Superconducting Phase with a Chiral f-Wave Pairing Symmetry and Majorana Fermions Induced in a Hole-Doped Semiconductor

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We show that a chiral $(f + if)$-wave superconducting pairing may be induced in the lowest heavy hole band of a hole-doped semiconductor thin film through proximity contact with an s-wave superconductor. The chirality of the pairing originates from the 3π Berry phase accumulated for a heavy hole moving along a close path on the Fermi surface. There exist three chiral gapless Majorana edge states, in consistence with the chiral $(f + if)$-wave pairing. We show the existence of zero-energy Majorana fermions in vortices in the semiconductor-superconductor heterostructure by solving the Bogoliubov–de Gennes equations numerically as well as analytically in the strong confinement limit.

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Superconductors or superfluids with unconventional pairings have been an important subject in condensed matter physics for many decades because of their rich physics and important applications. There has been considerable experimental evidence to support that the pairing symmetry in high-T_c superconductors is d wave [1]. The pairing symmetry in the superfluid ^{3}He was found to be p wave [2]. The superconducting order parameters in Sr_2RuO_4 and some heavy-fermion materials are suggested to be chiral $p_x + ip_y$ wave [3], although the true nature of the order parameters in these materials has not been fully settled in experiments [4,5]. The importance of chiral p-wave superconductors or superfluids is that the quasiparticle excitation inside a vortex is a zero-energy Majorana fermion with non-Abelian exchange statistics, which is a crucial ingredient for topological quantum computation (TQC) [6].

However, in contrast to the simple s-wave superconductor described by the BCS theory, the theoretical description and experimental identification of unconventional superconductivity and the associated exotic physics in natural solid state systems are often difficult and, in many systems, controversial. For instance, despite the tremendous technological potential, the observation of the exotic properties such as quantum half-vortices and non-Abelian statistics in Sr_2RuO_4 has been a serious problem because of the small quasiparticle excitation energy gap as well as the intrinsic spin-orbit coupling in the suggested p-wave order parameter [7]. Therefore, it should be not only interesting but also important to investigate whether various unconventional superconducting pairings and the associated exotic physics can be externally induced from conventional s-wave superconductors or superfluids [8–11]. For instance, schemes have been proposed recently to induce Majorana fermions in the vortex core of conventional s-wave superconductors that are proximately coupled to topological insulators or electron-doped semiconductors [9–11].

In this Letter, we propose that a chiral $(f + if)$-wave superconducting pairing can be induced in a hole-doped semiconductor thin film through the proximity contact with an s-wave superconductor. To the best of our knowledge, a chiral $(f + if)$-wave superconducting pairing and the associated exotic physics have not been unequivocally identified in any condensed matter system. The induced chiral $(f + if)$-wave pairing symmetry has a topological origin: the geometric phase [12] of holes in the Bloch band. It is well known that an electron or hole evolving adiabatically in the reciprocal space accumulates a geometric phase associating with the adiabatic change of the quasimomentum [12], in analogy to the Aharanov-Bohm phase acquired by an electron moving in the real space in the presence of a magnetic field. The geometric phase is nonzero in the hole-doped semiconductors with nonvanishing spin-orbit coupling, which tunes an original s-wave pairing into a chiral $(f + if)$-wave pairing for holes in the lowest energy band. The induced chiral $(f + if)$-wave superconductor has a full pairing gap in the 2D bulk, and 3 gapless chiral Majorana fermions at the edge. By solving the Bogoliubov–de Gennes (BdG) equations analytically and numerically, we show that there exists a Majorana zero-energy state in the vortex core of the semiconductor-superconductor heterostructure in some parameter regions. The corresponding quasiparticle exchange statistics in this system is the same as that for a chiral p-wave superconductor or superfluid; therefore, the proposed heterostructure can be used as a platform for observing non-Abelian statistics and performing TQC. The advantage of using hole-doped, instead of electron-doped, semiconductors for TQC is that hole-doped semiconductors have stronger spin-orbit coupling due to the larger effective mass of holes and the p-like symmetry of the valence band, resulting in larger carrier densities.

