

Quantum temperature fluctuations in the magnetization of antiferromagnetic semimetals

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(Submitted February 17, 1998)

Fiz. Tverd. Tela (St. Petersburg) **40**, 1674–1680 (September 1998)

It is shown that in semimetallic, low-temperature antiferromagnetic materials located in a quantizing magnetic field, the part of the band magnetization M_{\sim} which oscillates in H can have a nonmonotonic temperature dependence. This non-Fermi liquid behavior will show up experimentally in the form of quantum temperature fluctuations of the magnetization when the decrease with rising temperature is oscillatory, rather than the usual monotonic decrease.

It is shown that the magnetization from an individual spin electron (or hole) subband has the form of weakly damped periodic oscillations as a function of T^2 . This result makes it possible to develop an efficient method for studying the electronic structure of antiferromagnetic semimetals based on an examination of the quantum temperature fluctuations. Calculations show that quantum temperature fluctuations can be observed, for example, in the cerium monpnictides CeP and CeAs, which are strongly correlated, antiferromagnetic, compensated semimetals with low Neel temperatures. © 1998 American Institute of Physics. [S1063-7834(98)02409-5]

Studies of the electronic structure of strongly correlated systems have stimulated experimental studies of the de Haas-van Alphen effect in compounds with mixed valence, heavy fermions,^{1–3} and high-temperature superconductors.^{4,5} The class of strongly correlated systems includes compounds with a low current-carrier concentration. The cerium monpnictides CeX, with X=Sb, Bi, As, and P are striking representatives of this type of compound.^{6–8} The presence of a long-range antiferromagnetic order in these compounds has led to the creation of the concept of magnetopolaron liquids and crystals⁹ for describing the ground state of the electronic system. This has made it possible to explain the features of the de Haas-van Alphen effect in CeAs.¹⁰

In addition to the ordinary de Haas-van Alphen effect, which involves a fluctuating magnetic field dependence of the magnetization of band charge carriers, experimental studies have recently been made¹¹ of a new type of fluctuations in the magnetization. These involve a nonmonotonic variation in the magnetization as the temperature is changed. They have been referred to, therefore, as quantum temperature fluctuations. The degenerate magnetic semiconductor n -HgCr₂X₄ has been chosen for testing. A theoretical analysis¹² of quantum temperature fluctuations showed that the major factors determining the possibility of observing quantum temperature fluctuations are the existence of strong single-site correlations, magnetic ordering, and s - d coupling between localized and collectivized electrons. The principal sources of the motion of the Landau levels, as the temperature is varied, were the s - d -exchange interaction, along with a change in the average magnetization. Since the Curie temperature is quite high ($T_c = 130$ K), it was not possible to observe many spikes in the magnetization (before the fluctuations were damped out).

Quantum temperature fluctuations are evidently best observed using materials with low magnetic ordering tempera-

tures ($T_c \sim 1$ – 10 K). Then the reduction in the spontaneous magnetization will be fairly strong over a small temperature interval and the number of spikes in the quantum temperature fluctuations will be large. In this regard, the cerium monpnictides are extremely promising. For them $T_N \approx 7$ K and the de Haas-van Alphen effect shows up quite well. Since these compounds have an antiferromagnetic order, and the antiferromagnetic sublattices become tapered in strong magnetic fields, there is some interest in analyzing the quantum temperature fluctuations in the antiferromagnetic semimetals taking this tapering into account.

In this paper we examine the quantum temperature fluctuations in the magnetization of antiferromagnetic materials theoretically under conditions such that the quantizing magnetic field causes a reordering of the ground state. Taking the strong tapering of the antiferromagnetic sublattices into account in a spin-wave approximation, we study the low-temperature thermodynamics of a localized subsystem and determine the dependence of the magnetic-order parameters on the magnetic field and temperature. It is shown that, even at the low temperatures where the spin-wave approximation is justified, a change in the temperature leads to a large number of spikes in the fluctuating magnetization of the band electrons. The contributions from individual electron- and hole-spin subbands to the quantum temperature fluctuations are analyzed and it is found that these contributions are weakly damped functions periodic in T^2 . This makes it possible to use Fourier analysis to study quantum temperature fluctuations and to develop an effective technique for testing the electronic structure of antiferromagnetic semimetals.

