Characteristic feature of dynamical susceptibility in noncentrosymmetric system

T Takimoto and P Thalmeier
Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Str. 40, 01187 Dresden, Germany
E-mail: takimoto@cpfs.mpg.de

Abstract. The static spin susceptibility $\chi_{\alpha\beta}(q)$ of spin components $S_\alpha$ and $S_\beta$ is examined in the non-centrosymmetric system with the antisymmetric spin-orbit coupling (so-called Rashba coupling), where $S_\alpha$ is $\alpha$-component of spin. Unlike in centrosymmetric case, off-diagonal spin susceptibilities do not vanish due to the Rashba coupling. The anomalous spin susceptibilities show significant momentum dependences like $\chi_{xx}(q) - \chi_{yy}(q) \sim q_x^2 - q_y^2$ and $\chi_{xy}(q) + \chi_{yx}(q) \sim q_xq_y$. Increasing the on-site Coulomb interaction, not only usual spin susceptibility but also anomalous spin susceptibilities are enhanced, especially, around the magnetic instability. As the direct probe to observe the anomalous spin susceptibility, a polarized neutron scattering experiment is proposed.

Since the discovery of unconventional superconductivity in a non-centrosymmetric compound CePt$_3$Si [1], the intensive investigation is carried out from experimental and theoretical sides. In addition to CePt$_3$Si, it has been observed that CeRhSi$_3$ and CeIrSi$_3$ also show superconductivity around magnetic phases under applying pressure [2, 3]. Recently, it has been reported that the NMR relaxation rate of CeIrSi$_3$ shows $\sqrt{T}$ temperature dependence above the superconducting transition temperature [4]. Due to the fact that the anomalous behavior is observed around the critical pressure, above which the antiferromagnetism disappears, it has been suggested that the critical antiferromagnetic spin fluctuation dominates the anomalous behavior. Therefore, it is desirable to study the spin susceptibility in non-centrosymmetric compounds.

Theoretically, the property of breaking inversion symmetry is incorporated by an effective spin-orbit coupling (so-called Rashba coupling) [5, 6], which has an antisymmetric momentum dependence. Due to the Rashba term, electron bands split to show a large Van-Vleck-type uniform spin susceptibility [7, 8]. In addition, it is known that a magnetic anisotropy for uniform susceptibility is also induced by the Rashba term. However, the study on magnetic response is not so extensive so far. In this proceedings, we examine dynamical susceptibilities in a non-centrosymmetric system with the Rashba term.

In order to describe the non-centrosymmetric system, we use the Hubbard model including the Rashba coupling, given as

$$H = \sum_{k\sigma\sigma'} \left[ (\varepsilon_k - \mu)\hat{\sigma}_0 + g_{k} \cdot \hat{\sigma} \right]_{\sigma\sigma'} c_{k\sigma}^\dagger c_{k\sigma'} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}, \quad (1)$$

where $c_{k\sigma}$ and $c_{k\sigma}^\dagger$ are annihilation and creation operators of an electron with a momentum $k$ and a spin $\sigma$. Here, $\varepsilon_k$ and $\mu$ are the energy dispersion of electrons and the chemical potential,
respectively, while $g_k$ describes the Rashba field satisfying $g_k = -g_{-k}$, which breaks the inversion symmetry. Then, eigenenergies of the non-interacting part are given by $\varepsilon_{k\pm} = \varepsilon_k \pm |g_k| - \mu$. In addition, $U$ is the on-site interaction.

In the non-interacting case ($U = 0$), the electron Green’s function is given by

$$G(0)(k, i\omega_n) = G^+(0)(k, i\omega_n)\hat{\sigma}_0 + \frac{g_k}{|g_k|} \cdot \hat{\sigma} G^-(0)(k, i\omega_n),$$

with

$$G^+(0)(k, i\omega_n) = \frac{1}{2} \left[(i\omega_n - \varepsilon_{k+})^{-1} \pm (i\omega_n - \varepsilon_{k-})^{-1}\right],$$

where $\omega_n$ is a fermionic Matsubara frequency. It should be noted that $G^-(0)(k, i\omega_n)$ vanishes in the limit of $|g_k| \to 0$, since $G^-(0)(k, i\omega_n)$ is expanded only in odd powers of $|g_k|$.

