Low Temperature Physics/Fizika Nizkikh Temperatur, 2017, v. 43, No. 1, pp. 15–21

Antiferromagnetic order in $CeCoIn_5$ oriented by spin-orbital coupling

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Received June 14, 2016, published online November 25, 2016

An incommensurate spin-density wave (Q phase) confined inside the superconducting state at high basal plane magnetic field is an unique property of the heavy-fermion metal $CeCoIn_5$. The neutron scattering experiments and the theoretical studies point out that this state come out from the soft mode condensation of magnetic resonance excitations. We show that the fixation of direction of antiferromagnetic modulations by a magnetic field reported by Gerber *et al.*, *Nat. Phys.* **10**, 126 (2014), is explained by spin-orbit coupling. This result, obtained on the basis of quite general phenomenological arguments, is supported by the microscopic derivation of the χ_{zz} susceptibility dependence on the mutual orientation of the basal plane magnetic field and the direction of modulation of spin polarization in a multiband metal.

PACS: 74.70.Tx Heavy-fermion superconductors;
75.30.Gw Magnetic anisotropy;
71.70.Ej Spin-orbit coupling, Zeeman and Stark splitting, Jahn–Teller effect;
74.25.Ha Magnetic properties including vortex structures and related phenomena.

Keywords: superconductor, heavy fermion, spin-density wave.

1. Introduction

$CeCoIn_5$ is a tetragonal, d-wave-pairing superconductor with the highest critical temperature $T_c = 2.3$ K among all the heavy-fermion compounds [1–3]. The superconducting state of $CeCoIn_5$ at a magnetic field above 9.8 T applied in the basal plane (Fig. 1) of its tetragonal crystal structure co-exists with incommensurate antiferromagnetic (AF) ordering or spin-density wave (SDW) [4] with $\mathbf{Q}_{IC} = (0.45, \pm 0.45, 0.5)$ independent of the field magnitude. Its 2D incommensurate part $\mathbf{q}_{IC} = (0.45, \pm 0.45, 0)$ is parallel to the nodal directions of the d-wave order parameter

$$\Delta(\mathbf{k}) = \Delta(\cos k_x^2 - \cos k_y^2).$$

Here we use reciprocal lattice units. The existence of the magnetic order was first detected by the technique of NMR [6] and its precise field-dependence later determined [7]. The antiferromagnetic modulation is concentrated on the cerium sites with amplitude $m = 0.15\mu_B$ (μ_B is the Bohr magneton) and polarized along the tetragonal axis. The incommensurate SDW is confined inside the superconducting phase, meaning that here superconductivity is an essential ingredient for SDW to develop. Different theoretical models have been proposed to explain why the SDW order occurs only in the high field-low temperature region of the d-wave superconducting state [8–16]. The choice

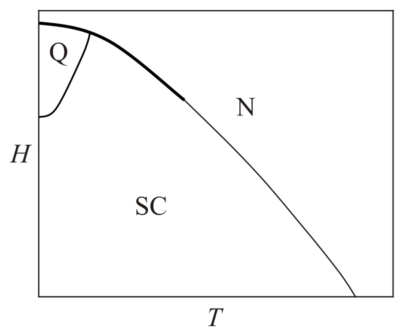

Fig. 1. Schematic (H, T) phase diagram of $CeCoIn_5$. N and SC are the normal and the superconducting states correspondingly. The upper critical field in $CeCoIn_5$ is mostly determined by paramagnetic limiting ($H_{c2}(T = 0) \simeq 11.7$ T) and due to this the phase transition to the superconducting state below $T = 0.4T_c$ ($T_c = 2.3$ K) is of the first order (thick line on the figure) [5]. The Q phase is the incommensurate antiferromagnetic state coexisting with the superconducting mixed state.

between these models can be made with the help of results of neutron scattering.