The physical system we consider is a heterostructure composed of an s-wave superconductor, a hole-doped semiconductor thin film, and a magnetic insulator [Fig. 1(a)]. In the semiconductor thin film, the dynamics of holes can be described by a single particle effective Hamiltonian that contains both the Luttinger four band model and the spin-3/2 Rashba term [13]:

$$H_0 = [(\gamma_1 + 5\gamma_2/2)\mathbf{k}^2 - 2\gamma_2(\mathbf{k}\cdot\mathbf{J})^2]/2m + \alpha(\mathbf{J}\times\mathbf{k})\cdot\hat{z} + 2h_0 J_z - \mu, \quad (1)$$

where $\mathbf{J}$ is the total angular momentum operator for a spin-3/2 hole, γ_1 and γ_2 are the Luttinger parameters, and μ is the chemical potential. Henceforth we set $\hbar = 1$. The confinement of the quantum well along the z direction yields the quantized momentum $\langle k_z\rangle \approx 0$, $\langle k_z^2\rangle = (\pi/a)^2$, where a is the thickness of the quantum well. α is the Rashba spin-orbit coupling strength. The crucial difference between the Rashba terms in the 2D hole and electron gases is that $\mathbf{J}$ in the 2D hole gas (2DHG) is a spin-3/2 matrix, describing both the heavy holes (HH) and light holes (LH). The term $2h_0J_z$ describes a Zeeman splitting induced either through the polarization of the local magnetic moments in the semiconductor [14] or the exchange field through the contact with a magnetic insulator.

The eigenstates of the Hamiltonian (1) can be written as

$$\Psi_{\mathbf{k}} = (u_0 e^{-i3\theta_{\mathbf{k}}}, iu_1 e^{-i2\theta_{\mathbf{k}}}, -u_2 e^{-i\theta_{\mathbf{k}}}, -iu_3)^T, \quad (2)$$

where $\theta_{\mathbf{k}}$ is the azimuthal angle of $\mathbf{k}$, u_i are functions of k only, and the eigenstates of the reduced Hamiltonian

$$\bar{H}_0 = -\gamma_2 k^2 J_y^2/m - \alpha k J_x - \gamma_2\langle k_z^2\rangle J_z^2/m + 2h_0 J_z. \quad (3)$$

Equation (2) ensures that the wave function for the lowest HH band is single valued at $\mathbf{k} = 0$ (i.e., only $u_3 \neq 0$ at $\mathbf{k} = 0$). The additional phase $e^{im\theta_{\mathbf{k}}}$ needs to be multiplied by the wave functions for the other bands to ensure the single value. In Fig. 1(b), we plot the energy spectrum for the 2DHG. The degeneracy between different HH and LH bands at $k = 0$ is lifted due to nonzero $\langle k_z^2\rangle$ and h_0. In the strong (weak) confinement region $2\gamma_2\langle k_z^2\rangle/m > (<)\ 4h_0$, the second lowest energy band is the HH (LH) with the corresponding wave function $\Psi_{\mathbf{k}} e^{i3\theta_{\mathbf{k}}}$ ($\Psi_{\mathbf{k}} e^{i\theta_{\mathbf{k}}}$).

The proximity-induced superconductivity is described by the Hamiltonian [15]

$$\hat{H}_p = \sum_{m_J=1/2,3/2} \int d\mathbf{r}\{\Delta_s(\mathbf{r}) c^{\dagger}_{m_J} c^{\dagger}_{-m_J} + \text{H.c.}\}, \quad (4)$$

where $c^{\dagger}_{m_J}$ are the creation operators for holes with the angular momentum m_J and $\Delta_s(\mathbf{r})$ is the proximity-induced gap. When μ lies between the lowest two bands [Fig. 1(b)], and only the lowest HH band is occupied, the effective superconducting pairing for holes becomes

$$\Delta_{\text{eff}} \propto \langle a_{\mathbf{k}} a_{-\mathbf{k}}\rangle \propto i\Delta_s g(k)\exp(i3\theta_{\mathbf{k}}), \quad (5)$$

where $a_{\mathbf{k}} = \sum_{m_J} \chi_{m_J} c_{\mathbf{k}m_J}$ is the annihilation operator for holes at the lowest HH state $\Psi_{\mathbf{k}}$, with the coefficient $\chi_{m_J} = \Psi^*_{\mathbf{k}m_J}$, $g(k) = 2(u_0u_3 + u_1u_2)$. We have used $\Delta_s \propto \langle a_{\mathbf{k}m_J} a_{-\mathbf{k}(-m_J)}\rangle$ and $\langle a_{\mathbf{k}m_J} a_{-\mathbf{k}m'_J}\rangle = 0$ if $m_J \neq -m'_J$ to derive Eq. (5). Clearly the pairing order Δ_{eff} has a chiral $(f + if)$-wave symmetry. Around the Fermi surface $g(k) \to 1$; that is, $\Delta_{\text{eff}} \to i\Delta_s \exp(i3\theta_{\mathbf{k}})$.

