i-Josephson Junction as Topological Superconductor

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Superconducting states with broken time reversal symmetry are rarely found in nature. Here we predict that it is inevitable that the time reversal symmetry is broken spontaneously in a superconducting Josephson junction formed by two superconductors with different pairing symmetries dubbed as i-Josephson junction. While the leading conventional Josephson coupling vanishes in such an i-Josephson junction, the second order coupling from tunneling always generates chiral superconductivity orders with broken time reversal symmetry. Josephson frequency in the i-junction is doubled, namely $\omega = 4eV/h$. The result can not only provide a way to engineer topologically trivial or nontrivial time-reversal breaking superconducting states, but also be used to determine the pairing symmetry of unconventional superconductors.

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Introduction—Van der Waals (vdW) Josephson junction[1], which is contacted by two close-by superconducting (SC) layers by vdW forces, has been realized in layered dichalcogenide superconductors recently[1, 2]. This provides a platform to investigate the properties of two SC layers with different pairing symmetries forming in the junction. In general, the physics of the junction is controlled by the relative phase between the two SC order parameters, $\Delta \theta$. In a conventional Josephson junction which is formed by two s-wave SC layers, $\Delta \theta$ is typically zero in the absence of external or internal magnetic fields. It can be turned to nonzero by magnetic fields that break the time reversal symmetry of the system explicitly. However, in the unconventional Josephson junction, $\Delta \theta$ can be nonzero in the ground state without external nor internal magnetic fields[3–5]. A special case $\Delta \theta = \pm \pi/2$, which breaks time-reversal symmetry, is called chiral SC in the literature[6].

Superconductors with spontaneous time-reversal symmetry breaking (TRB) pairing states[7–15] have been widely sought. The most intriguing property of a TRB SC is the nontrivial topology, namely, a TRB SC can be a topological superconductor (TSC)[16–19], e.g. topological $p + ip[20–22]$ and $d + id[23–28]$ superconductors. The former $p + ip$ TSC can be realized in many spin-orbital coupling systems[22, 29–37], while the latter $d + id$ TSC has only been proposed in honeycomb lattice systems[38], such as doped graphene[24, 28, 39–41], single TiSe$_2$ layer[42] and bilayer Silicene[25]. Although the $d + id$ TSC exhibits many interesting phenomena, such as quantized boundary current[23, 28], spontaneous magnetization[23, 43], quantized spin and thermal Hall conductance[28, 43], and geometric effects[44], there is no strong experimental evidence to support the presence of this chiral SC state.

Here, we ask whether a TRB SC can be spontaneously formed in a vdw Josephson junction. We show that the TRB takes place spontaneously in this Josephson junction formed by two SC layers with different pairing symmetries as illustrated in FIG. 1. For example, a $d + id$ TRB SC can be engineered in a junction with a $d_{x^2−y^2}$ SC layer close to a $d_{xy}$ one. Furthermore, we prove that this $d + id$ SC constructed in this way is also a TSC. The junction has a distinct Josephson frequency, $\omega = 4eV/h$, which is twice of the conventional Josephson frequency $2eV/h$. We discuss possible experimental realizations for this type of junctions. The results can not only help to realize novel SC states and design new SC qubit devices[45, 46], but also be used to determine the pairing symmetry of an unknown SC by the unique feature of Josephson frequency.

Before we discuss specific models, we first present a general argument. Considering a general Bogoliubov-De Gennes (BDG) Hamiltonian of two SC layers connected through tunneling and expanding the free energy up to the fourth order of the tunneling, the free energy can be generally written as[3–5, 47]

$$F = F_0 − J \cos \Delta \theta + g \cos^2 \Delta \theta,$$

where the first term is the relative phase independent term, the second term is the conventional Josephson coupling term.
resentations, namely, they have different pairing symmetries, \( \Delta \) and \( J \), except the point group. One can notice all the parameter functions are represented by the red dashed lines, which coincide the arcs in BZ.