In the zero-field superconducting state, a spin resonance was found at a frequency ω = 0.6 meV ≈ 7 K, which corresponds approximately to $3T_c$. Initially, the resonance was observed [17] at a wave vector $\mathbf{Q} = (0.5, 0.5, 0.5)$ associated with the nested parts of the Fermi surface corresponding to antiferromagnetic correlations. Theoretically Eremin and collaborators [18] have attributed the resonance to the proximity to the threshold of the particle-hole excitations continuum which is at energy $\omega_c = \min(|\Delta_{\mathbf{k}}| + |\Delta_{\mathbf{k+Q}}|)$. Another scenario related to a magnon excitation was proposed by Chubukov and Gor'kov [19].

Recent, more precise inelastic neutron scattering measurements [20] have demonstrated that the spin resonance is peaked at the same wave vector as the incommensurate static AF modulation in a high fields. Moreover, the fluctuations associated with the resonance are polarized along the tetragonal c axis that corresponds to the direction of the ordered magnetic moments in the Q phase. Thus, the dynamical mode at zero field and the field induced static order share the same properties as if the resonance is a dynamical precursor of the Q phase. Also there were observed the Zeeman splitting of the resonance under magnetic field and the softening of the lowest energy mode of the Zeeman-split resonance [21–23]. All these observations point on the soft mode condensation caused by magnetic field as the mechanism for AF ordering formation. Such type theoretical model was put forward in Ref. 16.

In a random phase approximation the spin susceptibility is

$$\chi(\mathbf{q},\omega) = \frac{\chi^{(0)}(\mathbf{q},\omega)}{1 - U_q \chi^{(0)}(\mathbf{q},\omega)},$$

where $\chi^{(0)}(\mathbf{q},\omega))$ is the electron gas susceptibility in superconducting state and U_q is a momentum-dependent Hubbard–Coulomb repulsion potential. In this model the conditions for a collective excitation (called spin exciton) to occur are $U_q \Re e \chi^{(0)}(\mathbf{q},\omega) = 1$, and $U_q \Im m \chi^{(0)}(\mathbf{q},\omega) \ll 1$. The static antiferromagnetic state at some $\mathbf{q}$ is realized when the real part of the spin susceptibility along the tetragonal c axis in the presence of a finite basal plane magnetic field $\mathbf{H}_\perp$ exceeds the inverse constant of the AF interaction

$$\Re e \chi^{(0)}_{zz}(\omega = 0, \mathbf{q}, H_\perp) > U^{-1}_{\mathbf{q}}. \qquad (1)$$

In a two-dimensional model (Ref. 16) it was found that $\chi^{(0)}_{zz}(\omega = 0, \mathbf{q}_{IC}, H_\perp)$ in d-wave superconducting state increases with the field and exceeds the corresponding normal state susceptibility at fields essentially smaller than the paramagnetic limiting field [24]. The physical reason for this behavior is that the incommensurate wave vector connects the points on the Fermi surface where $\Delta(\mathbf{k}) = -\Delta(\mathbf{k} + \mathbf{q}_{IC})$. The same is true in real 3D case with modulation along $\mathbf{Q}_{IC}$. As a result, the tendency for AF instability in $CeCoIn_5$ is much more effective in the superconducting d-wave state.

An important observation made recently [25] is that the degeneracy between the two possible directions of antiferromagnetic modulation $\mathbf{Q}_{IC} = (0.45, \pm 0.45, 0.5)$ is lifted by the magnetic field orientation. Namely, for field parallel to $[1\bar{1}0]$, a Bragg peak was with $\mathbf{Q}_h = (0.45, 0.45, 0.5)$ but no peaks corresponding to $\mathbf{Q}_v = (0.45, -0.45, 0.5)$ were detected. For field precisely parallel to [100], the direction of the incommensurate part of AF modulation can take either of the two directions parallel to the gap nodes of $d_{x^2-y^2}$ pairing. But a tiny deviation of the field orientation from [100] toward [110] lifts this degeneracy and fixes the AF modulation along $[1\bar{1}0]$ direction. Correspondingly, a deviation of the field from [100] toward $[1\bar{1}0]$ fixes the AF modulation along [110] direction. In other words, the incommensurate AF modulation chooses that orientation which is the "most perpendicular" to the field direction (see Fig. 2).