1. MODEL HAMILTONIAN AND SPECTRUM OF FERMION QUASIPARTICLES

Before considering quantum temperature fluctuations in antiferromagnetic semimetals such as CeP, CeAs, and CeSb,

let us recall the general properties of their electronic structure. The cerium monopnictides have an NaCl cubic structure. Low-energy states of the conduction band lie as the X points of the Brillouin zone. The top of the valence band lies at the Γ point. A slight overlap of these bands is responsible for the semimetallic properties of these compounds. At low temperatures ($T_N=7$ and 10.5 K for CeAs and CeP, respectively), a long-range antiferromagnetic order develops in the subsystem of localized electronic states. The antiferromagnetic sublattices undergo tapering in the presence of a magnetic field H , influencing the energy spectrum of the current carriers through an interaction between the electrons in localized and collectivized states. The major features of these interactions are modelled by the following hamiltonian for an antiferromagnetic semimetal:

$$\begin{aligned} \mathcal{H} = & \sum_{\lambda f f' \sigma} \{t_{ff'}^\lambda - \delta_{ff'}(2\sigma\mu_B H + \mu_\lambda)\} c_{\lambda f \sigma}^+ c_{\lambda f' \sigma} \\ & + \sum_{\lambda g g' \sigma} \{t_{gg'}^\lambda - \delta_{gg'}(2\sigma\mu_B H + \mu_\lambda)\} c_{\lambda g \sigma}^+ c_{\lambda g' \sigma} \\ & + \sum_{\lambda f g \sigma} f_{fg}^\lambda (c_{\lambda f \sigma}^+ d_{\lambda g \sigma} + d_{\lambda g \sigma}^+ c_{\lambda f \sigma}) + \sum_{f g} K_{fg} (\mathbf{S}_f \mathbf{S}_g) \\ & - \frac{1}{2} \sum_{ff'} I_{ff'} (\mathbf{S}_f \mathbf{S}_{f'}) - \frac{1}{2} \sum_{gg'} I_{gg'} (\mathbf{S}_g \mathbf{S}_{g'}) \\ & - \sum_f g \mu_B H S_f^z - \sum_g g \mu_B H S_g^z - \sum_{f \lambda} J_\lambda (\mathbf{S}_f \boldsymbol{\sigma}_{f \lambda}) \\ & - \sum_{g \lambda} J_\lambda (\mathbf{S}_g \boldsymbol{\sigma}_{g \lambda}). \end{aligned} \quad (1)$$

Here the first three terms describe the free-electron-hole subsystem in the Wannier representation. To describe effects associated with the antiferromagnetic order in the localized subsystem, one performs the conventional separation into two sublattices, F and G . The Fermi operator $c_{\lambda f \sigma}$ annihilates an electron for $\lambda=e$ or hole for $\lambda=h$ at site f with projection σ ($\sigma = \pm 1/2$) of the spin angular momentum. The operator $d_{\lambda g \sigma}$ corresponds to the same kind of process, but for site g from the sublattice G . For electrons $\mu_e = \mu$ and for holes $\mu_h = -\mu$. The next group of operators in Eq. (1) describes the Heisenberg interaction among the spin angular momenta of the localized electronic states, which brings about an antiferromagnetic order, as well as an interaction of the spin angular momenta with the magnetic field H . Here we have included both the interaction within the sublattices and the interaction among spin angular momenta from the F and G sublattices. Finally, the last two terms account for the $s-f$ exchange coupling among the spin angular momenta of the localized and collectivized states.

The energy spectrum of the electrons and holes in the tapered antiferromagnetic phase is conveniently found by first going to local coordinate systems for the F and G sublattices. The procedure for transforming to local coordinates and obtaining the electron and hole spectra in the noncolinear geometry of this problem has been described in detail

elsewhere.¹³ Thus, here we only give the final expression for the lower branches of the spectrum for the electrons ($\lambda=e$) and holes ($\lambda=h$),

$$\begin{aligned} E_{\mp}^\lambda(\mathbf{k}) = & \varepsilon^\lambda + t_{\mathbf{k}} - \left\{ \left[\Gamma_{\mathbf{k}\mp}^\lambda \left(\mu_B H + \cos \theta \frac{J_\lambda R}{2} \right) \right]^2 \right. \\ & \left. + \sin^2 \theta \left(\frac{J_\lambda R}{2} \right)^2 \right\}^{1/2}, \end{aligned} \quad (2)$$

where

$$\varepsilon^\lambda = t_{\mathbf{k}}^\lambda = \sum_{f'} t_{ff'}^\lambda \exp\{-i\mathbf{k}(\mathbf{R}_f - \mathbf{R}_{f'})\},$$

$$\Gamma_{\mathbf{k}}^\lambda = \sum_g t_{fg}^\lambda \exp\{-i\mathbf{k}(\mathbf{R}_f - \mathbf{R}_g)\}.$$