The dynamical susceptibility is defined as

$$\chi_{\alpha\beta}(q, i\Omega_n) = \int_0^T d\tau e^{i\omega_n\tau} \langle T_\tau [\left( \hat{S}_{\alpha}(\tau) - \langle \hat{S}_{\alpha}\rangle \right) \left( \hat{S}_{\beta}(0) - \langle \hat{S}_{\beta}\rangle \right)] \rangle,$$

where $\langle \cdots \rangle$ means the thermal average of $\cdots$, $T_\tau$ denotes the imaginary-time ordering operator, and $\Omega_n$ is a bosonic Matsubara frequency. Here, charge and spin operators with a wave vector $q$ are given by $S^c_q = \frac{1}{2} \sum_{\mu\nu} c^\dagger_{\mu\nu} c_{\mu+q\nu}$ and $S^\alpha_q = \frac{1}{2} \sum_{\sigma\sigma'} \sigma^\alpha \sigma' c^\dagger_{\sigma\nu} c_{\mu+q\sigma'} (\alpha = x, y, z)$, respectively, where $\hat{\sigma}^\alpha$ is an $\alpha$-component of Pauli matrices. In centrosymmetric systems, all off-diagonal susceptibilities disappear. On the other hand, it should be noted that off-diagonal susceptibilities do not always vanish in non-centrosymmetric systems [9, 10], and even susceptibilities between spin and charge operators $\chi_{ac}(q, i\Omega_n)$ and $\chi_{\alpha\alpha}(q, i\Omega_n)$ ($\alpha = x, y, z$) have non-zero values for $\Omega_n \neq 0$.

With use of the Green’s function $G(0)^\alpha_q(k, i\omega_n)$ given above, we provide expressions of dynamical susceptibilities $\chi_{\alpha\beta}(q, i\Omega_n)$. In the non-interacting case, the susceptibility $\chi_{\alpha\beta}^{(0)}(q, i\Omega_n)$ is calculated through a transformation from $\tilde{\chi}_{\sigma_1\sigma_2\sigma_3\sigma_4}(q, i\Omega_n)$ defined by [11],

$$\chi_{\sigma_1\sigma_2\sigma_3\sigma_4}(q, i\Omega_n) = \frac{1}{N_0^2} \sum_k \sum_m G(0)^{\sigma_1}_{\alpha\beta}(k, i\omega_n) G(0)^{\sigma_2}_{\sigma_3\sigma_4}(k + q, i\omega_m + i\Omega_n),$$

where $N_0$ is the number of unit cells. As a result, we have the following expressions for $\chi_{\alpha\beta}^{(0)}(q, i\Omega_n)$

$$\chi_{cc}^{(0)}(q, i\Omega_n) = \frac{1}{8N_0} \sum_k \sum_{\xi, \zeta} \left( 1 + \xi g_k \cdot g_{k+q} \right) \Delta_{\xi\zeta}(k; q, i\Omega_n),$$

$$\chi_{\alpha\beta}^{(0)}(q, i\Omega_n) = \frac{1}{8N_0} \sum_k \sum_{\xi, \zeta} \left[ \delta_{\alpha\beta} \left( 1 - \xi \frac{g_k \cdot g_{k+q}}{|g_k| |g_{k+q}|} \right) + \xi \frac{g_{\sigma\alpha} g_{k+q\beta} + g_{\beta\sigma} g_{k+q\alpha}}{|g_k| |g_{k+q}|} \right] \Delta_{\xi\zeta}(k; q, i\Omega_n),$$