The authors of Ref. 25 have attributed this phenomenon to the presence in the Q phase of an additional modulated on atomic scale superconducting component with triplet p-pairing with order parameter $\hat{\Delta}_Q = i(\mathbf{d}_Q \sigma)\sigma_y$ called pair density wave (PDW) interacting with d-wave order Δ and the AF order M^z_Q

$$V \propto i M^z_Q \left(\Delta^\dagger d^z_{-Q} - \Delta (d^z_Q)^\dagger\right) + \text{c.c.}$$

For the $\mathbf{H} \parallel [1\bar{1}0]$ then p-wave state with maximal spin-susceptibility along field direction and the zeros of the order parameter along perpendicular to the field direction $d^z_Q \propto (k_x - k_y)$ does not disturb the d-wave superconducting state and can stimulate the emergence of Q state with $\mathbf{Q} = (0.45, 0.45, 0.5)$. While possible phenomenologically this idea was not supported by any argument in favor of a specific mechanism for space modulated triplet pairing in this material.

Another interpretation of the same phenomenon, developed quite recently [26], is based on the AF modulation interaction with the Fulde–Ferrel–Larkin–Ovchinnikov (FFLO)

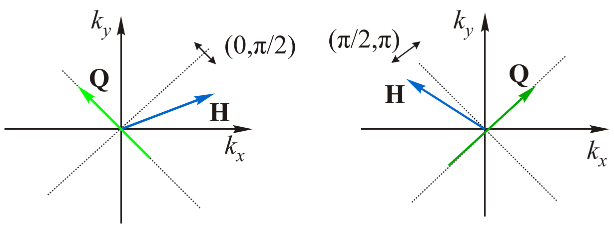

Fig. 2. (Color online) (Left) Basal plane magnetic field lies in the sector $(0, \pi/2)$ or in the sector $(\pi, 3\pi/2)$, the AF modulation is directed along $(1, \bar{1}, 0)$ direction. (Right) Basal plane magnetic field lies in the sector $(\pi/2, \pi)$ or in the sector $(3\pi/2, 2\pi)$, the AF modulation is directed along $(1,1,0)$ direction.

modulation parallel to the magnetic field direction. One can remark, however, that the phase diagram for the coexistence of the superconducting Q state and the FFLO state found theoretically in the previous paper of the same authors [13] does not resemble on the phase diagram of superconducting Q state shown on Fig. 1. Moreover, the isothermal measurements [27] at $H \parallel [100]$ did not reveal an entropy increase at phase transition from the superconducting state mixed state to the superconducting Q state which would indicate nodal quasiparticles in FFLO SC state. By contrast, a clear reduction of the entropy is found at a second-order transition at 10.4 T. This transition coincides with the incommensurate AF order [4,6]. The observed reduction of DOS is in perfect agreement with the expectation for a SDW formation without the additional FFLO state.

Here we propose an explanation of the Q-phase anisotropy governed by magnetic field based not on an imaginary additional ordering, but arising from the ordinary spin-orbit coupling. In the next section, on the basis of quite general phenomenological arguments, we demonstrate, that in a tetragonal crystal under the basal plane magnetic field, the static magnetic susceptibility along the tetragonal axis $\chi_{zz}^{(0)}(\mathbf{q}_\perp, \mathbf{H}_\perp)$ at finite $\mathbf{q}_\perp = (q_x, q_y)$ is largest either at $\mathbf{q}_\perp \parallel \mathbf{H}_\perp$ or at $\mathbf{q}_\perp \perp \mathbf{H}_\perp$. As a result, if the maximum of the susceptibility occurs for a space modulation perpendicular to the field, then the inequality given by Eq. (1) is realized first on the $\mathbf{Q}_{IC}$ direction, which is closer to being perpendicular to the magnetic-field direction. Thus, the degeneracy of directions of antiferromagnetic instability is lifted.

