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Electronic structures and NMR T_1^{-1} in quasi-one-dimensional organic superconductor $(TMTSF)_2PF_6$

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Abstract

On the basis of the Bogoliubov de Gennes theory, electronic structures around a vortex in quasi-one-dimensional organic superconductor $(TMTSF)_2PF_6$ are studied at the quarter-filling electron density in magnetic fields applied parallel to the conduction chain. We consider three pairing symmetries (d-, p- and f-wave) in superconductors. In d- and f-wave symmetries, nuclear relaxation rate T_1^{-1} is proportional to temperatures because quasiparticles around the vortex relax spins.

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1. Introduction

Recently much attention has been focused on superconductivity in quasi one-dimensional (Q1D) organic compound $(TMTSF)_2PF_6$, which is called Bechgaard salt. Under a pressure, the superconducting phase appears above the SDW phase. A number of studies have been made on analyzing the superconducting pairing symmetry so far. In theories, three kinds of pairing symmetry have been proposed: d-wave [1–3], p-wave [3–6] and f-wave [7–11]. The d- and f-wave pair potentials have line nodes on the Fermi surface, whereas p-wave potential has no nodes. Experimentally, the spin–triplet pairing symmetry has been suggested because the Knight shift does not change across T_C. A NMR experiment by Lee et al. [12] revealed that the relaxation rate T_1^{-1} has two characteristics (i) $T_1^{-1} \propto T$ in low temperatures ($T \ll T_c$) and (ii) T_1^{-1} has a small peak at T_c. Since the NMR experiment was done under magnetic fields in the chain direction, we should consider effects of quasiparticles around the vortices on T_1^{-1} to understand the experimental results. In this paper, we will explain experimental behaviors of T_1^{-1} in the mixed state of Q1D organic superconductor.

2. Formulation

To study electronic structures in Q1D superconductor under magnetic fields in the conduction chain, we solve the Bogoliubov de Gennes (BdG) equation self-consistently on the three-dimensional tight-binding lattices. Hamiltonian is given by

$$H = \sum_{i,j,\sigma} t_{i,j} a^{\dagger}_{j,\sigma} a_{i,\sigma} - \mu + \sum_{i,j,\sigma} V_{i,j} \left(\Delta^{\dagger}_{ji,\sigma} a_{i,-\sigma} a_{j,\sigma} + \Delta_{ji,\sigma} a^{\dagger}_{i,\sigma} a^{\dagger}_{j,-\sigma'} \right), \quad (1)$$

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where $a^{+}_{i,\sigma}(a_{i,\sigma})$ is a creation (annihilation) operator of an electron at a lattice site i with spin σ and $V_{i,j}$ represents the attractive interaction in the z-direction (chain direction). The pairing interactions are working between second nearest neighbor sites for d- and p-wave symmetries and the fourth nearest neighbor sites for f-wave symmetry. After the Fourier translation in the z-direction, we obtain $\Delta_{i,j} = \varphi(k_z)\Delta_i$, $\varphi(k_z) = \cos 2k_z$ for d-wave, $\sin 2k_z$ for p-wave, and $\cos 4k_z$ for f-wave symmetries. The transfer integral in the xy-plane is expressed as $\tilde{t}_{ij} = t_{ij}\exp[\mathrm{i}(\pi/\phi_0)\int_{r_i}^{r_j} A(r)\cdot \mathrm{d}r]$, where the vector potential $A(r) = \frac{1}{2}H \times r$ is given in the symmetric gauge with external fields $\boldsymbol{H} = (0,0,H)$ and ϕ_0 is the flax quantum. The hopping integrals t_{ij} between nearest neighbor sites are chosen as $t_x{:}t_y{:}t_z = 1{:}0.03{:}10$ to reproduce the Q1D Fermi surface of $(TMTSF)_2PF_6$. In calculations, we take the paring interaction $U = -38t_x$. The charge density is kept to be at the quarter-filling. By the Bogoliubov transformation, the BdG equation is given by

$$\sum_i \begin{pmatrix} K_{ji} & \Delta_{ji} \\ \Delta^{\dagger}_{ji} & -K^{*}_{ji} \end{pmatrix} \begin{pmatrix} u_\varepsilon(r_i) \\ v_\varepsilon(r_i) \end{pmatrix} = E_\varepsilon \begin{pmatrix} u_\varepsilon(r_j) \\ v_\varepsilon(r_j) \end{pmatrix}, \tag{2}$$

where $K_{ij} = -\tilde{t}_{ij} + \delta_{ij}(-2t_z\cos k_z - \mu)$, $D_{ij} = U\Delta_i\delta_{ij}\varphi(k_z)$, and $u_\alpha(r_i)$, $v_\alpha(r_i)$ are wave functions at the lattice site i belonging to the energy E_α. The expressions for the pair potential and the charge density are given by

$$\tilde{\Delta}(r_i) = \sum_{\alpha,k_z} u_\alpha(r_i)v^{*}_\alpha(r_i)f(E_\alpha)\varphi(k_z), \tag{3}$$

$$n_i = n_{i\uparrow} + n_{i\downarrow} = \sum_\alpha (|u_\alpha(r_i)|^2 f(E_\alpha) + |v_\alpha(r_i)|^2(1 - f(E_\alpha))), \tag{4}$$

where $\Delta(r_i) = \tilde{\Delta}(r_i)\exp[\mathrm{i}(\pi/\phi_0)\int_{r_i}^{r_j} A(r)\cdot \mathrm{d}r]$.