$$\chi_{cc}^{(0)}(q, i\Omega_n) = \frac{1}{8N_0} \sum_k \sum_{\xi, \zeta} \left[ \xi \frac{g_{k+q\alpha} g_{k+q\beta} + g_{\beta\alpha} g_{k+q\beta}}{|g_k| |g_{k+q}|} \right] \Delta_{\xi\zeta}(k; q, i\Omega_n),$$

$$\chi_{cc}^{(0)}(q, i\Omega_n) = \frac{1}{8N_0} \sum_k \sum_{\xi, \zeta} \left[ \xi \frac{g_{k+q\beta} g_{k+q\alpha} + g_{\beta\alpha} g_{k+q\beta}}{|g_k| |g_{k+q}|} \right] \Delta_{\xi\zeta}(k; q, i\Omega_n),$$

where $\xi, \zeta$ are Matsubara frequencies.
The matrix elements of $\hat{U}$ are given by $U_{\alpha\beta} = \delta_{\alpha\beta} U_{\alpha\alpha}$ with $U_{cc} = U_{zz} = U_{xx} = U_{yy} = U$.

Then, we calculate $\chi_{\alpha\beta}(q, i\Omega_n)$ numerically, based on a two-dimensional noncentrosymmetric system with an energy dispersion $\varepsilon_k = 2t_1 (\cos k_x + \cos k_y) + 4t_2 \cos k_x \cos k_y$, and a Rashba-field $g_k = g_i (\sin k_x, -\sin k_y, 0)$. For chosen parameters $t_2/t_1 = 0.35$ and $g/t_1 = 0.2$, we can reproduce quasi two dimensional Fermi surfaces of CePt$_3$Si obtained by the band structure calculation [14, 15]. In Fig. 1, we show momentum dependences of static spin susceptibilities in the non-interacting case. Diagonal components of $\hat{\chi}(q, i\Omega_n)$ are shown in Fig. 1(a), where Fermi surfaces and the momentum path are also shown in insets. Unlike in centrosymmetric systems, all momentum dependences of $\chi_{xx}(q)$, $\chi_{zz}(q)$, $\chi_{zx}(q)$, and $\chi_{yy}(q)$ are different from each other. Especially, in a path from $(0, \pi)$ to $(\pi, 0)$, $\chi_{xx}(q)$ is antisymmetric around the mid-point $(\pi/2, \pi/2)$, and it vanishes in a diagonal path from $(\pi, \pi)$ to $(0, 0)$. Therefore, the momentum dependence of $\chi_{xx}(q) - \chi_{yy}(q)$ has the typical $q_x^2 - q_y^2$ symmetry. Likewise, momentum dependences of $\chi_{xy}(q) + \chi_{yx}(q)$, $\chi_{yx}(q) - \chi_{xy}(q)$, and $\chi_{zx}(q) - \chi_{xz}(q)$ are shown in Fig. 1(b), where the momentum path is depicted in the inset. In the figure, $\chi_{xy}(q)$ is symmetric around $(0, 0)$ and $(2\pi, 0)$, while it is antisymmetric around $(\pi, \pi)$. Accordingly, the momentum dependence of $\chi_{xy}(q) + \chi_{yx}(q)$ is a $q_x q_y$-type. Similarly, it can be understood easily that momentum dependences of $\chi_{yz}(q) - \chi_{zy}(q)$ and $\chi_{xz}(q) - \chi_{zx}(q)$ are of $q_y^2$- and $q_x^2$-type, respectively. Thus, spin susceptibilities have significant and unusual momentum dependences related with corresponding spin indices.