The $\chi_{zz}^{(0)}(\omega = 0, \mathbf{q}, \mathbf{H}_\perp)$ calculated in a single band model [16] is completely independent of the mutual orientation of $\mathbf{q}$ and the basal plane magnetic field $\mathbf{H}_\perp$. One can show that this orientational independence persists in a single band metal even in the Abrikosov mixed state characterized by inhomogeneous superfluid velocity and field distributions. On the other hand, it is known that the spin-orbit interaction in a noncentrosymmetric tetragonal metal causes the magnetic susceptibility orthorhombic anisotropy [28] $\chi_{xx} - \chi_{yy} \sim q_x^2 - q_y^2$. Such type anomalous susceptibility anisotropy in noncentrosymmetric $CePt_3Si$ has been measureed recently by polarized neutron scattering reported in Ref. 29. A similar phenomenon can be expected in a multiband centrosymmetric material.

$CeCoIn_5$ is the multiband metal that has been established by the de Haas–van Alphen measurements [30], by the band structure calculations and by the band spectroscopy studies [31–34]. In the third section to illustrate the phenomenological conclusions we show that, owing to the interband spin-orbit interaction, the static spin susceptibility $\chi_{zz}^{(0)}(\mathbf{q}_\perp, \mathbf{H}_\perp)$ in a tetragonal multiband metal depends on the mutual orientation of the wave vector $\mathbf{q}_\perp$ and the magnetic field $\mathbf{H}_\perp$. The spin-orbit coupling originating from the interaction of conducting electrons with the ionic crystal field can in principle be another source of violation of tetragonal symmetry by the basal plane magnetic field.

The presented microscopic calculations of susceptibility are performed for a two-band tetragonal metal in the normal state. However, it should be stressed that antiferromagnetism and antiferromagnetic domain switching are phenomena originating from different mechanisms. As it was demonstrated in Ref. 16, the antiferromagnetism arises from an anomalous enhancement of the $\chi_{zz}^{(0)}(\mathbf{q}_{IC})$ susceptibility in the d-wave superconducting state under the basal plane magnetic field. The domain switching is caused by spin-orbit coupling violating the crystal tetragonal symmetry at finite basal plane magnetic field and space modulation. The susceptibility $\chi_{zz}^{(0)}(\mathbf{q}_\perp, \mathbf{H}_\perp)$ is proved to be dependent from the mutual orientation of the magnetic field and the direction of the space modulated spin polarization. This dependence takes place already in the $CeCoIn_5$ normal state, but reveals itself in the d-wave superconducting state where the antiferromagnetic modulation developes. To demonstrate the violation of tetragonal symmetry by the basal plane magnetic field, it is sufficient to perform a microscopic derivation of the susceptibility in the normal state. The corresponding calculation in the superconducting state is much more cumbersome, but does not add any qualitative changes to the conclusions based on the normal state calculations.

2. Phenomenological approach

We consider a tetragonal paramagnet in a magnetic field having a constant basal plane (x, y) part and coordinate-dependent small additions

$$\mathbf{H}(\mathbf{r}) = [H_x + \delta H_x(\mathbf{r})]\hat{x} + [H_y + \delta H_y(\mathbf{r})]\hat{y} + \delta H_z(\mathbf{r})\hat{z}. \quad (2)$$

Its free energy in the quadratic approximation has the following form:

$$F = \int dV \left\{ \alpha(M_x^2 + M_y^2) + \alpha_z M_z^2 + \gamma\left[\left(\frac{\partial \mathbf{M}}{\partial x}\right)^2 + \left(\frac{\partial \mathbf{M}}{\partial y}\right)^2\right] + \right.$$
$$+ \gamma_z \left(\frac{\partial \mathbf{M}}{\partial z}\right)^2 + \gamma_{xy} \frac{\partial M_x}{\partial x}\frac{\partial M_y}{\partial y} + \gamma_{\perp z}\left(\frac{\partial M_x}{\partial x} + \frac{\partial M_y}{\partial y}\right)\frac{\partial M_z}{\partial z} +$$
$$\left. + \delta_1\left(H_x \frac{\partial M_z}{\partial y} - H_y \frac{\partial M_z}{\partial x}\right)^2 + \delta_2\left(H_x \frac{\partial M_z}{\partial x} + H_y \frac{\partial M_z}{\partial y}\right)^2 - \mathbf{HM} \right\}. \quad (3)$$

Here all terms besides the terms proportional to δ_1 and δ_2 have the tetragonal symmetry, whereas these two terms depend on the mutual orientation of the basal plane field and the direction of the space modulation of the M_z component of magnetization. This dependence originates from the spin-orbit interaction. Disregarding the spin-orbit coupling corresponds to the equality $\delta_1 = \delta_2$, recreating the functional tetragonal symmetry. For $\delta_1 > \delta_2$, the direction of the M_z basal-plane modulation is preferentially parallel to

$$\mathbf{H}_\perp = H_x\hat{x} + H_y\hat{y}.$$

On the other hand, for $\delta_1 < \delta_2$, the direction of the M_z basal-plane modulation tends to be perpendicular to $\mathbf{H}_\perp$.