The $3\theta_{\mathbf{k}}$ phase in Δ_{eff} originates from a 3π Berry phase accumulated when the holes move in the momentum space. In the lowest HH band, the Berry phase along a loop on the Fermi surface is $\phi = \int_{\mathbf{k}_1}^{\mathbf{k}_2} \mathbf{A}\cdot d\mathbf{k} = A(k_F)\delta\theta_{\mathbf{k}}$, where the Berry connection $\mathbf{A} = i\langle\Psi_{\mathbf{k}}|\nabla_{\mathbf{k}}|\Psi_{\mathbf{k}}\rangle = A(k)\nabla\theta_{\mathbf{k}}$ with $A(k) = (3u_0^2 + 2u_1^2 + u_2^2)$, $\delta\theta_{\mathbf{k}} = \theta_{\mathbf{k}_2} - \theta_{\mathbf{k}_1}$ is the change of the azimuthal angle from $\mathbf{k}_1$ to $\mathbf{k}_2$. In Fig. 2(a), we see $A(k) \to 3/2$ around the Fermi surface for the lowest HH state, indicating a $3\delta\theta_{\mathbf{k}}/2$ Berry phase (3π for a close loop) for a single hole and a $3\delta\theta_{\mathbf{k}}$ phase for a Cooper pair. Therefore, Δ_{eff} in the lowest band has a phase factor $\exp(i3\theta_{\mathbf{k}})$. Similarly, we find the Berry phases for the upper HH, lower LH, and upper LH bands are -3π, π, and $-\pi$ [Fig. 2(a)], respectively, which means that their superconducting pairing symmetries are chiral $f - if$, $p_x + ip_y$, $p_x - ip_y$ waves, respectively.

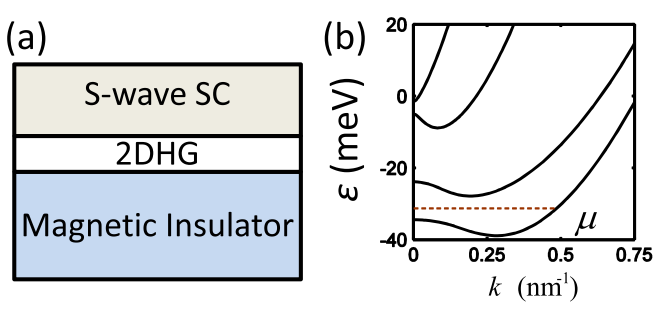

FIG. 1 (color online). (a) A schematic illustration of the heterostructure composed of a hole-doped semiconductor thin film, an s-wave superconductor (SC), and a magnetic insulator. (b) The band structure of the hole-doped semiconductor. The lower (upper) two bands are the HH (LH). $\alpha = 2\times 10^5$ m/s, $\hbar\sqrt{\langle k_z^2\rangle} = 3\times 10^{-26}$ kg·m/s, $\gamma_1 = 6.92$, $\gamma_2 = 2.1$, $h_0 = 1.75$ meV. The parameters are chosen from GaAs [other materials (e.g., InAs, InSb) yield the same physics]. The hole density is $\sim 4\times 10^{12}$ cm^{-2}.

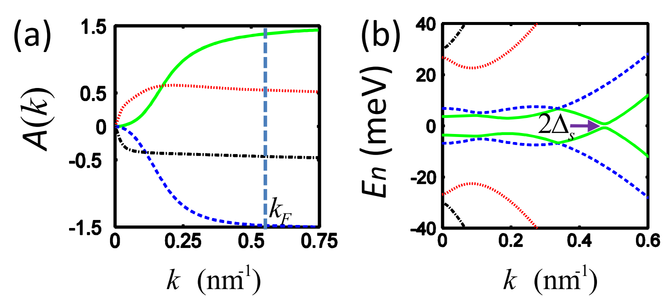

FIG. 2 (color online). (a) Plot of $A(k)$ with respect to k. (b) Plot of the bulk quasiparticle energy E_n of Eq. (7). Solid, dashed, dotted, and dash-dotted lines correspond to the lowest to the highest bands in Fig. 1(b). $\mu = -32.5$ eV. The other parameters are the same as in Fig. 1.