The angle θ defines the orientation \mathbf{R} of the equilibrium magnetization of the sublattice relative to the z axis along which the external magnetic field H is directed. For $H=0$, $\theta = \pi/2$, while at the spin-flip transition point $\theta=0$. We are interested in the fairly high magnetic fields when the tapering of the antiferromagnetic sublattices is large ($\theta \geq \pi/4$). In this case, the lower energy states have energies given by the simpler expressions

$$\begin{aligned} E_{\mp}^e(\mathbf{k}) = & \mp \left(\mu_B H + \cos \theta \frac{J_e R}{2} \right) + \frac{\hbar^2 \mathbf{k}^2}{2m_e}, \\ E_{\mp}^h(\mathbf{k}) = & -\Delta \mp \left(\mu_B H + \cos \theta \frac{J_h R}{2} \right) + \frac{\hbar^2 \mathbf{k}^2}{2m_h}, \end{aligned} \quad (3)$$

in which the effective masses are related to the jump parameters by the following equations

$$\frac{\hbar^2}{2m_\lambda} = -\frac{1}{6} \left\{ \sum_g t_{fg}^\lambda (\mathbf{R}_f - \mathbf{R}_g)^2 + \sum_{f'} t_{ff'}^\lambda (\mathbf{R}_f - \mathbf{R}_{f'})^2 \right\}. \quad (4)$$

Here the cubic structure of the lattice is taken into account. In Eq. (3), the choice of reference scale for the energy is such that, in the paramagnetic phase with $H=0$, the bottom of the conduction band corresponds to zero energy. Then the degree of overlap of the valence band with the conduction band is determined by the parameter $\Delta > 0$. In order to determine the temperature dependence of this energy spectrum it is necessary to study the low-temperature thermodynamics of this system and to calculate the temperature dependence of $R \cos \theta$ in a noncolinear geometry.

2. TEMPERATURE EVOLUTION OF THE SUBLATTICE MAGNETIZATION

The parameters which determine the magnetic structure of the localized subsystem (R and $\cos \theta$) can be calculated in our case using an exchange hamiltonian. In local coordinates this hamiltonian is obtained by rotation through an angle θ for the F sublattice and by an angle $-\theta$ for the G sublattice. Then (for details, see Ref. 13),

$$\begin{aligned}
 H_{mz} = & -\frac{1}{2} \sum_{ff'} I_{ff'} (\mathbf{S}_f \mathbf{S}_{f'}) - \frac{1}{2} \sum_{gg'} I_{gg'} (\mathbf{S}_g \mathbf{S}_{g'}) \\
 & + \sum_{fg} K_{fg} \{ \cos 2\theta (S_f^x S_g^x + S_f^z S_g^z) \\
 & + S_f^y S_g^y + \sin 2\theta (S_f^z S_g^z - S_f^x S_g^x) \} \\
 & - g \mu_B H \cos \theta \left(\sum_f S_f^z + \sum_g S_g^z \right) \\
 & + g \mu_B H \sin \theta \left(\sum_f S_f^x - \sum_g S_g^x \right). \quad (5)
 \end{aligned}$$

For examining the low-temperature thermodynamics in the localized subsystem we use the Dyson–Maleev representation,

$$\begin{aligned}
 S_f^+ &= \sqrt{2S} (a_f - a_f^+ a_f), \quad S_f^- = \sqrt{2S} a_f^+, \\
 S_f^z &= S - a_f^+ a_f, \quad S_g^+ = \sqrt{2S} (b_g - b_g^+ b_g), \\
 S_g^- &= \sqrt{2S} b_g^+, \quad S_g^z = S - b_g^+ b_g, \quad (6)
 \end{aligned}$$

where a_f (a_f^+) are the annihilation (creation) operators for excitation at site f for sublattice F . For the G sublattice the corresponding operators are denoted by b_g (b_g^+).

