Inverse coherence effects in nuclear magnetic relaxation rates as a sign of topological superconductivity

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We reveal that topological superconductivity is detectable by a bulk measurement, i.e., the temperature dependence of nuclear magnetic relaxation (NMR) rates. Below a critical temperature $T_c$, the NMR rate in a topological state has an anti-peak behavior (inverse coherence effect), which is opposite to the conventional s-wave state. The sign reversal of coherence factors comes from a twist of order parameters with respect to orbital and spin degrees of freedom. Our self-consistent calculations in the model for Cu$_2$Bi$_2$Se$_3$ show that the inverse coherence effect appears as a concave temperature dependence of the NMR rates. We propose that the temperature dependence of the NMR rate is a definitive sign of the bulk topological superconductors.

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The Hebel-Slichter peak\cite{1,2} is one of the most significant signatures of s-wave superconductivity. The nuclear magnetic relaxation (NMR) rate ($T_1^{-1}$) is enhanced just below a critical temperature $T_c$. This coherence peak comes from the formation of superconducting gaps and directly supports the validity of the Bardeen-Cooper-Schrieffer theory. The temperature dependence of $T_1^{-1}$ also offers the information on gap functions of unconventional superconductors\cite{3,4}. The inverse of $T_1$ shows the absence of the coherence peak at $T_c$ and a power-law behavior at lower temperatures owing to the existence of low-energy excitations. The NMR rate differentiates the unconventional features of the superconducting gap.

Topological superconductors have attracted intense theoretical and experimental attention\cite{5,6,7}. They have their own topological invariants and gapless bound states on the boundaries between different topological phases (e.g., superconductors and vacuum). These features allow to renew the list of unconventional superconductors since any conventional s-wave states never produce such surface bound states. Superconducting topological insulators, e.g., Cu$_2$Bi$_2$Se$_3$ and Sn$_1$-In$_x$Te provide the opportunity to study bulk topological superconducting materials\cite{7,10,11,12,13}.

A way of finding the signatures of bulk topological superconductors is highly desirable for condensed matter physics and materials science. A primary probe is to observe gapless bound states on surfaces at low temperatures. However, the setups of surface measurements would be sensitively affected by the characteristics of the interfaces between materials and probes. Thus, it is necessary for supporting some results in the surface measurements to perform experiments from a different point of view. Bulk measurements, especially the NMR rates have played such a role in superconducting studies\cite{4}. Moreover, the previous calculations of impurity effects\cite{16,17} indicate that a model of Cu$_2$Bi$_2$Se$_3$ possesses both s- and p-wave properties\cite{10,11,12,13}. This point also motivates us to seek a sign of topological superconductors by bulk quantities.

In this paper, we show an inverse coherence effect of the NMR rates in odd-parity topological superconductors. The sign of the coherence factor is opposite to that of the conventional s-wave state owing to a twist of the order parameter with respect to orbital and spin degrees of freedom. Our self-consistent calculations in the model of Cu$_2$Bi$_2$Se$_3$ show that this sign reversal leads to an anti-peak behavior of the NMR rates below $T_c$. Therefore, we claim that the detection of this inverse coherence effect in NMR-rate measurements of bulk samples leads to an evidence of the odd-parity topological superconductivity.

We formulate the NMR rate of a multi-orbital superconductor, with a mean-field approach. The mean-field Bogoliubov-de Gennes (BdG) Hamiltonian is $\mathcal{H} = (1/2) \sum_k \psi_k^\dagger \mathcal{H}(k) \psi_k$, with $\psi_k^\dagger = (c_k^\dagger, c_k^T)$ and $\psi_k^T = (c_k, c_k^T)^T$. The $2n_o$-component column (raw) vector $c_k$ ($c_k^\dagger$) contains electron’s annihilation (creation) operators, with the number of orbitals $n_o$. The arrangement of the components is, e.g., ($c_1^\dagger, c_1$, $c_2^T, c_2^T$) when $n_o = 2$. The BdG matrix is

$$\mathcal{H}(k) = \begin{pmatrix} \hat{H}_0(k) & \hat{\Delta}(k) \\ \hat{\Delta}^\dagger(k) & -[\hat{H}_0(-k)]^* \end{pmatrix}.$$ (1)