The physics origin of the chiral $(f + if)$-wave superconducting pairing in the lowest HH band is more transparent in the strong confinement limit ($k \ll \sqrt{\langle k_z^2 \rangle}$), where the four band Hamiltonian (1) can be diagonalized into two effective two-band Hamiltonians for the HH and LH, respectively. The effective Hamiltonian H_{HH} for the HH is

$$H_{\mathrm{HH}} = \eta_0 k^4 + \eta_1 k^2 + i\beta(k_-^3 \sigma_+ - k_+^3 \sigma_-) + 3h_0 \sigma_z - \bar{\mu}. \tag{6}$$

Here $k_\pm = k_x \pm ik_y$, $\sigma_\pm = (\sigma_x \pm i\sigma_y)/2$ are Pauli matrices applied on the two HH states (denoted as pseudospin $\uparrow$ and $\downarrow$), η_i are the reduced coefficients, β is the effective coupling strength, $\bar{\mu}$ is the effective chemical potential. The Hamiltonian (6) is similar to the Rashba type of Hamiltonian for electron-doped semiconductors except that $k_x + ik_y$ is now replaced with $(k_x + ik_y)^3 = k\exp(i3\theta_{\mathbf{k}})$ and there is a k^4 term to ensure the bands bend up for a large k. Therefore, a chiral $(f + if)$-wave superconducting pairing is obtained when only the lowest HH band is occupied with holes.

A chiral $(f + if)$-wave superconductor should have a full pairing gap in the 2D bulk, and $\mathcal{C} = 3$ gapless chiral Majorana fermions at the edge [16], where $\mathcal{C} = \frac{1}{2\pi}\sum_{E_n<0}\int d^2\mathbf{k}\,\mathbf{\Omega}_z^n$ is the first Chern number and $\mathbf{\Omega}_z^n = -2\,\mathrm{Im}\langle\partial\Phi_n/\partial k_x|\partial\Phi_n/\partial k_y\rangle$ is the Berry curvature of the nth band. E_n and Φ_n are eigenenergies and wave functions of the BdG equation

$$\begin{pmatrix} H_0 & \Delta_s(\mathbf{r}) \\ \Delta_s^*(\mathbf{r}) & -\bar{\sigma}_x\tau_y H_0^*\tau_y\bar{\sigma}_x \end{pmatrix}\Phi_n(\mathbf{r}) = E_n\Phi_n(\mathbf{r}) \tag{7}$$

in the Nambu spinor basis. Here, $\Phi_n(\mathbf{r}) = [u_{n,3/2}u_{n,1/2}u_{n,-1/2}u_{n,-3/2}v_{n,-3/2}v_{n,-1/2} - v_{n,1/2} - v_{n,3/2}]^T$ is the quasiparticle wave function, $\bar{\sigma}_x = \mathrm{diag}(\sigma_x, \sigma_x)$,

$$\tau_y = \begin{pmatrix} 0 & -iI_{2\times2} \\ iI_{2\times2} & 0 \end{pmatrix}.$$

In a uniform system with a constant $\Delta_s(\mathbf{r})$, Eq. (7) can be solved in the momentum space, and the quasiparticle energy dispersions $E_n(k)$ are plotted in Fig. 2(b). We see a $2\Delta_s$ energy gap is opened at the Fermi surface. Using the eigenwave functions Φ_n for bands with $E_n < 0$, we confirm that the Chern number $\mathcal{C} = 3$, which is consistent with the chiral $(f + if)$-wave pairing and yields 3 gapless chiral Majorana fermions at the edge of the superconductor.