Substituting Eqs. (6) in the Hamiltonian (5), taking the Fourier transform, and proceeding as usual,¹⁴ we obtain the Hamiltonian in the second quantization representation. The quadratic form is given by

$$\begin{aligned}
 H_{mz}^{(2)} = & \sum_{\mathbf{q}} \{ \varepsilon_{\mathbf{q}} (a_{\mathbf{q}}^+ a_{\mathbf{q}} + b_{\mathbf{q}}^+ b_{\mathbf{q}}) + \nu_{\mathbf{q}} (a_{\mathbf{q}}^+ b_{\mathbf{q}} + b_{\mathbf{q}}^+ a_{\mathbf{q}}) \\
 & + \xi_{\mathbf{q}} (a_{\mathbf{q}}^+ b_{-\mathbf{q}}^+ + b_{-\mathbf{q}} a_{\mathbf{q}}) \}, \quad (7)
 \end{aligned}$$

where we have introduced the following notation;

$$\begin{aligned}
 \varepsilon_{\mathbf{q}} &= g \mu_B H \cos \theta - SK_0 \cos 2\theta + S(I_0 - I_{\mathbf{q}}), \\
 \nu_{\mathbf{q}} &= SK_{\mathbf{q}} \cos^2 \theta, \quad \xi_{\mathbf{q}} = -SK_{\mathbf{q}} \sin^2 \theta. \quad (8)
 \end{aligned}$$

Here the Fourier transforms of the exchange integrals are given in the form

$$\begin{aligned}
 K_{\mathbf{q}} &= \sum_g K_{fg} \exp\{-i\mathbf{q}(\mathbf{R}_f - \mathbf{R}_g)\}, \\
 I_{\mathbf{q}} &= \sum_{f'} I_{ff'} \exp\{-i\mathbf{q}(\mathbf{R}_f - \mathbf{R}_{f'})\}.
 \end{aligned}$$

In order to write down the Hamiltonian in the $a_{\mathbf{q}}$, $a_{\mathbf{q}}^+$, $b_{\mathbf{q}}$ and $b_{\mathbf{q}}^+$ operator representation, we equate the terms in first order in these operators to zero and obtain a condition for the equilibrium angle θ ,

$$\cos \theta = g \mu_B H / 2SK_0. \quad (9)$$

To find the equilibrium magnetization

$$R = \frac{1}{N} \sum_g \langle S_g^z \rangle = S - \frac{1}{N} \sum_{\mathbf{q}} \langle b_{\mathbf{q}}^+ b_{\mathbf{q}} \rangle \quad (10)$$

we use the ideology of the two-time temperature Green functions.^{14,15} For this purpose, we introduce the following four functions into the discussion:

$$\begin{aligned}
 & \langle \langle b_{\mathbf{q}}(t) | b_{\mathbf{q}}^+(t') \rangle \rangle, \quad \langle \langle a_{\mathbf{q}}(t) | b_{\mathbf{q}}^+(t') \rangle \rangle, \\
 & \langle \langle b_{-\mathbf{q}}^+(t) | b_{\mathbf{q}}^+(t') \rangle \rangle, \quad \langle \langle a_{-\mathbf{q}}^+(t) | b_{\mathbf{q}}^+(t') \rangle \rangle.
 \end{aligned}$$

A closed system of equations for the Fourier transforms of these functions can be written in the form

$$\begin{aligned}
 (\omega - \varepsilon_{\mathbf{q}}) \langle \langle b_{\mathbf{q}} | b_{\mathbf{q}}^+ \rangle \rangle_{\omega} &= 1 + \nu_{\mathbf{q}} \langle \langle a_{\mathbf{q}} | b_{\mathbf{q}}^+ \rangle \rangle_{\omega} + \xi_{\mathbf{q}} \langle \langle a_{-\mathbf{q}}^+ | b_{\mathbf{q}}^+ \rangle \rangle_{\omega}, \\
 (\omega - \varepsilon_{\mathbf{q}}) \langle \langle a_{\mathbf{q}} | b_{\mathbf{q}}^+ \rangle \rangle_{\omega} &= \nu_{\mathbf{q}} \langle \langle b_{\mathbf{q}} | b_{\mathbf{q}}^+ \rangle \rangle_{\omega} + \xi_{\mathbf{q}} \langle \langle b_{-\mathbf{q}}^+ | b_{\mathbf{q}}^+ \rangle \rangle_{\omega}, \\
 (\omega + \varepsilon_{\mathbf{q}}) \langle \langle b_{-\mathbf{q}}^+ | b_{\mathbf{q}}^+ \rangle \rangle_{\omega} &= -\nu_{\mathbf{q}} \langle \langle a_{-\mathbf{q}}^+ | b_{\mathbf{q}}^+ \rangle \rangle_{\omega} - \xi_{\mathbf{q}} \langle \langle a_{\mathbf{q}} | b_{\mathbf{q}}^+ \rangle \rangle_{\omega}, \\
 (\omega + \varepsilon_{\mathbf{q}}) \langle \langle a_{-\mathbf{q}}^+ | b_{\mathbf{q}}^+ \rangle \rangle_{\omega} &= -\nu_{\mathbf{q}} \langle \langle b_{-\mathbf{q}}^+ | b_{\mathbf{q}}^+ \rangle \rangle_{\omega} - \xi_{\mathbf{q}} \langle \langle b_{\mathbf{q}} | b_{\mathbf{q}}^+ \rangle \rangle_{\omega}. \quad (11)
 \end{aligned}$$