The normal-state Hamiltonian is $\hat{H}_0$. The pairing potential (matrix) fulfills $\hat{\Delta}(k) = -\hat{\Delta}^\dagger(-k)$, owing to the Fermion anticommutation property. The check symbol (') indicates a matrix in the Nambu space, whereas the hat symbol (\hat{\cdot}) does that in an orbital-spin space. The NMR rate\cite{5,10} is

$$\frac{1}{T_1(T)T} = \pi \sum_{\alpha, \alpha'} \int_{-\infty}^{\infty} d\omega \left[ -\frac{df(\omega)}{d\omega} \right] \times \text{Re} \left\{ \rho_{\uparrow\uparrow}^{G\alpha\alpha'}(\omega)\rho_{\downarrow\downarrow}^{G\alpha\alpha'}(\omega) - \rho_{\uparrow\downarrow}^{F\alpha\alpha'}(\omega)\rho_{\downarrow\uparrow}^{F\alpha\alpha'}(\omega) \right\}.$$ (2)

We use the unit system of $\hbar = k_B = 1$ throughout this paper. The indices $\alpha$ and $\alpha'$ represent...
The Fermi-Dirac distribution function is denoted by $f(\omega)$. The spectral functions $\hat{\rho}^G(\omega)$ and $\hat{\rho}^F(\omega)$ are the submatrices of $\hat{\rho}^G(\omega) = (-1/2\pi i)\sum_{k} [\hat{G}_k(i\omega_n \rightarrow \omega + i0) - \hat{G}_k(i\omega_n \rightarrow \omega - i0)]$. Temperature Green’s function is $\hat{G}_k(i\omega_n) = [i\omega_n - \hat{H}(k)]^{-1}$, with the fermionic Matsubara frequency $\omega_n = \pi T(2n + 1) \, (n \in \mathbb{Z})$. The matrix form in the Nambu space is

$$\hat{G}_k(i\omega_n) = \left( \begin{array}{cc} \hat{G}_k(i\omega_n) & \hat{F}_k(i\omega_n) \\ \hat{F}_k(i\omega_n) & \hat{G}_k(i\omega_n) \end{array} \right). \hspace{1cm} (3)$$

The diagonal block, $\hat{G}_k$, leads to $\hat{\rho}^G$, relevant to electron’s density of states. The off-diagonal block, $\hat{F}_k$, contributes to the anomalous spectral function $\hat{\rho}^F$.

The presence of the coherence peak just below $T_c$ is predominated by the second term in Eq. (2). The Hebel-Slichter peak appears when this term (including the minus sign in front of the spectral functions) has a positive contribution to $T_c^{-1}$. To intuitively understand the behaviors of the second term, we evaluate anomalous Green’s functions near $T_c$. Linearizing $\hat{G}$ with respect to $\hat{\Delta}$, we obtain $\sum_k \hat{F}_k(i\omega_n) = \sum_k \hat{G}_k(i\omega_n) \Delta(k) \hat{G}_k(i\omega_n)$, with normal-state Green’s functions, $\hat{G}_k^N$ and $\hat{G}_k^N$. The spin-singlet property of s-wave states, for example, indicates $\Delta_{\uparrow\downarrow} = -\Delta_{\uparrow\uparrow}$; we obtain $-\rho^F_{\uparrow\uparrow}(\rho^F_{\uparrow\downarrow})^* = +|\rho^F_{\uparrow\downarrow}|^2$, with $\rho^F \neq 0$. In contrast, the $k$-integral with a spin-triplet p-wave gap leads to $\hat{\rho}^F = 0$ [19].

Now, we apply the above arguments to topological superconducting insulators. We focus on the model of Cu$_2$Bi$_2$Se$_3$. The normal electrons are effectively described by a two-orbital model ($n_o = 2$), leading to a massive Dirac Hamiltonian,

$$\hat{H}_0(k) = \gamma^0 \left[ -\mu \Gamma^0 + \sum_{i=1}^{3} v_i k_i \Gamma_i + i\Gamma^4 + h_5(k) \Gamma^5 \right]}, \hspace{1cm} (4)$$

