Nuclear Magnetic Relaxation Rate in Iron-Pnictide Superconductors

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Abstract

Nuclear magnetic relaxation rate $1/T_1$ in iron-pnictide superconductors is calculated using the gap function obtained in a microscopic calculation. Based on the obtained results, we discuss the issues such as the rapid decrease of $1/T_1$ just below the transition temperature and the difference between nodeless and nodal s-wave gap functions. We also investigate the effect of Coulomb interaction on $1/T_1$ in the random phase approximation and show its importance in interpreting the experimental results.

Key words: Iron pnictides, multi-orbital Hubbard model, gap structure, NMR

Iron-pnictide superconductors have been one of the central issues in condensed matter physics since its discovery. Many experimental and theoretical works have been carried out to elucidate the symmetry and the structure of the superconducting gap function since the information on the gap structure gives a vital clue to determine the origin of the superconductivity. Recently, it is recognized that the iron-pnictide superconductors show varieties of the structure of the gap function[1], i.e., nodeless behavior in some systems and nodal behavior in other systems.

NMR measurement of $1/T_1 T$ is useful in determining such detailed structure of the gap function and many experimental results have been published[2] [3] [4] [5] [6]. Thus, we calculate $1/T_1 T$ based on some models for iron pnictides and compare the obtained results with experiments. Since many theoretical works exist[7] [8] [9] [10] [11], we concentrate on the unresolved issues such as the rapid decrease of $1/T_1 T$ just below the transition temperature and the discussion on the difference between nodeless and nodal s-wave gap functions.

For this purpose, we use the five-orbital Hubbard model proposed in ref[12]. Since we want to discuss the difference between the nodeless s-wave and nodal s-wave, we use following two models. One is a simplified model downfolded from the LDA calculation on the LaFeAsO system. Here “simplify” means that we neglect the three dimensionality and take hopping integrals only up to the fifth nearest neighbors. Other is a three dimensional model of the LaFePO system. All results shown below are obtained with band filling $n = 6.1$.

Assuming that the coupling between the conduction electrons and nuclear spins is diagonal in the orbital basis and using the constant form factor $A(q) = 1$, $1/T_1 T$ can be written as

$$
\frac{1}{T_1 T} = \lim_{\omega \to 0} \frac{1}{N} \sum_{q} \sum_{ab} \frac{\text{Im} \chi_{ab}(q, \omega)}{\omega}.
$$

(1)

Note that $a$ and $b$ denote the orbital indices. Without Coulomb interaction, we have

$$
\chi_{abcd}(q) = -\frac{T}{N} \sum_{q'} [G_{ac}(q + q')G_{db}(q') + F_{bc}(q + q')F_{da}(q')] \tag{2}
$$

where $q = (\omega, \vec{q})$ and $G_{ab}(q) (F_{ab}(q))$ is the normal (anomalous) Green’s function in the orbital representation. We also take account of the Coulomb interaction within the random phase approximation (RPA), where the enhancement factor $(\hat{1} - \hat{\chi}(q)\hat{V}^{s})^{-1}$ is included. Note that $\hat{\chi}(q)$ is the matrix form of eq. (2) and $\hat{V}^{s}$ is the spin vertex defined as $V^{s}_{abcd} = U (a = b = c = d), U' (a = c, b = d, a \neq b), J_H (a = b, c = d, a \neq c), J (a = d, b = c, a \neq b), 0$ (others). In what follows, we use $U = 1.0$ eV, $J_H = 0.2$ eV, $U = U' + J_H + J$ and $J_H = J$.

As is noted above, we describe the coupling between electrons and nuclear spins and the Green’s function in the orbital basis. Thus, we describe the gap function also in the orbital basis. In this orbital representation, the gap function becomes matrix form as $\Delta(\vec{k})$. Limiting the discussion on the s-wave channel, physically important entries of $\Delta(\vec{k})$ can be written as

$$
\Delta_{22}(\vec{k}) = a_2 + 2b_2(\cos k_x + \cos k_y) + 4c_2 \cos k_x \cos k_y - 4\delta \sin k_x \sin k_y, \tag{3}
$$

$$
\Delta_{33}(\vec{k}) = a_3 + 2b_3(\cos k_x + \cos k_y) + 4c_2 \cos k_x \cos k_y + 4\delta \sin k_x \sin k_y, \tag{4}
$$