The chiral $(f + if)$-wave pairing may lead to novel exotic physics that has not been explored before (e.g., fractional Josephson effects [17]). Here we focus on the Majorana fermions in vortices in the heterostructure that can be used for TQC. In the presence of a vortex in the heterostructure, the pairing order parameter takes the form $\Delta_s(\mathbf{r}) = \Delta_s(r)e^{i\theta}$. For simplicity of the calculation, we consider a 2D cylinder geometry with a hard wall at the radius $r = R$ and a single vortex at $r = 0$. This system preserves the rotation symmetry, and the BdG equation can be decoupled into different angular momentum channels indexed by l with the corresponding spinor wave function $\Phi_n^l(\mathbf{r}) = e^{il\theta}[u_{n,3/2}^l e^{-i\theta}, u_{n,1/2}^l, u_{n,-1/2}^l e^{i\theta}, u_{n,-3/2}^l e^{2i\theta}, v_{n,-3/2}^l e^{-2i\theta}, v_{n,-1/2}^l e^{-i\theta}, v_{n,1/2}^l, v_{n,3/2}^l e^{i\theta}]^T$. Here u and v are functions of r only. The special form of $\Phi_n^l(\mathbf{r})$ is chosen to preserve the particle-hole symmetry at $l = 0$ and to remove the θ dependence in the BdG equation (7). If $\Phi_n^l(\mathbf{r})$ is a solution with an energy E, then there is another solution with the energy $-E$ in the $-l$ channel. Henceforth we only consider $E \geq 0$ solutions.

Generally, the BdG Eq. (7) with a vortex cannot be solved analytically. Here we numerically solve Eq. (7) and calculate the quasiparticle eigenenergies and eigenwave functions. We use the pairing gap Δ_s from a self-consistence solution of the BdG equation for a pure s-wave superconductor with a small $R = 25k_c^{-1}$ (the Fermi vector k_c for the s-wave superconductor is chosen as 0.5 nm^{-1}). Because the pairing gap approaches the bulk value in a distance much larger than k_c^{-1}, we can extend the pairing gap to a larger $R = 300k_c^{-1}$ by inserting the uniform bulk value (see the inset in Fig. 3). We find that there exists a unique zero-energy solution when μ lies in the gap between the lowest two HH bands [Fig. 1(b)]. In Fig. 3, we plot the two components $u_{0,1/2}^0(r)$ and $v_{0,1/2}^0(r)$ of the zero-energy wave function $\Phi_0^0(\mathbf{r})$ and find $u_{0,1/2}^0(r) = -v_{0,1/2}^0(r)$. We also confirm that $u_{0,m_J}^0(r) = -v_{0,m_J}^0(r)$ for other m_J. Therefore the Bogoliubov quasiparticle operator

$$\gamma_n^\dagger = i\int d\mathbf{r}\sum_{m_J}[u_{nm_J}(\mathbf{r})c_{m_J}^\dagger(\mathbf{r}) + v_{nm_J}(\mathbf{r})c_{m_J}(\mathbf{r})] \tag{8}$$

satisfies $\gamma_0^\dagger = \gamma_0$, which is a self-Hermitian Majorana operator. Consider two Majorana operators γ_A and γ_B in two vortices. It is easy to show $\gamma_A \to \gamma_B$, $\gamma_B \to -\gamma_A$ upon an exchange of two vortices [18]. Therefore the Majorana zero-energy modes satisfy the same non-Abelian braiding statistics as that in a chiral p-wave superconductor or superfluid [19,20] and can be used for TQC.

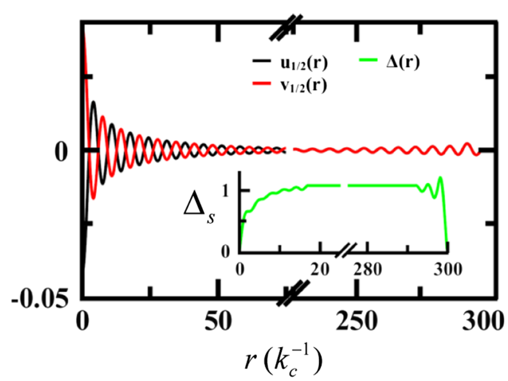

FIG. 3 (color online). Plot of the wave function of the zero-energy state. $\mu = -32.5$ meV. The other parameters are the same as in Fig. 1. Inset: Plot of the s-wave pairing gap with a vortex.