From this system we obtain a dispersion equation for the energy spectrum of the elementary excitations,

$$\begin{vmatrix}
 \omega - \varepsilon_{\mathbf{q}} & -\nu_{\mathbf{q}} & -\xi_{\mathbf{q}} & 0 \\
 -\nu_{\mathbf{q}} & \omega - \varepsilon_{\mathbf{q}} & 0 & -\xi_{\mathbf{q}} \\
 \xi_{\mathbf{q}} & 0 & \omega + \varepsilon_{\mathbf{q}} & \nu_{\mathbf{q}} \\
 0 & \xi_{\mathbf{q}} & \nu_{\mathbf{q}} & \omega + \varepsilon_{\mathbf{q}}
 \end{vmatrix} = 0. \quad (12)$$

On solving Eq. (12), we find two branches of the energy spectrum,

$$\begin{aligned}
 \omega_1(\mathbf{q}) &= \sqrt{(\varepsilon_{\mathbf{q}} - \nu_{\mathbf{q}})^2 - \xi_{\mathbf{q}}^2}, \\
 \omega_2(\mathbf{q}) &= \sqrt{(\varepsilon_{\mathbf{q}} + \nu_{\mathbf{q}})^2 - \xi_{\mathbf{q}}^2}. \quad (13)
 \end{aligned}$$

Given Eqs. (8) and (9), the expressions for the spectrum in the noncollinear phase, where $\theta > 0$, can be written in the form

$$\begin{aligned}
 \omega_1(\mathbf{q}) &= S \{ (I_0 - I_{\mathbf{q}} + K_0 - K_{\mathbf{q}}) (I_0 - I_{\mathbf{q}} + K_0 - K_{\mathbf{q}} \cos 2\theta) \}^{1/2}, \\
 \omega_2(\mathbf{q}) &= S \{ (I_0 - I_{\mathbf{q}} + K_0 + K_{\mathbf{q}}) (I_0 - I_{\mathbf{q}} + K_0 + K_{\mathbf{q}} \cos 2\theta) \}^{1/2}. \quad (14)
 \end{aligned}$$

It is clear that the lower branch is gapless, consistent with the Goldstone theory. The exchange Hamiltonian is invariant with respect to rotation by an arbitrary angle about the z axis, while the ground state of the system in the tapered phase does not have this invariance. This explains the presence of the Goldstone boson in the system.

The second branch of the spectrum has an activation character. The energy gap for this branch is given by

$$\Delta = \omega_1(0) = 2SK_0 \cos \theta = g \mu_B H. \quad (15)$$

In the right-hand neighborhood of the spin-flip transition, when $\theta = 0$ and the subsystem of localized spins undergoes a transformation to the colinear phase, the two branches of the spectrum obey

$$\omega_{1,2}(\mathbf{q}) = g \mu_B H + S(I_0 - I_{\mathbf{q}}) - S(K_0 \pm K_{\mathbf{q}}). \quad (16)$$