$$
\Delta_{44}(\vec{k}) = a_4 + 2b_4(\cos k_x + \cos k_y) + 4c_4 \cos k_x \cos k_y, \tag{5}
$$

$$
\Delta_{23}(\vec{k}) = 2d_{23} \cos k_y - \cos k_x, \tag{6}
$$

$$
\Delta_{24}(\vec{k}) = 2i(\cos k_y - \sin k_x). \tag{7}
$$

Note that subscript 2, 3 and 4 represent $zx$, $yz$ and $x^2 - y^2$ orbital respectively. To determine the parameters in eqs. (3-7), we solve the linearized Eliashberg equation with the effective interaction calculated within RPA (we follow the formalisms in...
Figure 1: $T_c^* T_c / T_c T$ without Coulomb interaction where $T_c^*$ is the $T_c$ value at $T_c$. Calculation is done with 192x192 (100x100x8) meshes in the momentum space for LaFeAsO (LaFePO) system. Upper (lower) panel shows the results without (with) Coulomb interaction.

Then, we obtain the gap function with interband sign reversal which can be parameterized as $(a_2, b_2, c_2, \bar{\alpha}, a_4, b_4, c_4, d_2, p_2) = (0.0075, -0.038, -0.0155, 0.0075, 0.21, 0.11, -0.047, -0.0054, 0.045)$ for LaFeAsO and $(0.060, -0.030, -0.011, 0.047, -0.0054, 0.045)$ for LaFePO. For studying the gap function below $T_c$, we assume the usual temperature dependence, i.e., we use

$$\tilde{\Delta}(T, \bar{k}) = \alpha \tilde{\Delta}(\bar{k}) \tanh \left(1.74 \sqrt{T_c(T - 1)}\right). \tag{8}$$

In this work, $T_c$ is fixed to a large value of 0.02 eV to avoid the numerical difficulty. Scaling factor $\alpha$ in eq. (8) is determined to have $2\Delta_{\text{max}}/k_B T_c \sim 8$ that is typical for iron-pnictide superconductors with $\Delta_{\text{max}}$ being the largest gap value on the Fermi surface.

First, we show the results without Coulomb interaction in the upper panel of Fig. 1. In this calculation, we use the damping factor $\gamma = 0.05 T_c$ to discuss the clean limit ($\gamma$ is defined as $i\omega_n = \omega + i\gamma$). Although the used gap functions have unconventional property (interband sign reversal), the results show that the small coherence peaks appear in both of LaFeAsO and LaFePo system. (The coherence peak in LaFePO is negligibly small.) Inset of the upper panel of Fig. 1 shows that $1/T_1$ decreases slower in LaFePO system that has the nodal gap function compared with LaFeAsO system as is expected. Actually, $1/T_1$ in LaFePO decreases slower than $T^3$ just below $T_c$.

Next, we show the results with Coulomb interaction treated within RPA in the lower panel of Fig. 1. The most important difference between results with and without Coulomb interaction is the disappearance of the coherence peaks. Here, we use the same damping factor $\gamma = 0.05 T_c$ as in the case of without Coulomb interaction, i.e., we assume the same strength of the impurity scattering. This means that we can eliminate the coherence peaks without including the impurity effects. The reason for this disappearance is that Coulomb interaction makes the interband contribution to $1/T_1$ more dominant than the intraband contribution and the dominance of the interband contribution leads to the disappearance of the coherence peak for the gap function with an interband sign reversal. Another important point is that Coulomb interaction gives faster decrease of $1/T_1$ just below $T_c$ as can be seen by comparing the inset of upper and lower panel of Fig. 1. Paying attention to the temperature just below $T_c$, the result for LaFeAsO system shows more rapid decrease than $T^3$, which is the experimentally claimed rapid decrease, and the result for LaFePO system shows the decreasing rate close to $T^3$. Note that such details depend on the value of $\alpha$ as is the case without Coulomb interaction.

In summary, we have investigated the difference of the nodeless and nodal s-wave gap function through calculating $1/T_1 T$ using the microscopically determined gap functions. We have also demonstrated that Coulomb interaction can be a possible reason for the non existence of the coherence peaks in the clean limit. Further, we have shown the importance of Coulomb interaction in the discussion of the power of $1/T_1$ just below $T_c$.

Acknowledgment

We thank K. Kuroki for useful comments and for sharing the data of downfolded models.

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