One can formulate the same conclusion in terms of the susceptibility. Namely, by making the variation of Eq. (3) with respect to the magnetization components, taking into account the expressions for the equilibrium parts of the magnetization

$$M_x = H_x / 2\alpha, \quad M_y = H_y / 2\alpha,$$

and performing a Fourier transform, one arrives that the following equations for the magnetization response to the coordinate-dependent part of the magnetic field $\delta\mathbf{H}(\mathbf{r})$:

$$2\left[\alpha + \gamma(q_x^2 + q_y^2) + \gamma_z q_z^2\right]\delta M_x + \gamma_{xy} k_x k_y \delta M_y + \\ + \gamma_{\perp z} q_x q_z \delta M_z = \delta H_x, \tag{4}$$

$$\gamma_{xy} k_x k_y \delta M_x + 2\left[\alpha + \gamma(q_x^2 + q_y^2) + \gamma_z q_z^2\right]\delta M_y + \\ + \gamma_{\perp z} q_y q_z \delta M_z = \delta H_y, \tag{5}$$

$$\gamma_{\perp z}(q_x q_z \delta M_x + q_y q_z \delta M_y) + \\ + 2\left[\alpha_z + \gamma(q_x^2 + q_y^2) + \gamma_z q_z^2 + \delta_1(H_x q_y - H_y q_x)^2 + \right. \\ \left. + \delta_2(H_x q_x + H_y q_y)^2\right]\delta M_z = \delta H_z. \tag{6}$$

The solution of these equations yields the Fourier components of magnetization,

$$\delta M_x(\mathbf{q}) = \chi_{xx}\delta H_x(\mathbf{q}) + \chi_{xy}\delta H_y(\mathbf{q}) + \chi_{xz}\delta H_z(\mathbf{q}), \tag{7}$$

$$\delta M_y(\mathbf{q}) = \chi_{yx}\delta H_x(\mathbf{q}) + \chi_{yy}\delta H_y(\mathbf{q}) + \chi_{yz}\delta H_z(\mathbf{q}), \tag{8}$$

$$\delta M_z(\mathbf{q}) = \chi_{zx}\delta H_x(\mathbf{q}) + \chi_{zy}\delta H_y(\mathbf{q}) + \chi_{zz}\delta H_z(\mathbf{q}). \tag{9}$$

The coefficients γ_{xy} and $\gamma_{\perp z}$ have relativistic smallness relative to the exchange-determined coefficients α and γ. Neglecting the entanglement between the components of magnetization in Eqs. (4)–(6), which gives only small corrections of order $O(\gamma_{xy}^2)$ and $O(\gamma_{xy}\gamma_{\perp z})$ to the susceptibilities, we obtain

$$\chi_{zz}(\mathbf{q}) \cong \frac{1}{2\left[\alpha_z + \gamma(q_x^2 + q_y^2) + \gamma_z q_z^2 + \delta_1(H_x q_y - H_y q_x)^2 + \delta_2(H_x q_x + H_y q_y)^2\right]}. \tag{10}$$

Thus, for $\delta_1 > \delta_2$ the magnetic susceptibility along the tetragonal axis is largest for $\mathbf{H}_\perp \parallel \mathbf{q}_\perp$, where $\mathbf{q}_\perp = (q_x, q_y)$. On the other hand, for $\delta_1 < \delta_2$, the perpendicular mutual orientation of $\mathbf{H}_\perp$ and $\mathbf{q}_\perp$ corresponds to a maximum in the z component of susceptibility. This conclusion becomes evident if we rewrite the susceptibility as

$$\chi_{zz}(\mathbf{q}) \cong \frac{1}{2\left[\alpha_z + \gamma\mathbf{q}_\perp^2 + \gamma_z q_z^2 + (\delta_1 - \delta_2)[\mathbf{H}_\perp \times \mathbf{q}_\perp]^2 + \delta_2 \mathbf{H}_\perp^2 \mathbf{q}_\perp^2\right]}. \tag{11}$$

