 1,2,\ldots,N$. Here n is the row index and N is the width of ribbon, i.e., the number of unit cells along the transverse cross section. $H_{\rm ribbon}(k_x)$ is a $4N \times 4N$ matrix:

$$H_{\rm ribbon}(k_x) = \begin{pmatrix} H_\uparrow(k_x) & 0 \\ 0 & H_\downarrow(k_x) \end{pmatrix}, \qquad (5)$$

where $H_{\sigma=\uparrow\downarrow}(k_x)$ are $2N \times 2N$ tridiagonal matrices. The detail of the expression is given in the Appendix. Approximating the interaction term within the mean-field theory, we have

$$H_U = -\sum_{nk_x}[\Delta_{An}a^\dagger_\uparrow(k_xn)a^\dagger_\downarrow(-k_xn) + \Delta_{Bn}b^\dagger(k_xn)b^\dagger(-k_xn)] + \text{H.c.}, \qquad (6)$$

where $\Delta_{An} = \frac{|U|}{N_r}\sum_{k_x}\langle a_\downarrow(-k_xn)a_\uparrow(k_xn)\rangle$. Δ_{An} (Δ_{Bn}) is the pairing potential on sublattice A (B) of row n. N_r is the number of the unit cell of each row. Therefore, with the basis in Nambu representation $\Psi^\dagger(k_x) = [\ldots, a^\dagger_\uparrow(k_xn), b^\dagger_\uparrow(k_xn), \ldots, a_\downarrow(-k_xn), b_\downarrow(-k_xn), \ldots]$, the mean-field BCS Hamiltonian can be expressed as $H_{\rm MF} = \int \frac{dk_x}{2\pi}\Psi^\dagger(k_x)H_{\rm sc}(k_x)\Psi(k_x)$

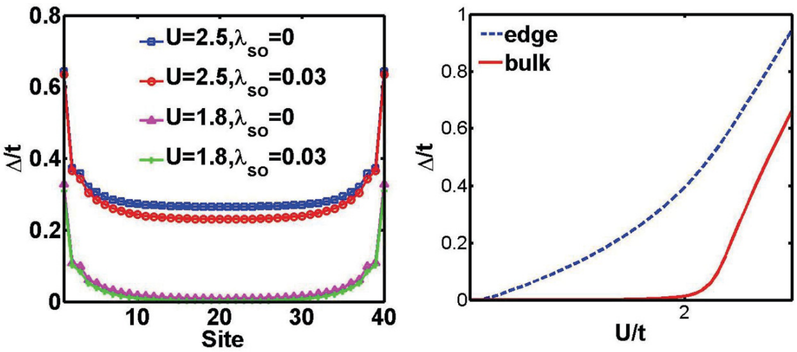

FIG. 3. (Color online) (a) Mean-field zero-temperature superconducting gap Δ across the zigzag ribbon at half filled ($N = 20$, i.e., 40 sites across the ribbon). (b) Dashed line (blue), $\Delta(U)$ at the ribbon edge; solid line (red), $\Delta(U)$ inside the ribbon (middle site).

where

$$H_{\mathrm{sc}} = \begin{pmatrix} H_{\uparrow}(k_x) & -\Delta_R \\ -\Delta_R^* & -H_{\downarrow}^T(-k_x) \end{pmatrix}.$$

Here Δ_R is a diagonal matrix, the diagonal elements of which are $(\ldots,\Delta_{An},\Delta_{Bn},\ldots)$. Given Δ_{An}, Δ_{Bn}, and the chemical potential (i.e., the average electron density $n_e = N_e/[2N_r \cdot N]$), H_{sc} can be diagonalized numerically and we can get the energy dispersion and eigenfunction of the Bogoliubov quasiparticles. Thus, Δ_{An} and Δ_{Bn} can be determined self-consistently. We remark that Δ_{An} and Δ_{Bn} are no longer equivalent in the calculation of the ribbon structure because of the ribbon edge. The results for the half filled case are shown in Fig. 3.