At zero temperature, the free energy is \( \mathcal{F} = \sum_{\mathbf{k}} (E^+ + E^-) \). We can expand the free energy up to the fourth order of \( t(k) \). The free energy is given by Eq. (1), in which the parameters can be specified as

\[
J = \sum_{\mathbf{k}} \frac{t^2(k) g_1(k) + t^4(k) g_3(k)}{\Delta_\alpha(k) \Delta_\beta(k)} \quad \text{and} \quad g = \sum_{\mathbf{k}} t^4(k) g_2(k) \Delta_\alpha^2(k) \Delta_\beta^2(k).
\]

The explicitly form of \( g_i(k) \) are shown in the Supplementary Materials. While the functions of \( g_i(k) \) are very lengthy, we can analyze their symmetry characters. For convenience, we consider a square lattice symmetry classified by the \( C_{4v} \) point group. One can notice all the parameter functions except \( \Delta_1(k) \) belong to the \( A_1 \) irreducible representation of \( C_{4v} \).

The magnitudes and phases of pairing orders are represented by the lengths and directions of the arrows; (c) and (d) show the real and image parts of \( d_{xy} + id_{xy} \) order in the first layer with \( J_1 = 3.1 \) and \( J_2 = 3 \). The Fermi surfaces of the two layer Hamiltonian are represented by the red dashed lines, which coincide the arcs in BZ.

\[
E^{\pm \pm} = \pm \frac{1}{\sqrt{2}} \left[ \epsilon_\alpha^2 + \epsilon_\beta^2 + \Delta_\alpha^2 + \Delta_\beta^2 + 2t^2 \pm \sqrt{(\epsilon_\alpha^2 - \epsilon_\beta^2 + \Delta_\alpha^2 - \Delta_\beta^2)^2 + 4t^2 (\epsilon_\alpha + \epsilon_\beta)^2 + |\Delta_\alpha e^{i\theta_\alpha} - \Delta_\beta e^{i\theta_\beta}|^2} \right].
\]
top and bottom layers respectively. Including the tunneling coupling between the two layers, the overall Hamiltonian can be written as \( H = H_{J_1} + H_{J_2} + H_t \), where

\[
H_{J_\alpha} = \sum_{\mathbf{k},\sigma} \xi_\alpha(\mathbf{k}) d_{\mathbf{k},\sigma}^{\dagger} d_{\mathbf{k},\sigma} + \sum_{i,\delta=x,y} J_\alpha (\hat{S}^i_{\delta} \cdot \hat{S}^{i+\delta}_{\delta}) - \frac{1}{4} n_i^\alpha n_{i+\delta}^\alpha,
\]

\[H_t = t \sum_{\alpha,\mathbf{k},\sigma} d_{\mathbf{k},\sigma}^{\dagger} d_{\mathbf{k},\sigma} + h.c.\]  

(7)

Here the tunneling term \( t \) is chosen to be real and independent of \( \mathbf{k} \) for simplicity. We also drop the double occupancy projection operators which is required in the standard \( t - J \) model because the double occupancy projection in the mean field level can be treated as an overall renormalization factor to the band dispersion[50, 51]. Therefore, it does not affect the qualitative result. The sketch of this model is shown in FIG. 2 (a).

In the mean field solution, we can compare the energies of the \( s \)-wave and \( d \)-wave SC states. The self-consistent mean field solutions for the \( d \)-wave SC states are given by[52]

\[
\frac{\Delta_{x^2-y^2}(\mathbf{k})}{\cos k_x - \cos k_y} = \sum_{\mathbf{k}'} \frac{2J_1}{N} (\cos k'_x \pm \cos k'_y) (d_{-\mathbf{k}',\sigma}^{\dagger} d_{\mathbf{k}',\sigma})
\]

(8)

\[
\frac{\Delta_{xy}(\mathbf{k})}{\sin k_x \sin k_y} = \sum_{\mathbf{k}'} -\frac{8J_2}{N} \sin k'_x \sin k'_y (d_{-\mathbf{k}',\sigma}^{\dagger} d_{\mathbf{k}',\sigma})
\]

(9)