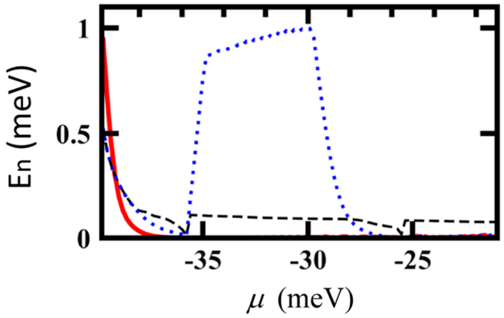

FIG. 4 (color online). Plot of the quasiparticle energies in a vortex core with respect to the chemical potential μ. Solid curve, zero-energy state; dashed curve, the minigap; dotted curve, the bulk excitation gap. The parameters are the same as in Fig. 1.

In Fig. 4, we plot the zero-energy state (the lowest energy level at the $l = 0$ channel), the bulk excitation gap (the first excitation at the $l = 0$ channel), and the minigap energy (the lowest energy level in the vortex core at the $l = 1$ channel) with respect to μ. When μ lies in the gap between the lowest two HH bands, there exists a unique zero-energy solution, which originates from the broken time reversal symmetry of the chiral $(f + if)$-wave superconducting pairing. The minigap is the topological gap protecting the Majorana fermions in the zero-energy states and the associated non-Abelian braiding statistics from finite temperature effects. The numerical results show that the magnitude of the minigap is at the order between Δ_s and Δ_s^2/E_F. Additional numerical calculation shows that Majorana fermions also exist for a vortex with a winding number -3 or other odd numbers. We also find that the Majorana fermions exist when the second lowest band is LH, instead of HH.

The existence of the Majorana zero-energy modes can also be demonstrated analytically in the strong confinement limit. In this limit, the single particle Hamiltonian H_0 is replaced with H_{HH} in (6). The spinor wave function at the l channel changes to $\Phi_n^l(\mathbf{r}) = e^{il\theta}[u_{n\uparrow}^l e^{-i\theta}, u_{n\downarrow}^l e^{2i\theta}, v_{n\downarrow}^l e^{-2i\theta}, -v_{n\uparrow}^l e^{i\theta}]^T$. The BdG equation can be reduced to a 2×2 matrix form

$$\begin{pmatrix} F_0 - \bar{\mu} + 3h_0 & \beta F_1 + \lambda\Delta_s \\ -\beta F_2 - \lambda\Delta_s & F_4 - \bar{\mu} - 3h_0 \end{pmatrix}\begin{pmatrix} u_\uparrow(r) \\ u_\downarrow(r) \end{pmatrix} = 0 \qquad (9)$$

for a zero-energy state after θ is eliminated using the wave function $\Phi_n^l(\mathbf{r})$ and the particle-hole symmetry of the wave function is taken into account. Here, $F_0(r) = \eta_0(Q - r^{-2})^2 + \eta_1(Q - r^{-2})$, $F_1(r) = \partial_r(\partial_r + r^{-1}) \times (\partial_r + 2r^{-1})$, $F_2(r) = (\partial_r + r^{-1})\partial_r(\partial_r - r^{-1})$, $F_4(r) = \eta_0(Q - 4r^{-2})^2 + \eta_1(Q - 4r^{-2})$, $Q = \frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r}$, $u_\sigma(r) = \lambda v_\sigma(r)$. We approximate the radial dependence of Δ_s as a step function, i.e., $\Delta_s = 0$ for $0 \le r \le \xi$, and Δ_0 for $r > \xi$. Detailed analysis of the wave function $(u_\uparrow(r), u_\downarrow(r))^T$ shows that there are four and five independent solutions of Eq. (9) inside and outside the vortex core, respectively, in the parameter region $\lambda = -1$ and $\bar{\mu}^2 + \Delta^2 < 9h_0^2$. The corresponding 9 unknown superposition coefficients for the total wave function match with the 9 constraints from the continuity of the wave function (up to the third order derivative) and the normalization condition, yielding a unique zero-energy solution.

In summary, we show that a chiral $(f + if)$-wave superconducting pairing and the associated Majorana physics may be induced in a hole-doped semiconductor thin film through the proximity contact with an s-wave superconductor. The proposed Berry phase mechanism presents a new possibility for studying unconventional pairing symmetry, which is distinctly different from the conventional scenario in which the pairing is induced by the boson-exchange electron-electron interaction mechanism.

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