In Fig. 3(a), we show the gap across the ribbon. As we can see, for a large U the bulk becomes superconducting, and the gap Δ near the edges is larger than that in the bulk. For a small U, the gap is zero in bulk, but is nonzero near the edges, which means that the superconductivity only appears near the edges and the bulk is still insulating. This is the ESS, and is the main result of this paper. We note that the surface superconductivity in a topological flat band system has been studied recently.[42]

In Fig. 3(b), we show the U dependence of the gap Δ at the edge and in the bulk. Clearly, the bulk superconductivity acquires $U > U_c$ but the edge superconductivity does not. A small U immediately induces nonzero edge superconductivity. This is because that one-dimensional (1D) Dirac fermion (linear dispersion of the edge state) has a constant density of state, which is in sharp contrast to the 2D case. In two dimensions, the density of state of Dirac fermions is zero at the Dirac point, which acquires a finite critical U_c to induce the bulk superconductivity at half filled. Based on this analysis, we may argue that there is a critical U for the superconductivity on the surface of a 3D topological insulator. Due to the appearance of the ESS in the attractive Kane-Mele-Hubbard model, as the attractive U increases from zero, the topological insulating state is immediately developing into the ESS, and becomes bulk superconducting at $U > U_c$. We have examined the slightly doped case ($\mu \neq 0$ but still in the bulk gap) and the results are qualitatively similar.

For the ribbon geometry, a special case is $\lambda_{\mathrm{so}} = 0$, where the system becomes a graphene zigzag ribbon. It is well known that the edge states of a graphene zigzag ribbon are flat bands. Our calculations [see Fig. 3(a)] show that edge superconductivity also appears for any small U in this case. The peculiar feature of the flat band is its divergent density of states at Fermi level (the half filling case), which is believed to induce an extremely high superconducting critical temperature.[42]

We now examine the finite-size effect in the ribbon structure. We show the superconducting gap Δ in bulk for ribbons with different widths in Fig. 4. Increasing ribbon width, the U_c in bulk grows asymptotically to approach the value in an infinite system. It implies that the bulk superconductivity is easier to achieve in a narrow ribbon. On the other hand, the edge states are not influenced by the ribbon width; i.e., any small U can immediately induce edge superconductivity.

Finally, we study an effective model for the ESS. The effective model of the helical edge states is $H_0 = \hbar v_f \int dx(\Phi_{R\uparrow}^{\dagger} i\partial_x \Phi_{R\uparrow} - \Phi_{L\downarrow}^{\dagger} i\partial_x \Phi_{L\downarrow})$. The attractive interaction is $H_U = -U\int dx \Phi_{R\uparrow}^{\dagger}\Phi_{R\uparrow}\Phi_{L\downarrow}^{\dagger}\Phi_{L\downarrow}$. Since the electron spin is locked with its momentum, we ignore the right-moving (left-moving) index R (L) in the following. In momentum space, we have $H_0 = \int \frac{dk}{2\pi}\psi^{\dagger} H_0(k)\psi$ where $\psi^{\dagger} = [c_{k\uparrow}^{\dagger}, c_{k\downarrow}^{\dagger}]^T$, and

$$H_0(k) = \begin{pmatrix} \hbar v_f k - \mu & 0 \\ 0 & -\hbar v_f k - \mu \end{pmatrix}.$$

The eigenvalues are $E_{\nu=\pm} = -\mu \pm \hbar v_f |k|$ where $\nu = \pm$ is the band index. Since not the spin but the helicity is a good quantum number here, the upper ($\nu = +$) and lower ($\nu = -$) bands correspond to different helicity. Based on the BCS mean-field approximation, $H_U = -\int \frac{dk}{2\pi}(\Delta^* c_{-k\downarrow}c_{k\uparrow} + \Delta c_{k\uparrow}^{\dagger}c_{-k\downarrow}^{\dagger})$ with $\Delta = U\int \frac{dk}{2\pi}\langle c_{-k\downarrow}c_{k\uparrow}\rangle$. It should be noticed that when $k > 0$ ($k < 0$) $\langle c_{-k\downarrow}c_{k\uparrow}\rangle$ indicate the pairing in upper band $\nu = +$ (lower band $\nu = -$). Thus, Δ includes superconducting pairs in both bands.