The derivation presented here demonstrates the dependence of the susceptibility on the mutual orientation of the field and the direction of modulation in the long-wave limit. The effect, however, can be strong enough in the case of atomic scale antiferromagnetic orderings.

Let us now show that the established χ_{zz} susceptibility dependence from $[\mathbf{H}_\perp \times \mathbf{q}_\perp]^2$ really takes place in a two-band tetragonal metal.

3. Microscopic derivation

The Green function of a tetragonal two-band metal in an external magnetic field $\mathbf{H}_\perp$ satisfies the equation

$$\hat{H}\hat{G} = \hat{1} \tag{12}$$

with the 4×4 matrix Hamiltonian

$$\hat{H} = \begin{pmatrix} (i\omega - \xi_1)\sigma_0 + \mathbf{h}_\perp \boldsymbol{\sigma} & i\mathbf{l}\boldsymbol{\sigma} \\ -i\mathbf{l}\boldsymbol{\sigma} & (i\omega - \xi_2)\sigma_0 + \mathbf{h}_\perp \boldsymbol{\sigma} \end{pmatrix}, \tag{13}$$

where

$$\xi_i(\mathbf{k}) = \varepsilon_i(\mathbf{k}) - \mu, \quad i = 1, 2$$

are the band energies counted from the chemical potential, $\mathbf{h}_\perp = \mu_B \mathbf{H}_\perp$, μ_B is the Bohr magneton, and $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ are the Pauli matrices. The interband spin-orbit coupling [35] is given by the vector $\mathbf{l}(\mathbf{k})$ which is an even function $\mathbf{l}(-\mathbf{k}) = \mathbf{l}(\mathbf{k})$ subordinating all the symmetry operations g of the tetragonal point group $g\mathbf{l}(g^{-1}\mathbf{k}) = \mathbf{l}(\mathbf{k})$. For the sake of concreteness, we can choose it to have the following form:

$$\mathbf{l}(\mathbf{k}) = \gamma_\perp k_z (k_y \hat{x} - k_x \hat{y}) + \gamma_\parallel \hat{k}_x \hat{k}_y (\hat{k}_x^2 - \hat{k}_y^2)\hat{z}, \tag{14}$$

where $\hat{k}_x = k_x / k_F$, $\hat{k}_y = k_y / k_F$ such that $\gamma_\perp$ and $\gamma_\parallel$ have common dimensionality of inverse mass $[1/m]$. We are seeking a $\mathbf{q}_\perp$ dependent z component of the spin susceptibility given by the equation

$$\chi_{zz}^{(0)}(\mathbf{q}_\perp) = -\mu_B^2 T \sum_{\mathbf{k},\omega_n} \mathrm{Tr}\begin{pmatrix} \sigma_z & 0 \\ 0 & \sigma_z \end{pmatrix} \hat{G}(\mathbf{k} + \mathbf{q}_\perp / 2, \omega_n) \times \\ \times \begin{pmatrix} \sigma_z & 0 \\ 0 & \sigma_z \end{pmatrix} \hat{G}(\mathbf{k} - \mathbf{q}_\perp / 2, \omega_n). \tag{15}$$

Calculating the trace, we rewrite it in terms of the products of $\hat{G}$ matrix elements

$$\chi_{zz}^{(0)}(\mathbf{q}) = -\mu_B^2 T \sum_{\mathbf{k},\omega_n} \sum_{i=1,\, j=1}^{4} (-1)^{i+j} G_{ij}(\mathbf{k}+\mathbf{q}_\perp/2,\omega_n)\times \times G_{ji}(\mathbf{k}-\mathbf{q}_\perp/2,\omega_n). \quad (16)$$