Solving the system of Eqs. (11), we find the Green function

$$\langle \langle b_{\mathbf{q}} | b_{\mathbf{q}}^+ \rangle \rangle_{\omega} = \frac{[(\omega + \varepsilon_{\mathbf{q}})^2 - \nu_{\mathbf{q}}^2](\omega - \varepsilon_{\mathbf{q}}) + \xi_{\mathbf{q}}^2(\omega + \varepsilon_{\mathbf{q}})}{[\omega^2 - \omega_1^2(\mathbf{q})][\omega^2 - \omega_2^2(\mathbf{q})]}, \quad (17)$$

which allows us to obtain the desired expression for the equilibrium magnetization,

$$R = S - \delta S(0) - \delta S(T), \quad (18)$$

where $S(0)$ is a term which reduces the magnetization owing to the zero-point quantum fluctuations, with

$$\delta S(0) = \frac{1}{2} - \frac{1}{4N} \sum_{\mathbf{q}} \left\{ \frac{\varepsilon_{\mathbf{q}^-} \nu_{\mathbf{q}}}{\omega_1(\mathbf{q})} + \frac{\varepsilon_{\mathbf{q}^+} \nu_{\mathbf{q}}}{\omega_2(\mathbf{q})} \right\}. \quad (19)$$

The temperature reduction in the magnetization is given by

$$\delta S(T) = \frac{1}{2N} \sum_{\mathbf{q}} \left\{ \frac{\varepsilon_{\mathbf{q}^-} \nu_{\mathbf{q}}}{\omega_1(\mathbf{q})} n_{1\mathbf{q}} + \frac{\varepsilon_{\mathbf{q}^+} \nu_{\mathbf{q}}}{\omega_2(\mathbf{q})} n_{2\mathbf{q}} \right\}, \quad (20)$$

where

$$n_{i\mathbf{q}} = \{ \exp\{\omega_i(\mathbf{q})/T\} - 1 \}^{-1}, \quad i = 1, 2.$$

These equations will be used to study the temperature dependence of the band magnetization in a quantizing magnetic field.

3. QUANTUM TEMPERATURE FLUCTUATIONS

Landau quantization takes place in a strong magnetic field.¹⁶ In order to find the thermodynamic potential of the electrons and holes, whose spectrum is given by Eq. (3), it is sufficient to transform to the Landau representation and sum over the quantum numbers of this representation.^{17,18} Then the fluctuating part of the magnetization from the collectivized electrons is given by

$$M_{\sim}^e = - \frac{T \sqrt{\hbar \omega_c^e(m_e)}^{3/2}}{2 \pi \hbar^3 H} \sum_{\sigma} \tilde{\mu}_{e\sigma} \times \sum_{n=1}^{\infty} \frac{(-1)^n}{\sqrt{n}} \frac{\sin\{2\pi n \tilde{\mu}_{e\sigma} / \hbar \omega_c^e + \phi_{e\sigma}\}}{\sin h\{2\pi^2 n T / \hbar \omega_c^e\}}, \quad (21)$$

where

$$\phi_{e\sigma} = 2\pi\sigma m_e / m_0 - \pi/4,$$

m_0 is the free-electron mass, and $\omega_c^e = eH/m_e c$ is the cyclotron frequency for the conduction electrons. The important feature of this expression for M_{\sim}^e is that, instead of a chemical potential that depends weakly on the temperature and magnetic field in the ordinary Fermi-liquid case, Eq. (21) includes the renormalized chemical potential

$$\tilde{\mu}_{e\sigma} = \mu + \sigma(2\mu_B H + J_e R \cos \theta), \quad (22)$$

which, because of the term $\propto R \cos \theta$, can vary rather strongly as the temperature and magnetic field are changed, if the s - f -exchange interaction parameter is sizeable. The strong T dependence of $\tilde{\mu}_{e\sigma}$, therefore, lies at the basis of the quantum temperature fluctuation phenomenon in these antiferromagnetic semimetals. Before proceeding to a direct analysis of the quantum temperature fluctuations, we note that the contribution of the holes to the fluctuating part of the magnetization is given by an expression analogous to Eq. (21), with the subscript e for the electrons replaced by h . Then,

$$\tilde{\mu}_{h\sigma} = -\mu + \Delta + \sigma(2\mu_B H + J_h R \cos \theta). \quad (23)$$

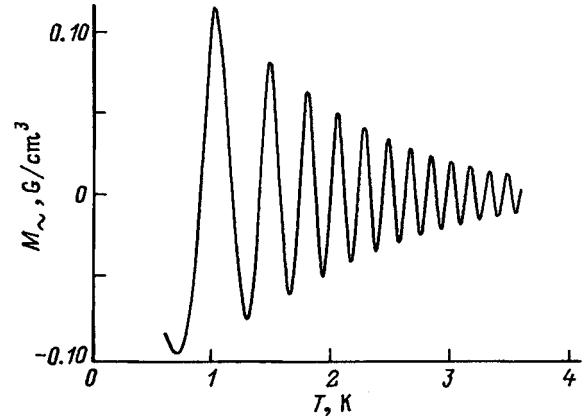


FIG. 1. Quantum temperature fluctuations of an antiferromagnetic semimetal. One electron and one hole subband are populated.