with chemical potential $\mu$, spin-orbit coupling constants $v_i$, and mass $m$. This Hamiltonian is the same as that in Ref. [17], except $h_5$. The last term corresponds to the effects of hexagonal warping in the Fermi surface of Cu$_2$Bi$_2$Se$_3$ [20]. We drop this term in most of our calculations, but argue the effects on the NMR rate at the end of this paper. Six kinds of 4 × 4 matrices $\Gamma^A$ ($A = 0, 1, 2, 3, 4, 5$) are composed of the gamma matrices $\gamma^\mu$ ($\mu = 0, 1, 2, 3$) [21] and the identity: $\Gamma^A = \gamma^A$ ($A \neq 4$) and $\Gamma^4 = \mathbb{I}_4$, with $\gamma^5 = i\gamma^0 \gamma^1 \gamma^2 \gamma^3$. Our choice [22] is that $\gamma^0 = \sigma_x \otimes \mathbb{I}_2$, $\gamma^1 = -i\sigma_y \otimes \mathbb{I}_2$, $\gamma^2 = i\sigma_y \otimes \mathbb{I}_2$, and $\gamma^3 = \sigma_z \otimes \mathbb{I}_2$, where $\sigma_x, \sigma_y, \sigma_z$ are the 2 × 2 Pauli matrices in the orbital (spin) space. In this paper, we study the momentum-independent pair potential $\Delta$, owing to the onsite interaction $[7, 8]$. The relation $\Delta^T = -\Delta$ leads to

$$\hat{\Delta} = \sum_{A=0}^{5} \Delta^A \Gamma^A \gamma^2 \gamma^5. \hspace{1cm} (5)$$

Since $\gamma^2 \gamma^5 = \mathbb{I}_2 \otimes s_y$, the case of $\Gamma^A$ to be the identity (i.e., $A = 4$) describes a spin-singlet s-wave state: $\Delta^5 \propto \sum (c_{k1}^\dagger c_{k1} + c_{k2}^\dagger c_{k2})$. The additional $\Gamma^A$ ($A \neq 4$) characterizes a twist of each order-parameter component in the orbital-spin space, compared to the conventional s-wave state. According to Ref. [2], even-parity order parameters ($A_{1g}$ states) are given by $\Delta^4$ and $\Delta^0$. Odd-parity states correspond to $\Delta^{1,2,3,5}$. The component $\Delta^5$ corresponds to an odd-parity fully-gapped ($A_{1u}$) state (a topological state) [3, 8]: $\Delta^5 \propto \sum (c_{k1}^\dagger c_{k1} + c_{k2}^\dagger c_{k2})$. Let us study the anomalous spectral function $\hat{\rho}^F$ of the odd-parity state near $T_c$. Normal-state Green’s functions are evaluated by focusing on an algebraic relation of $\hat{H}_0$; we find that $[\hat{H}_0(\omega)]^2 = |E(\omega)|^2$, with $\hat{H}_0 = \hat{H}_0 + \mu$. This property corresponds to the fact that the Dirac equation is the square root of the Klein-Gordon equation [21]. We obtain $\hat{G}_k^N(i\omega_n) = \sum_{k} \hat{\rho}_k^F(i\omega_n) = (1/2) \, \int \left[ \hat{H}_0(\omega) \hat{H}_0(\omega) \right]$, with $P_\omega = \langle 1/2 \rangle \left[ \hat{H}_0(\omega) \hat{H}_0(\omega) \right]$. The projector $\hat{P}_k$ is rewritten by $\hat{P}_k = \gamma^0 \sum_{A=0}^{5} w^A(k) \Gamma^A$. Then, when $\hat{\Delta}(k) = \Delta^5$, $\Delta^5 = \Gamma^5 \gamma^2 \gamma^5$ and $h_5 = 0$, we find that

$$\hat{\rho}_k^F(\omega; \Delta^5) = \chi^5(\omega) \Delta^5 + \chi^4(\omega) \gamma^5 \Delta^5, \hspace{1cm} (6)$$

near $T_c$. The coefficients are $\chi^5, \chi^4 = \sum_{k} \hat{\rho}^F_{\uparrow\uparrow} \hat{\rho}^F_{\uparrow\downarrow} = \sum_{\ell,\ell'} N_{\ell,\ell'}(k, \omega) \hat{W}^{\ell,\ell'}(k, \omega)$, where $N_{\ell,\ell'} = \{1/\left[ (\ell + \ell')E - 2\mu \right] \} \delta(\omega - (\ell + \ell')E - \mu)$, $\hat{W}_{\ell,\ell'}^{\uparrow\downarrow} = \sum_{A=0}^{5} w^A(k, \ell, \ell') - w^A(k, \ell', \ell)$, and $\hat{W}_{\ell,\ell'}^{\uparrow\uparrow} = \sum_{A=0}^{5} w^A(k, \ell, \ell') - w^A(k, \ell', \ell)$. Since $\Gamma^5 \gamma^2 \gamma^5 = -i\sigma_y \otimes \mathbb{x}^2$, $\Delta^5$ is odd under an orbital-index exchange, while is even under a spin-index exchange. The multiplication of $\gamma^0$ with $\Delta^5$ does not change these properties. Thus, we show that $\hat{\rho}^F_{\uparrow\downarrow}(\omega) = \hat{\rho}^F_{\downarrow\uparrow}(\omega)$. This property indicates that the second term in Eq. (2) negatively contributes to $T_1^{-1}$:

$$-\rho_{\uparrow\downarrow}^F(\omega) = -|\rho_{\uparrow\downarrow}^F(\omega)|^2. \hspace{1cm} (7)$$

An inverse coherence effect can occur in the presence of the odd-parity state.