Using the same parameter set as in Fig. 1, we show $q$-dependences of susceptibilities $\chi_{\alpha\beta}(q)$ calculated within RPA. With the critical interaction $U_c = 2.551t_1$, the paramagnetic
The state becomes unstable at an ordering wave vector \( \mathbf{Q} = (0.81\pi, 0.25\pi) \). We show momentum dependences of \( (\chi_{xx}(\mathbf{q}) + \chi_{yy}(\mathbf{q})) / 2 \) and anomalous \( (\chi_{xy}(\mathbf{q}) + \chi_{yx}(\mathbf{q})) / 2 \) in Figs. 2(a) and 2(b), respectively. \( (\chi_{xx}(\mathbf{q}) + \chi_{yy}(\mathbf{q})) / 2 \) is enhanced with increasing \( U \), where \( \mathbf{q} \)-dependence of \( \chi_{zz}(\mathbf{q}) \) is different from that of \( (\chi_{xx}(\mathbf{q}) + \chi_{yy}(\mathbf{q})) / 2 \) \[10\]. Furthermore, the amplitude of \( \chi_{xy}(\mathbf{q}) + \chi_{yx}(\mathbf{q}) \) increases considerably in comparison with the corresponding value of the non-interacting case. In addition, we note that the amplitude of \( (\chi_{xx}(\mathbf{q}) - \chi_{yy}(\mathbf{q})) / 2 \) is also enhanced with increasing \( U \), especially, around the ordering wave vector \( \mathbf{Q} \) \[10\].

In summary, we have calculated spin susceptibilities in a non-centrosymmetric system including the Rashba term. It has been shown that anomalous spin susceptibilities have significant momentum dependences like \( \chi_{xx}(\mathbf{q}) - \chi_{yy}(\mathbf{q}) \sim q_x^2 - q_y^2 \) and \( \chi_{xy}(\mathbf{q}) + \chi_{yx}(\mathbf{q}) \sim q_x q_y \), where the anomalous susceptibility vanishes in centrosymmetric system. Considering that not only usual susceptibilities but also anomalous susceptibilities are enhanced by the on-site Coulomb interaction, we suggest that these anomalous susceptibility characteristic in the non-centrosymmetric system can be observed by a polarized neutron scattering experiment, especially, just above the magnetic transition temperature at the ordering wave vector.

References

1. Bauer E, Hilscher G, Michor H, Paul Ch, Scheidt E W, Gribanov A, Seropegin Yu, Noël H, Sigrist M and Rogl P 2004 Phys. Rev. Lett. 92 027003
2. Kimura N, Ito K, Saito K, Umeda Y, Aoki H and Terashima T 2005 Phys. Rev. Lett. 95 247004
3. Sugitani I et al. 2006 J. Phys. Soc. Jpn. 75 043703
4. Mukuda H, Fujii T, Ohara T, Harada A, Yashima M, Kitaoka Y, Okuda Y, Settai R and Ōnuki Y 2008 Phys. Rev. Lett. 100 107003
5. Rashba E I 1960 Sov. Phys. Solid State 2 1109
6. Frigeri P A, Agterberg D F, Koga A and Sigrist M 2004 Phys. Rev. Lett. 92 097001
7. Samokhin K V 2005 Phys. Rev. Lett. 94 027004
8. Fujimoto S 2007 J. Phys. Soc. Jpn. 76 034712
9. Yanase Y and Sigrist M Preprint arXiv:0805.2791
10. Takimoto T Preprint arXiv:0806.3214
11. Frigeri P A, Agterberg D F, Milat I and Sigrist M 2006 Eur. Phys. J. B 54 435
12. Yanase Y and Sigrist M 2007 J. Phys. Soc. Jpn. 76 043712
13. Tada Y, Kawakami N and Fujimoto S 2008 J. Phys. Soc. Jpn. 77 054707
14. Samokhin K V, Zijlstra E S and Bose S K 2004 Phys. Rev. B 69 094514
15. Hashimoto S, Yasuda T, Kubo T, Shishido H, Ueda T, Settai R, Matsuda T D, Haga Y, Harima H and Ōnuki Y 2004 J. Phys.: Condens. Matter 16 L287