For low current-carrier concentrations and relatively large splitting of the electron- and hole-spin subbands, Fermi quasiparticles lie within the confines of spin subbands with a single spin polarization. This situation occurs when the following inequalities are satisfied:

$$n < \frac{4}{3} \frac{(m_e \Delta_e)^{3/2}}{\pi^2 \hbar^3}, \quad n < \frac{4}{3} \frac{(m_h \Delta_h)^{3/2}}{\pi^2 \hbar^3}, \quad (24)$$

where n is the concentration of electrons (and holes) per unit volume and

$$\Delta_e = \left| \mu_B H + \frac{1}{2} J_e R \cos \theta \right|, \quad \Delta_h = \left| \mu_B H + \frac{1}{2} J_h R \cos \theta \right|. \quad (25)$$

From the condition of electrical neutrality in the main approximation, we obtain

$$\tilde{\mu}_e = \frac{m_h}{m_e + m_h} \Delta_{eh}, \quad \tilde{\mu}_h = \frac{m_e}{m_e + m_h} \Delta_{eh}, \quad \Delta_{eh} = \Delta + \frac{R \cos \theta}{2} (|J_e| + |J_h|) + \mu_B H (\text{sign}(J_e) + \text{sign}(J_h)). \quad (26)$$

The above expressions for the Fermi energies of the electrons and holes determine their strong temperature and field dependences. Here the absolute changes in these quantities depend, in particular, on the ratio of their effective masses. Thus, for example, in the case of heavy holes, for which $m_h \gg m_e$, only the electron Fermi energy can change significantly. In this case, the quantum temperature fluctuations will be determined only by the conduction-electron subsystem.

For concrete calculations, we shall use Eqs. (9), (17)–(20), and (23). Figure 1 shows the results of a numerical calculation of the quantum temperature fluctuations for an antiferromagnetic semimetal with equivalent electron and hole bands. Here the following system parameters were used: $J_e = J_h = 0.2$ eV, $m_e = m_h = m_0$, and $T_N = 10$ K. The concentration of band carriers corresponded to the semimetal case and equalled 0.035 per lattice site. $M_{\sim}(T)$ was calculated for

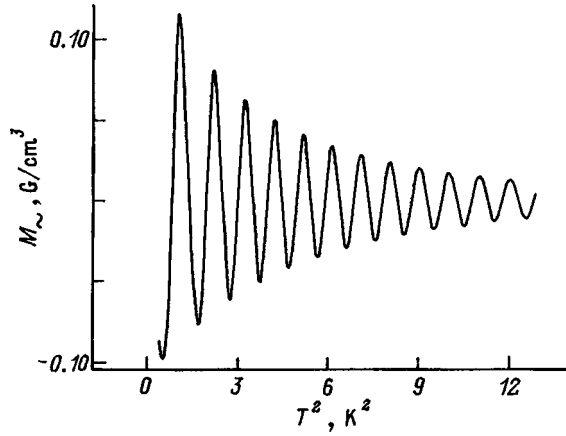


FIG. 2. Quantum temperature fluctuations of an antiferromagnetic semimetal as a function of T^2 .

temperatures $T=0.5\text{--}3.5$ K, where, as noted above, the spin-wave approximation is valid. It is quite clear from Fig. 1 that for these system parameters there are a substantial number of temperature fluctuations.

Let us analyze the results on quantum temperature fluctuations shown in Fig. 1. In the spin-wave approximation the drop in the magnetization owing to temperature is given by

$$\delta S(T) = \left(\frac{b^3}{48\alpha} \right) \left(\frac{1}{\sin \theta} \right) \left(\frac{1}{2K_0\alpha} \right)^{1/2} \left(\frac{T}{S} \right)^2, \quad (27)$$

where b is the magnetic cell parameter in the antiferromagnetic phase and the spin-wave rigidity is

$$\alpha = \frac{1}{6} \left\{ \sum_f I_{0f} \mathbf{R}_f^2 + \sum_g K_{0g} \mathbf{R}_g^2 \right\}. \quad (28)$$

In the nearest-neighbor approximation, where $\alpha = K_0 b^2/8$, we have

$$\delta S(T) = \left(\frac{1}{3 \sin \theta} \right) \left(\frac{T}{K_0 S} \right)^2.$$