It is convenient to express the superconducting Hamiltonian in the Nambu basis $\varphi^{\dagger} = [c_{k\uparrow}^{\dagger}, c_{-k\downarrow}]$ but not in the band basis.

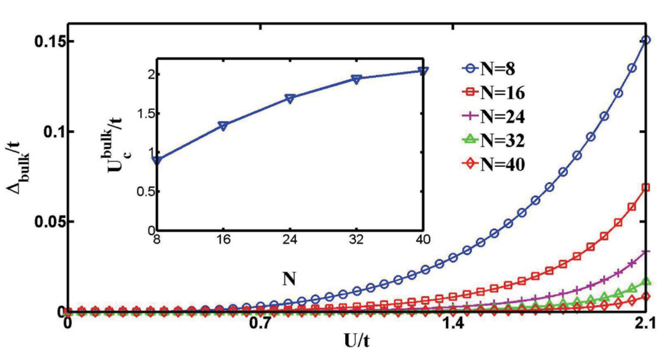

FIG. 4. (Color online) Bulk superconducting gap as a function of U for different ribbon widths N. Here, $\lambda_{\mathrm{so}} = 0.03$, and the results are similar for other values. Inset: U_c as a function of N.

We have

$$H_{\rm sc} = \begin{pmatrix} \hbar v_f k - \mu & -\Delta \\ -\Delta^* & -\hbar v_f k + \mu \end{pmatrix}.$$

The energy dispersion of the Bogoliubov quasiparticle is $\epsilon_B(k) = \sqrt{\Delta^2 + (\hbar v_f k - \mu)^2}$. We get the gap equation:

$$\frac{1}{U} = \frac{1}{2}\int \frac{dk}{2\pi}\frac{\tanh[\beta\epsilon_B(k)/2]}{\epsilon_B(k)}.$$

In order to determine μ and Δ, we need the number equation concerning the particle conservation (δ: filling):

$$\delta = \int \frac{dk}{\pi}\left\{\nu^2 + \frac{v_f k - \mu}{\epsilon_B(k)} f_F[\epsilon_B(k)]\right\} - N_-,$$

where $\nu^2 = \frac{1}{2}[1 - \frac{\hbar v_f k - \mu}{\epsilon_B(k)}]$, f_F is the usual Fermi function, and N_- is the electron number of the filled band $\nu = -$. With the above equations, we can determine the properties of the ESS with given U and δ. The gap $\Delta(U)$ is calculated self-consistently for cases $\delta = 0$ (half filling) and 0.15, for example (see Fig. 5). Since it is an effective model of a lattice system, it is natural to use the hopping t and 1D lattice constant $a_1 = \sqrt{3}a_0$ as the unit. We can deduce the parameters, e.g., v_f, via fitting the tight-binding band structure. In Fig. 5(a), the results show that when U is rather small the superconducting gap Δ is still nonzero, which is qualitatively consistent with the tight-binding calculation. We also calculate the temperature dependence of the gap Δ in Fig. 5(b).

The 1D superconducting order here is obtained in the mean-field level, which does not survive the quantum fluctuation. It is well known that such an interacting electron gas is described by 1D Luttinger liquid theory,[43] where the forward scattering term H_U contributes to a nontrivial Luttinger parameter $K = \sqrt{(v_f + U)/(v_f - U)}$ and does not open a gap. The *gapless* helical edge state is therefore rather robust, except in the case that both forward and Umklapp scattering exist at the same time that leads to a gap if $K < 1/2$.[44] Note that this Umklapp gap has nothing to do with our mean-field superconducting gap, because we are considering a negative-U model where $K > 1$. Nevertheless, the ESS we study here can actually be viewed as a quasi-one-dimensional superconducting system

