THEORETICAL STUDIES ON VORTICES IN UNCONVENTIONAL AND CONVENTIONAL SUPERCONDUCTORS*

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Vortex imaging method by the site selective NMR is explained by self-consistently solving the Bogoliubov–de Gennes equation for both s-wave and d-wave pairings. We analyze the temperature dependence of the relation time T_1 using the resonance frequency at the intensity maximum, namely the saddle point T_1 experiments. The site selective T_1 data are shown to yield valuable information on low-lying electronic excitations around a vortex core.

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1. Introduction

The low-lying excitations around a vortex core play an important role in type II superconductors. Many physical properties in a mixed state are determined by these excitation spectra, ranging from thermodynamic properties such as electronic specific heat and the upper critical field H_{c2} to various transport properties. Of particularly interesting is the difference between conventional s-wave pairing and unconventional pairing state where the energy gap vanishes at a certain point on the Fermi surface. The spatial structure of the excitation spectrum around a core is directly observed by Scanning Tunneling Microscopy (STM), which yields quite impressive structures for these two kinds of materials [1]. However, since STM is a surface sensitive probe, it is desirable to independently check these results by other bulk measurements. In this context we proposed a site-selective NMR experiment [2]. The method relies on a fact that each frequency in the resonance spectrum, or the Redfield pattern contains local information corresponding

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to each position in the vortex lattice through the magnetic field distribution. Thus by tuning the resonance frequency we can obtain the site-dependent relaxation time $T_1(r)$. According to this proposal, vortex imaging NMR experiments [3, 4] are performed on high T_c cuprates and yield valuable information on the core excitations. Through these theoretical and experimental studies it is now recognized in retrospect that vast majority NMR measurements in the past using the resonance at the maximum intensity give the information coming from the saddle point of the field distribution, which is far site from the core. Here we explain two unsolved results on the saddle point NMR for s-wave superconductors, namely, the suppression of the Hebel–Slichter peak below T_c by magnetic field [5] and the T-linear behavior of T_1^{-1} at lower T for d-wave superconductors [6–8].

2. Bogoliubov–de Gennes equation

We start with the Bogoliubov–de Gennes (BdG) equation for the extended Hubbard model in the s- and d-wave cases, which is given by

$$\sum_j \begin{pmatrix} K_{i,j} & D_{i,j} \\ D^*_{i,j} & -K^*_{i,j} \end{pmatrix} \begin{pmatrix} u_\alpha(\boldsymbol{r}_j) \\ v_\alpha(\boldsymbol{r}_j) \end{pmatrix} = E_\alpha \begin{pmatrix} u_\alpha(\boldsymbol{r}_i) \\ v_\alpha(\boldsymbol{r}_i) \end{pmatrix}, \tag{1}$$

where

$$\begin{aligned} K_{i,j} &= -t_{i,j} \exp\left[i\frac{\pi}{\phi_0} \int_{\boldsymbol{r}_i}^{\boldsymbol{r}_j} \boldsymbol{A}(\boldsymbol{r}) \cdot d\boldsymbol{r} \right] - \delta_{i,j}\mu\,, \\ D_{i,j} &= \delta_{i,j} U \Delta_{i,i} + \frac{1}{2} V_{i,j} \Delta_{i,j} \end{aligned}$$

with the on-site interaction U, the chemical potential μ and the flux quantum ϕ_0. The transfer integral $t_{i,j} = t$ and the nearest neighbor interaction $V_{i,j} = V$ for the NN site pair $\boldsymbol{r}_i$ and $\boldsymbol{r}_j$, and otherwise $t_{i,j} = V_{i,j} = 0$. The vector potential $\boldsymbol{A}(\boldsymbol{r}) = \frac{1}{2}\boldsymbol{H} \times \boldsymbol{r}$ in the symmetric gauge. The self-consistent condition for the pair potential is

$$\Delta_{i,j} = -\frac{1}{2} \sum_\alpha u_\alpha(\boldsymbol{r}_i) v^*_\alpha(\boldsymbol{r}_j) \tanh\left(\frac{E_\alpha}{2T}\right).$$

The band filling factor $\langle n \rangle \sim 0.9$ in our calculation.

We consider the square vortex lattice case where nearest neighbor vortex is located at the 45° direction from the a axis. The unit cell in our calculation is the square area of N_r^2 sites where two vortices are included. Then, the field strength $H_{N_r} = 2\phi_0/(cN_r)^2$ (c is the atomic lattice constant). The on-site s-wave pair potential $\Delta_s(\boldsymbol{r}_i) = U\Delta_{i,i}$. The $d_{x^2-y^2}$-wave pair potential is given by $\Delta_d(\boldsymbol{r}_i) = V(\Delta_{\hat{x},i} + \Delta_{-\hat{x},i} - \Delta_{\hat{y},i} - \Delta_{-\hat{y},i})/4$. We construct the Green functions from E_α, $u_\alpha(\boldsymbol{r})$ and $v_\alpha(\boldsymbol{r})$, and calculate the spin–spin correlation function $\chi_{+,-}(\boldsymbol{r},\boldsymbol{r}',i\Omega_n)$. Then, we obtain the nuclear spin relaxation rate