We take the band dispersion,

\[\xi_\alpha = -2t_1 \cos k_x - 4t_2 \cos k_y + \mu_\alpha - \mu\]  

(10)

where \( t_1^{(2)} \) indicates the NN (NNN) hopping and \( \alpha = 1, 2 \), corresponding the top and bottom layers. \( \mu_\alpha \) is the corresponding on-site energy in each layer and \( \mu \) is the chemical potential. Without the tunneling, in the mean field solution shown in the Supplementary Materials, we find that the \( d_{x^2-y^2} \) and \( d_{xy} \) orders are favored on the top and bottom layers respectively when the parameters are set as \( t_1 = 0.88, t_2 = -0.35, t_2' = 1.67, t_2'' = -0.33, \mu_1 = -0.4, \mu_2 = -1.2 \) and \( \mu + \mu_1 = 0 \).

Turning on the layer tunneling and taking \( t = 0.4 \), the phase diagram is plotted in the Fig. 2 (b) as the function of \( J_1, J_2 \). The lengths of the vectors in Fig. 2 (b) represent the strength of the orders and the directions relate to the phases. As \( J_1 \) and \( J_2 \) increase, both \( d \)-wave orders become stronger and the relative phase maintains to be \( \pm \pi/2 \). The imaginary and real parts of the order parameter in the first layer are shown in Fig. 2 (c) and (d). Clearly, the real part has \( d_{x^2-y^2} \) symmetry and the imaginary part has \( d_{xy} \) symmetry. The \( d_{xy} \) order in the first layer is induced through the proximity effect from the second layer. This result is consistent with our previous analysis.

**Topological analysis**—Now we discuss the topological properties of the above spontaneous TRB SCs. The state at the i-junction can be topologically nontrivial for a \( d \pm id \) state but trivial for an \( s \pm id \) state. To show this, we can analyze the symmetry property of the Berry curvature. Starting from the Hamiltonian (3) with \( \theta_1 = 0 \) and \( \theta_3 = \pi/2 \), the band dispersions \( \epsilon_\alpha(\mathbf{k}) \) and \( \epsilon_\beta(\mathbf{k}) \) both belong to the \( A_1 \) irreducible representation (IR) of \( C_{4v} \). We consider the \( \sigma_v \) symmetry operation which maps \( \mathbf{k} = (k_x, k_y) \rightarrow \mathbf{k} = (k_x, -k_y) \) or \( (k_x, k_y) \rightarrow (k_x, k_y) \). In the \( s \pm id \) state, if the tunneling term \( t(\mathbf{k}) \) belongs to \( A_1 \) or \( B_1 \) IR, the Hamiltonian is invariant under \( \sigma_v \) operation. If the tunneling term \( t(\mathbf{k}) \) belongs to \( B_2 \) IR, under a \( \sigma_v \) operation, the Hamiltonian becomes \( \tilde{H}(\mathbf{k}) \), which can be expressed as \( \tilde{H}(\mathbf{k}) = \tau_y H(\mathbf{k}) \tau_x \). The corresponding eigenstate becomes \( |\tilde{u}_\alpha(\mathbf{k})\rangle = \tau_x |u_\alpha(\mathbf{k})\rangle \). In both cases, considering the definition of Berry curvature

\[B(\mathbf{k}) = i \sum_{n \in \text{occ}} \epsilon_{k_x k_y} \langle \partial_{k_x} u_n(\mathbf{k}) | \partial_{k_y} u_n(\mathbf{k}) \rangle\]  

(11)

one can find that the Berry curvature changes sign under \( \sigma_v \) operation so that the total Chern number is zero. But for the \( d \pm id \) state, the Berry curvature is invariant under \( C_4, \sigma_v, \) and \( \sigma_d \) operation. This means that the nonzero Chern number is forbidden by any symmetry operations. Thus, under some suitable parameters, the system can be a topological \( d \pm id \) SC. This is clearly shown in FIG. 3.