In this complete expression, we seek the terms proportional to the combination $[\mathbf{H}_\perp \times \mathbf{q}_\perp]^2$. Let us take, for instance, the sum of the product of matrix elements

$$\mu_B^2 T \sum_{\mathbf{k},\omega_n} \left[G_{12}(\mathbf{k}+\mathbf{q}_\perp/2,\omega_n)G_{21}(\mathbf{k}-\mathbf{q}_\perp/2,\omega_n) + + G_{21}(\mathbf{k}+\mathbf{q}_\perp/2,\omega_n)G_{12}(\mathbf{k}-\mathbf{q}_\perp/2,\omega_n)\right]. \quad (17)$$

Among the many terms in this sum, we will keep only the $\mathbf{H}_\perp$ and $\mathbf{q}_\perp$ mutual orientation-dependent terms. They are

$$-2\mu_B^2 T \sum_{\mathbf{k},\omega_n} \frac{[(i\omega_n-\xi_2)^2 - h_\perp^2 - l_z^2]_{\mathbf{k}+\mathbf{q}_\perp/2}\,\Re e[(h_x+ih_y)^2(il_x+l_y)^2_{\mathbf{k}-\mathbf{q}_\perp/2}]}{D(\mathbf{k}+\mathbf{q}_\perp/2,\omega_n)D(\mathbf{k}-\mathbf{q}_\perp/2,\omega_n)} + + \frac{[(i\omega_n-\xi_2)^2 - h_\perp^2 - l_z^2]_{\mathbf{k}-\mathbf{q}_\perp/2}\,\Re e[(h_x+ih_y)^2(il_x+l_y)^2_{\mathbf{k}+\mathbf{q}_\perp/2}]}{D(\mathbf{k}+\mathbf{q}_\perp/2,\omega_n)D(\mathbf{k}-\mathbf{q}_\perp/2,\omega_n)}, \quad (18)$$

where

$$D(\mathbf{k},\omega_n) = [(i\omega_n-\xi_+)^2 - \xi_-^2 - \mathbf{h}_\perp^2 - \mathbf{l}^2]^2 - 4[\xi_-^2\mathbf{h}_\perp^2 + (\mathbf{h}_\perp \mathbf{l})^2], \quad (19)$$

and

$$\xi_\pm(\mathbf{k}) = \frac{\xi_1(\mathbf{k}) \pm \xi_2(\mathbf{k})}{2}. \quad (20)$$

Keeping the $\mathbf{q}_\perp$ dependence only in

$$\Re e[(h_x+ih_y)^2(il_x+l_y)^2_{\mathbf{k}\pm\mathbf{q}_\perp/2}],$$

we obtain

$$\mu_B^2\gamma_\perp^2 T \sum_{\mathbf{k},\omega_n} \frac{k_z^2[(i\omega_n-\xi_2(\mathbf{k}))^2 - h_\perp^2 - l_z^2(\mathbf{k})]}{D^2(\mathbf{k},\omega_n)} \times \times\left\{2[\mathbf{h}_\perp \times \mathbf{q}_\perp]^2 - \mathbf{h}_\perp^2\mathbf{q}_\perp^2\right\}. \quad (21)$$

The sum over the Matsubara frequencies is easily calculated. However, the further integration over the Brillouin zone can only be performed numerically, taking into account the actual intraband quasiparticle spectra and the interband spin-orbital momentum dependencies. The knowledge of the quasiparticle density of states energy dependence near the Fermi surface is also crucially important. Analytically, we can write a rough estimation for orientation-dependent part of the susceptibility as

$$\chi_{zz}^{\text{anis1}} \propto \mu_B^2 N_0 \left(\frac{\mu_B\gamma_\perp k_F}{\varepsilon_F^2}\right)^2 [\mathbf{H}_\perp \times \mathbf{q}_\perp]^2. \quad (22)$$

Taking in mind that the modulus of the wave vector of antiferromagnetic modulation in CeCoIn$_5$ is $|\mathbf{q}_\perp| \approx k_F$ one can write the estimation of the absolute value of the susceptibility anisotropy as

$$\chi_{zz}^{\text{anis1}} \propto \mu_B^2 N_0 \left(\frac{\mu_B H}{\varepsilon_F}\right)^2 \left(\frac{\gamma_\perp k_F^2}{\varepsilon_F}\right)^2. \quad (23)$$