$$\begin{aligned} R(\boldsymbol{r},\boldsymbol{r}') &= \frac{\mathrm{Im}\chi_{+,-}(\boldsymbol{r},\boldsymbol{r}',i\Omega_n \to \Omega + \mathrm{i}\eta)}{(\Omega/T)\,|_{\Omega\to 0}} \\ &= -\sum_{\alpha,\alpha'} u_\alpha(\boldsymbol{r}) u^*_{\alpha'}(\boldsymbol{r}) \Big[u_\alpha(\boldsymbol{r}') u^*_{\alpha'}(\boldsymbol{r}') + v_\alpha(\boldsymbol{r}') v^*_{\alpha'}(\boldsymbol{r}') \Big] \\ &\quad \times \pi T f'(E_\alpha)\delta(E_\alpha - E_{\alpha'})\,, \end{aligned} \tag{2}$$

with the Fermi distribution function $f(E)$. We consider the case $\boldsymbol{r} = \boldsymbol{r}'$ by assuming that the nuclear relaxation occurs locally. Then, $\boldsymbol{r}$-dependent relaxation time is given by $T_1(\boldsymbol{r}) = 1/R(\boldsymbol{r},\boldsymbol{r})$. In Eq. (2), we use $\delta(x) = \pi^{-1}\mathrm{Im}(x - \mathrm{i}\eta)^{-1}$ to consider the discrete energy level of the finite size calculation. We typically use $\eta = 0.01t$. To understand the behavior of $T_1(\boldsymbol{r})$, we also consider the Local Density of States (LDOS) given by $N(\boldsymbol{r},E) = -\sum_\alpha [|u_\alpha(\boldsymbol{r})|^2 f'(E_\alpha - E) + |v_\alpha(\boldsymbol{r})|^2 f'(E_\alpha + E)]$. It corresponds to the differential tunneling conductance of STM experiments.

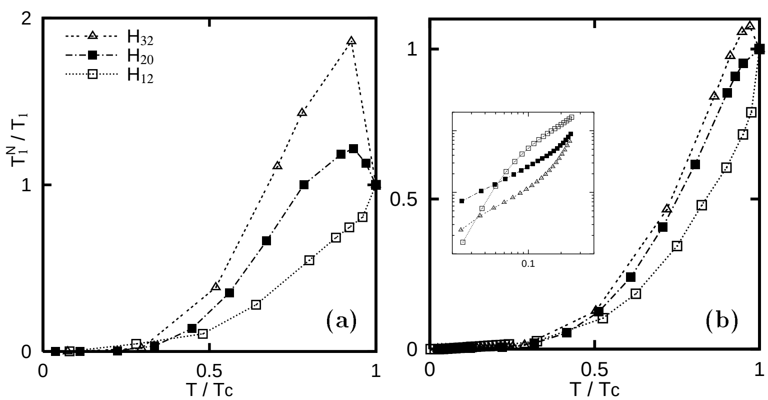

Fig. 1. T_1^{-1} at the saddle point. s-wave (a) and d-wave (b) cases for three magnetic field values. The inset in (b) shows the low T-behaviors.

3. Saddle point T_1

Fig. 1 shows the results of T_1^N/T_1 at the saddle point for selected field values with T_1^N normal state value. For the s-wave case (a) it is seen that the Hebel–Slichter peak at low field is suppressed for intermediate filed and completely disappears at higher field. This behavior is similar to ^{51}V-NMR result [5] of V_3Sn, which is a type II superconductor with s-wave pairing. At lower T, $T_1^{-1}(T)$ at the saddle point exhibits the T-dependence characterized by the activation type $e^{-\beta\Delta_{\rm mini}}$ where $\Delta_{\rm mini}$ is the vortex bound state energy. Several experiments [9,10] suggest a notable deviation from the BCS form $e^{-\beta\Delta_0}$ (Δ_0) and may indicate the above result.

We display the corresponding d-wave case in Fig. 1(b) where the saddle point $T_1^{-1}(T)$ is shown. It is seen from this that a reduced Hebel–Slichter peak is also suppressed by field because the singularity at the gap edge in DOS is smeared by the presence of vortices [11]. At lower T the T-linear behavior in $T_1^{-1}(T)$ can be seen from the inset in Fig. 1(b) except for the highest field case (H_{12}). These data imply that $1/TT_1 \sim \alpha H$ (α is a constant). Since $T_1^{-1}(T)$ contains a factor proportional to the square of the average DOS at the $E = E_F$, it is quite reasonable to consider that $1/TT_1 \propto \gamma(H)^2$ ($\gamma(H)$ is DOS at $E = E_F$). As shown previously [11] for d-wave $\gamma(H) \propto H^{0.41}$. Thus $1/TT_1 \propto H^{0.82}$ at the saddle point. This expectation is supported by NMR using ^{63}Cu [6] and ^{17}O [7] in $YBa_2Cu_3Y_7$ and ^{63}Cu [8] in $YBa_2Cu_4Y_8$.

4. Conclusion

By solving the Bogoliubov–de Gennes equation numerically we have shown the usefulness of the site selective NMR to know low-lying electronic excitations around a vortex core. The present study treats s-wave and d-wave cases. Although some of the important features of the latter case realized in the high T_c cuprates can be understood, more recent STM and NMR experiments [3,4] give results that sharply contradict the present calculation. Namely, it is suggested that in the vortex core antiferromagnetism is locally induced by external field. This interesting possibility belongs to a future problem.

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