Now, we show the inverse coherence effect of $T_1^{-1}$, solving the BdG equations self-consistently. We adopt the normal-state Hamiltonian [1] with $h_5 = 0$. We set $v_i = v$, for simplicity. We take a unit system with $v = 1$. It means that the energy and momentum are dimensionless. We vary $m$, with fixed chemical potential $\mu = 0.8$. The superconducting pairing model has two-orbital on-site density-density interaction $[2, 22]$: $H_{\text{int}}(x) = U \left[ n_1(x) n_2(x) \right] + 2V n_1(x) n_2(x)$ with $n_\alpha = \sum_{\sigma=\uparrow,\downarrow} c_{\alpha \sigma}^\dagger c_{\alpha \sigma}$. The gap equation is

$$\Delta_{\alpha\alpha} = -V_{\alpha\alpha} \hat{\rho}_{\alpha\alpha}^F, \hspace{1cm} (7)$$

with $\hat{\rho}^F = -\sum_k \lim_{\omega \to 0} \exp(-i\omega_n \tau) \hat{F}_k(i\omega_n)$. The label $a$ collectively represents orbital and spin: $a = (\alpha, s)$. 


The intra-orbital coupling constant \( U \) and the inter-orbital coupling constant \( V \) are bundled up by \( \mathcal{V}_{a\alpha a'} \), i.e., \( \mathcal{V}_{a\alpha a'} = U \) with \( a = a' \) and \( \mathcal{V}_{a\alpha a'} = V \) with \( a \neq a' \). Self-consistently solving Eq. (7), we evaluate the temperature dependence of Eq. (2). The momentum integral is performed by the trapezoidal rule in the spherical coordinate system, with cutoff momentum \( k_{\text{max}} = 9 \) and mesh \((N_k, N_\theta, N_\phi) = (128, 128, 128)\). The smearing factor of the delta function is set by 0.01. We tune either \( U \) or \( V \) so that the zero-temperature gap amplitude takes 0.01. In this paper, we focus on the odd-parity gap \( \Delta^5 \propto \sum (c_{k_1}^\dagger c_{k_1^\prime} + c_{k_1^\prime}^\dagger c_{k_1}) \) (\( \mathcal{A}_1 \)) and the even-parity gap \( \Delta^4 \propto \sum (c_{k_1} c_{k_1^\prime} + c_{k_2} c_{k_2^\prime}) \) (\( \mathcal{A}_2 \)). We set the chemical potential \( \mu = 0.8 \) and the Dirac mass \( m = 0.4 \) [See Eq. (4)]. We tune either \( U \) or \( V \) so that the zero-temperature gap amplitude takes 0.01. Inset: temperature dependence of the superconducting gaps.

FIG. 1. (Color online) Temperature dependence of nuclear magnetic relaxation rates in (a) an odd-parity gap \( \Delta^5 \propto \sum (c_{k_1}^\dagger c_{k_1^\prime} + c_{k_1^\prime}^\dagger c_{k_1}) \) (\( \mathcal{A}_1 \)) and the even-parity gap \( \Delta^4 \propto \sum (c_{k_1} c_{k_1^\prime} + c_{k_2} c_{k_2^\prime}) \) (\( \mathcal{A}_2 \)). The sign of the coherence effect is determined by the spin \( s \). Spin parity \( p_s \) is related to the exchange of spin: \( \Delta_{ss'}^{\alpha\alpha'}(k) = p_s \Delta_{ss'}^{\alpha\alpha'}(k) \) with \( p_s = \pm 1 \). Similarly, momentum (orbital) parity \( p_{m}(p_o) \) is determined by exchange of momentum (orbital): \( \Delta_{ss'}^{\alpha\alpha'}(k) = p_m \Delta_{ss'}^{\alpha\alpha'}(k) \) \( \Delta_{ss'}^{\alpha\alpha'}(k) = p_o \Delta_{ss'}^{\alpha\alpha'}(k) \) with \( p_m = \pm 1 \). The fundamental relation of \( \Delta \) is \( \Delta_T(\tilde{k}) = -\Delta(\tilde{k}) \), leading to \( p_m p_o = -1 \). Table I summarizes \( p_s, p_m, p_o \) of different gaps. The non-zero contributions of \( \tilde{p}^F \) to \( T_1^{-1} \) is allowed when \( p_m = 1 \). In fast, as discussed above, a single-orbital spin-triplet \( p \)-wave state \( (p_m = -1) \) has no peak. The sign of the coherence effect is determined by the spin parity \( p_s \). A multi-orbital odd-parity state allows both \( p_m = 1 \) and \( p_o = 1 \).