The above conclusion can be numerically verified. We perform numerical calculation for the model in Eq. (7). We calculate the topologically protected edge states in a stripe lattice as shown in FIG. 4. The parameters in the calculation are set to be \( J_1 = 3.4, J_2 = 3 \) in Eq. (7), and the correspond-
For the i-junction, the modified Josephson parameters, there are four chiral modes on each edge, which are corresponding to a Chern number equal to minus four, as shown in FIG. 4.

Experimental signatures—There are three smoking-gun signatures for the above topological $d + id'$ superconductivity in the Hamiltonian (6), the parameter we choose is $J_1 = 3.4$, $J_2 = 3$, and the corresponding self-consistent mean field SC orders are $\Delta_{x^2-y^2} = 0.8183$, $\Delta_{xy} = 0.5562i$. On the top panel is the band structure with left edge state blue and right red. The bottom panel are the corresponding distribution of edge states.

The AC Josephson current is $I = I_0 \sin(2\Delta\theta_0 - 4eV_0t/\hbar)$. The corresponding Josephson frequency is $\omega_i = 2\omega_0 = 4eV_0/\hbar$, which is twice of the ordinary Josephson frequency.

The third experimental signature is the magnetic field dependence of the critical current. When a magnetic field $B$ is applied to a conventional Josephson junction with a length $L$ and the penetration depth $W$, the critical current is

$$I_c = j_0 \frac{\sin(\pi \Phi/\Phi_0)}{2\pi \Phi/\Phi_0}.$$

The oscillation pattern is changed. Notice the last two experimental signatures are valid for all i-Josephson junctions.

Engineering TSC—Previously, the TSCs have already been proposed in $p$-wave superconductors[21], TI surface states[29–31] and semiconductor nanowires[22, 32–37]. These proposals all focus on the 0$d$ Majorana bound states, not the 1$d$ Majorana chiral edge states. Recently, the chiral Majorana modes have been observed in the quantum anomalous Hall insulator-superconductor structure[54]. Compared to the previous work, the major advantage here is that TSC and the corresponding chiral edge state can be realized with conventional $d$-wave superconductors, such as cuprates, and no external magnetic field[55] or topological non-trivial band structures are needed. Thus, in principle, our method allows TSC to operate at very high temperature because of the high SC transition temperature of cuprates.

Recently, the advances in vdW heterostructure technology provide an effective way to engineer the rotation angle between the two SC layers with a high accuracy[56, 57]. Furthermore, the vdW junction is defect-free contacted and has a strong proximity coupling[1, 2], which renders a larger value of $g$ in Eq. (1). Thus an explicit design of a TSC i-junction is to align two identical $d$-wave superconductors along the $z$ direction with a relative $\pi/4$ in-plane angle[58]. This design can be implemented by recent rapid technological progress in engineering heterostructures.

Engineering TRB state—The result also allows us to engineer new exotic SC states with TRB, e.g. $s + id$ pairing state. Superconductors with these type of pairing states have been widely searched. However, success has been very limited. So far, spontaneous TRB in SC states have been rarely observed.

The above physics can also be potentially realized in bulk materials. For example, it has been theoretically suggested that the FeAs layer, the building block in iron-based superconductors, and the CuO$_2$ layer, the building block in cuprates, can be hybridized to form a hybrid crystal[59]. Following our results, in such a hybrid crystal, the time reversal symmetry must be broken as FeAs[51, 60] and CuO$_2$[48, 49] are known to favor $s$-wave and $d$-wave pairing symmetries respectively.

The superconducting state in such a material must be $s \pm id$.

Applications—The i-Josephson junction can be used to determine the pairing symmetry of an unknown superconductor. This is based on the fact that the Josephson frequency will be doubled if two SC layers have different pairing symmetries. The i-Josephson junction can also be used to make a quantum qubit because the free energy has two minima. It becomes a natural two-level system to form a qubit. Other excited states have much higher energy so that the two-level system is well protected.

In summary, we have shown that the i-Josephson junction is an inevitable result when a Josephson junction is formed by two superconductors with different pairing symmetries. The
Josephson frequency is doubled. A TSC with a $d \pm id$ pairing symmetry can be achieved in this way. The result also provides a method to design TRB $s + id$ superconductor.

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