We consider that two vortices accommodate in a unit cell with 20×6 lattice sites in the xy plane. We also assume that the vortex core is located in the plaquette. By introducing the quasimomentum of the magnetic Bloch state, we obtain the wave function under the periodic boundary condition whose region covers a large number of unit cells. The spin–spin correlation function $\chi_{+-}(\boldsymbol{r},\boldsymbol{r}',\mathrm{i}\Omega_n)$ is calculated from Green's functions and the nuclear spin relaxation rate is given by

$$\begin{aligned} R(r,r') &= \mathrm{Im}\chi_{+,-}(r,r',\mathrm{i}\Omega_n \to \Omega + \mathrm{i}\eta)/(\Omega/T)|_{\Omega\to 0} \\ &= -\sum_{\alpha,\alpha'}[u_\alpha(r)u_{\alpha'}(r')v_\alpha(r)v_{\alpha'}(r') - v_\alpha(r)u_{\alpha'}(r') \\ &\quad \times u_\alpha(r)v_{\alpha'}(r')] \times \pi T f'(E_\alpha)\delta(E_\alpha - E_{\alpha'}), \end{aligned} \tag{5}$$

where $f(E)$ is the Fermi distribution function. We assume that $\boldsymbol{r} = \boldsymbol{r}'$ because site-diagonal spin relaxations are considered to be dominant. The $\boldsymbol{r}$-dependent relaxation time is given by $T_1(\boldsymbol{r}) = 1/R(\boldsymbol{r},\boldsymbol{r})$. In calculations, we use $\delta(\boldsymbol{r}) = \pi^{-1}\mathrm{Im}(x - \mathrm{i}\eta)$ to handle the discrete energy levels due to the finite size effect with $\eta = 0.02t_x$. In Eq. (5), the first term is proportional to $N(\boldsymbol{r},E)^2$ for $\boldsymbol{r} = \boldsymbol{r}'$. To understand the behavior of $T_1(\boldsymbol{r})$, we also calculate local density of states (LDOS) given by

$$N(E,\boldsymbol{r}) = \sum_\alpha [|u_\alpha(\boldsymbol{r})|^2\delta(E - E_\alpha) + |v_\alpha(\boldsymbol{r})|^2\delta(E + E_\alpha)].$$

3. Local density of state and NMR T_1^{-1} around vortices

Three pair potentials have different topology from one another in the k-space as shown in Fig. 1. The pair potentials for d- and f-waves change their sign at $k_z = \pm\pi/4$, and they have line nodes on the Fermi surface. The sign of pair potentials for p- and f-waves is also changed at the $k_z = 0$. The pair potential for p-wave, however, has no nodes on the Fermi surface. By solving the Eq. (2) self-consistently with Eq. (3), we obtain electronic states and order parameters. The critical temperature T_c/t_x results in 1.3 (d-wave), 2.6 (p-wave), and 2.2 (f-wave) and $|\Delta_i(\boldsymbol{H} = 0)|$ at the lowest temperature are calculated to be 0.065 (d-wave), 0.135 (p-wave) and 0.11 (f-wave). Since the vortex core is located at the central of the plaquette in the xy-plane, the spatial variation of $|\Delta_i|$ is very small (it is about $0.1 \sim 1\%$ of their bulk values). Therefore, the modulation of the LDOS around the vortex is also expected to be small.

Fig. 2 shows LDOS at the nearest lattice site to the core (solid line) and density of states in $H = 0$ (dashed line) and normal density of states (dotted line) at the lowest T. In d-

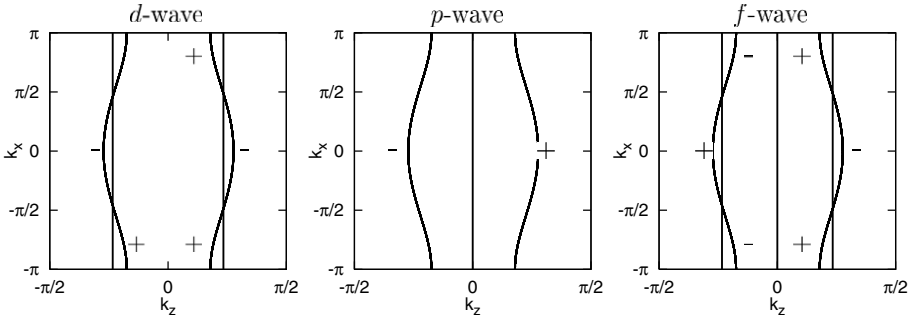

Fig. 1. The Fermi surface and signs of pairing symmetries are shown for (a) d-wave, (b) p-wave and (c) f-wave symmetries. At $k_z = \pi/4$, pair potentials for d- and f-wave have line nodes.