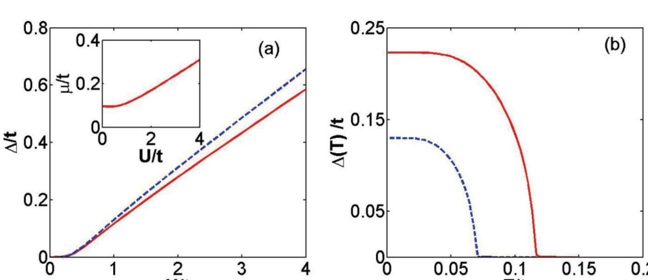

FIG. 5. (Color online) (a) Mean-field superconducting gap of the effective model for ESS at zero temperature. Dashed line (blue): half filled case $\delta = 0$. Solid line (red): $\delta = 0.15$. We set $\hbar v_f = 0.2t \times a_1$ and momentum cutoff $k_c = \frac{\pi}{3a_1}$, where t is the hopping amplitude and $a_1 = \sqrt{3}a_0$ is the 1D lattice constant of the tight-binding model. Inset: chemical potential μ vs U for $\delta N = 0.15$. (b) T dependence of Δ for half filled case. Dashed line (blue): $U = 1t$. Solid line (red): $U = 1.5t$.

which is similar to the ultrathin superconducting nanowire.[45,46] A key feature of a quasi-one-dimensional superconducting nanowire is that thermally activated phase slip and quantum phase slip processes will induce finite resistance when $T < T_c$. *Therefore, the ESS illustrated in our mean-field theory should be viewed as superconducting correlation at the edge, rather than a thermodynamically stable superconducting state.*

In summary, we have studied the phase transition from the topological insulating state to the superconducting state in the attractive Kane-Mele-Hubbard model by using a self-consistent mean-field theory. The mean-field theory shows an edge superconducting state, which is superconducting at the edge but insulating in the bulk. In this model, as the attractive U increases from zero, the edge superconducting state occurs immediately and the bulk becomes superconducting only at $U > U_c$. We have also proposed an effective model to discuss the edge superconducting state. While the 1D superconducting state is unstable against quantum fluctuation, the edge superconducting state we demonstrated may be viewed as an edge state with strong superconducting correlation.

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APPENDIX

Here, we give the expression of $H_{\sigma=\uparrow\downarrow}$ in Eq. (5). We have

$$H_\sigma(k_x) = \begin{pmatrix} H^\sigma_{11} & H^\sigma_{12} & 0 & \cdots & 0 \\ H^{\uparrow\sigma}_{21} & H^\sigma_{22} & H^\sigma_{23} & & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & & H^\sigma_{N-1N-2} & H^\sigma_{N-1N-1} & H^\sigma_{N-1N} \\ 0 & \cdots & 0 & H^\sigma_{NN-1} & H^\sigma_{NN} \end{pmatrix},$$

with

$$H^\sigma_{nn} = \begin{pmatrix} -\eta S_{k_x} - \mu & \chi_{k_x} \\ \chi^*_{k_x} & \eta S_{k_x} - \mu \end{pmatrix},$$

$$H^\sigma_{nn-1} = \begin{pmatrix} \eta \bar{S}_{k_x} & -t \\ 0 & -\eta \bar{S}_{k_x} \end{pmatrix}, \quad H^\sigma_{nn+1} = \begin{pmatrix} \eta \bar{S}^*_{k_x} & 0 \\ -t & -\eta \bar{S}^*_k \end{pmatrix}.$$

Here $S_{k_x} = 2\lambda_{\rm so}\sin(k_x a_1)$ and $\bar{S}_{k_x} = 2\lambda_{\rm so}\sin(\frac{k_x a_1}{2})e^{i\frac{k_x a_1}{2}}$ concerning the spin-orbit coupling; $\chi_k = -t\cdot(1 + e^{-ik_x a_1})$ is related with the next neighborhood hopping; $\eta = +1(-1)$ for spin-up (spin-down). $a_1 = \sqrt{3}a_0$ is the 1D lattice constant, i.e., the distance between adjacent unit cells along the x direction [see Fig. 1(b)].

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