Finally, we discuss the NMR rate with anisotropic odd-parity states labeled by \( E_{o\nu}: \Delta^5 \propto \sum (c_{k_1}^\dagger c_{k_1^\prime} + c_{k_1^\prime}^\dagger c_{k_1}) \) [20, 24, 25]. According to Ref. [20], this pairing can be just below \( T_c \). Thus, we obtain the inverse coherence effect in \( \Delta^5 \). It is worth noting that the temperature dependence of the gap function (insets in Fig. 1(a)) has no significant difference between \( \Delta^5 \) and \( \Delta^4 \). Moreover, we can find that the exponential temperature dependence of \( (T_1 T)^{-1} \) occurs at lower temperatures; this is consistent with the fully-gaped feature of \( \Delta^5 \). Thus, the temperature dependence of the NMR rate definitely signals the emergence of \( \Delta^5 \) in superconducting topological insulators.
TABLE I. Parity table of different gap functions. The coherence effect is characterized by spin parity $p_s \left[ \Delta^{\alpha' \alpha}_\uparrow (\mathbf{k}) = p_s \Delta^{\alpha' \alpha}_\uparrow (-\mathbf{k}) \right]$, momentum parity $p_m \left[ \Delta^{\alpha' \alpha}_\downarrow (\mathbf{k}) = p_m \Delta^{\alpha' \alpha}_\downarrow (-\mathbf{k}) \right]$, and orbital parity $p_o \left[ \Delta^{\alpha' \alpha}_\downarrow (\mathbf{k}) = p_o \Delta^{\alpha' \alpha}_\downarrow (\mathbf{k}) \right]$.

| Gap type          | Spin parity $p_s$ | Momentum parity $p_m$ | Orbital parity $p_o$ | Coherence effect |
|-------------------|-------------------|-----------------------|----------------------|-----------------|
| 2-orbital s-wave SC. ($A_{1g}$) | -1               | +1                    | -1                   | negative       |
| 2-orbital topo. SC. ($A_{1u}$)    | +1               | +1                    | +1                   | positive       |
| 1-orbital s-wave SC.             | -1               | -1                    | +1                   | positive       |
| 1-orbital chiral p-wave SC.      | +1               | -1                    | +1                   | 0              |

FIG. 2. (Color online) Nuclear magnetic relaxation rates of an odd-parity gap $\Delta^5 \left( A_{1u} \right)$ or $\Delta^2 \left( A_1 \right)$, changing $m/\mu$ (Dirac mass/chemical potential). The total rate (a), the normal part (b), and the anomalous part (c) are shown.

induced in the presence of a hexagonal warping term $h_5 = i\lambda(k_+^3 + k_2^3)$ with $k_2 \equiv k_2 \pm i\eta$. Near $T_c$, we can find that $\rho^{\alpha' \alpha}_{\uparrow \downarrow} (\omega; \Delta^1) \propto \lambda$. Since the orbital parity is odd but the spin parity is even, the inverse coherence effect can occur within $|\lambda| \neq 0$. We will conclusively discuss the coherence effect of the NMR rate in topological superconductors elsewhere, including anisotropy and momentum dependence in the gap functions.

In summary, we showed a bulk measurement, the NMR rate near $T_c$ as a sign of topological superconductivity. The inverse coherence effect was predicted in the NMR rate below $T_c$. Our self-consistent calculations in the model of Cu$_3$Bi$_2$Se$_3$ lead to the temperature dependence of $(T_1 T)^{-1}$, with a concave behavior below $T_c$. This notable effect originates from the anomalous part of the NMR rate in the odd-parity gap $\Delta^5 \propto \sum (c_{k_+} \lambda^3 + c_{k_2} \lambda^3)$. Moreover, the negative height when $m/\mu \to 1$ is proportional to an indicator of normal-electron relativistic effects. Therefore, we claim that the detection of the inverse coherence effect definitely signals the emergence of bulk topological superconductors.

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