CeCoIn$_5$ is the heavy-fermion compound with the electron effective mass about hundred times larger than the bare electron mass $m^* \approx 100m$ [30]. This means that the Fermi energy is quite small and can be of the order of spin-orbit interaction $\varepsilon_F \sim \gamma_\perp k_F^2$. At the same time, the magnetic energy $\mu_B H$ in fields about 10 T is about 10 K. Hence the anisotropy of susceptibility can have noticeable magnitude in comparison with the Pauli susceptibility $\chi_P = 2N_0\mu_B^2$.

Parametrically similar contributions to the orientation-dependent part of the susceptibility originate from all the Green-function products in Eq. (16) with indices $i \neq j$. On the other hand, the products with $i = j$ give rise to contributions such as

$$\chi_{zz}^{\text{anis2}} \propto \mu_B^2 N_0 \left(\frac{\mu_B\gamma_\parallel\gamma_\perp k_F^3}{\varepsilon_F^3}\right)^2 [\mathbf{H}_\perp \times \mathbf{q}_\perp]^2 \approx \approx \mu_B^2 N_0 \left(\frac{\mu_B H}{\varepsilon_F}\right)^2 \left(\frac{\gamma_\parallel\gamma_\perp k_F^4}{\varepsilon_F^2}\right)^2. \quad (24)$$

Thus, we have demonstrated by direct microscopic calculation that the violation of tetragonal symmetry by a basal plane magnetic field discussed in previous section on a purely phenomenological basis, really takes place in multiband metals.

Depending on the relative value and signs of expressions (22) and (24), the mutual orientations of $\mathbf{q}_\perp$ and $\mathbf{H}_\perp$ can either be parallel or perpendicular to each other. The preferred mutual orientation can be changed at some pressure if the orientation-dependent part of the susceptibility changes sign.

4. Conclusion

Some time ago [16], we have demonstrated the softening of spin resonance mode in the d-wave superconducting $CeCoIn_5$ under a basal plane magnetic field at a wave vector $\mathbf{q}_{IC}$ that connects the points of the Fermi surface with a finite gap $\Delta(\mathbf{k}) = -\Delta(\mathbf{k}+\mathbf{q}_{IC})$. In the strong enough field this leads to the formation of static incommensurate AF state with two possible types of antiferromagnetic domains. Here, we have shown that the spin-orbit interaction in a tetragonal metal under the basal plane magnetic field acts to favor an inhomogeneous spin density modulation directed either perpendicular or parallel to the field direction. Hence, in general, only one type of antiferromagnetic domain is energetically favorable. This allows us to explain the puzzle of antiferromagnetic domain switching initiated by the basal plane magnetic field rotation observed [25] in superconducting $CeCoIn_5$.

In $CeCoIn_5$ at ambient pressure, the incommensurate AF modulation prefers to be directed along the direction that is “the most perpendicular” to the field direction. At some pressure, the preferred orientation can change to “the most parallel” one.

The mechanism described for the orienting influence of the magnetic field on the direction of antiferromagnetic modulation has a general character and should reveal itself in an itinerant antiferromagnet. The phenomenon of antiferromagnetic domain switching is suppressed by domain pinning and can be observable only in clean enough metals, but not in doped antiferromagnets such as $CeRh_{1-x}Co_xIn_5$.

The susceptibility $\chi_{zz}(\mathbf{q}_\perp, \mathbf{H}_\perp)$ dependence from the mutual orientation $\mathbf{q}_\perp$ and $\mathbf{H}_\perp$ characterizing the intensity of spin-orbit coupling in a tetragonal material can be measured by neutron scattering.

I hope that this paper will stimulate quantitative numerical calculations of $\chi_{zz}(\mathbf{q}_\perp, \mathbf{H}_\perp)$ both in the normal and in the superconducting states based on the real band structure of $CeCoIn_5$.

Acknowledgments

I am grateful to S. Raymond for the interest to this study and to S. Blundell for the help in the manuscript preparation.

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