These equations show that as the temperature changes, the phase shift in the argument of the sine in Eq. (21) is determined by

$$\begin{aligned} \frac{\delta \tilde{\mu}_e(T)}{\hbar \omega_c^e} &= - \left(\frac{g}{2} \right) \left(\frac{m_{eh}}{m_0} \right) \left(\frac{|J_e| + |J_h|}{4SK_0} \right) \left(\frac{1}{3 \sin \theta} \right) \left(\frac{T}{K_0 S} \right)^2 \\ &= \frac{\delta \tilde{\mu}_h(T)}{\hbar \omega_c^h}, \end{aligned} \quad (29)$$

where m_{eh} is the reduced electron-hole mass, $m_{eh} = m_e m_h / (m_e + m_h)$. Equation (29) yields an important result for practical application of quantum temperature fluctuations. If we construct the part of the magnetization that oscillates with changing temperature as a function of T^2 , then a plot of “damped” but still periodic oscillations is obtained. Figure 2 shows the results of such a construction using the same values as in Fig. 1. Clearly, in the new coordinates (neglecting the drop in amplitude of the oscillations) the curve is indeed periodic in T^2 . Small deviations in this periodicity are re-

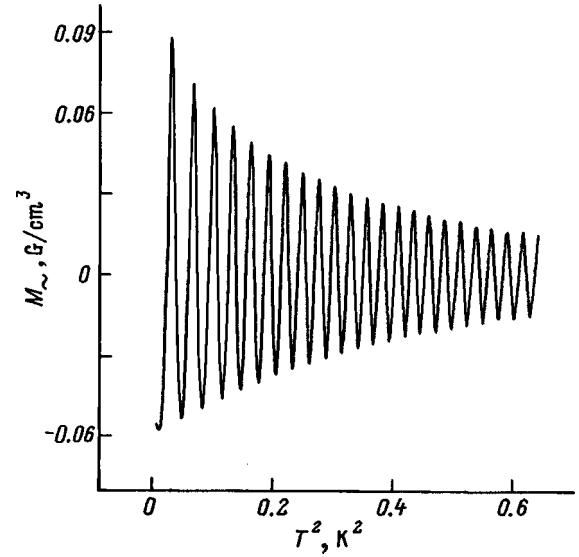


FIG. 3. Quantum temperature fluctuations of a low-temperature antiferromagnetic semimetal as a function of T^2 .

lated to the contribution of the second branch of the spin-wave perturbations and to the presence of Brillouin zone effects which were neglected in Eq. (27).

The equation for the phase shift implies that the period of the oscillations with respect to T^2 is given by

$$P = \left(\frac{2 \sin \theta}{g} \right) \left(\frac{m_0}{m_{eh}} \right) \left(\frac{12SK_0}{|J_e| + |J_h|} \right) \left(\frac{K_0 S}{k_B} \right)^2, \quad (30)$$

where k_B is the Boltzmann constant. This equation can be used to derive an important relationship among the parameters of the electronic structure of this antiferromagnetic semimetal from experimental data on quantum temperature fluctuations (after plotting the fluctuating part of the magnetization in the M_{\sim}, T^2 plane and measuring the period P of the oscillations).

Here we note two other features which are immediately evident from Eq. (30). First, with other conditions the same, the period of the oscillations decreases as K_0^3 when the exchange integral decreases. Given that the temperature range in which the spin-wave approximation is applicable decreases linearly (as the Neel temperature, itself) as K_0 becomes smaller, we conclude that the number of spikes in the quantum temperature fluctuations increases rapidly for antiferromagnetic semimetals with lower Neel temperatures. This feature is illustrated in Fig. 3. In calculating the quantum temperature fluctuation curve shown in this figure, the Neel temperature was taken to be 3 K (instead of 10 K, as in the earlier cases), while all the other characteristic parameters were unchanged.

The second feature is related to the dependence of the period of the quantum temperature fluctuations on the taper of the antiferromagnetic sublattices. As the spin-flip-transition point is approached, the period of the oscillations decreases $\propto \sin \theta$. Then, by measuring the periods P_1 and P_2 of the oscillations for two values of the external magnetic field $H_1 < H_2 < H_c$, it is possible to obtain the field for the spin-flip transition from the simple relation

$$H_c^2 = \frac{(P_1 H_2)^2 - (P_2 H_1)^2}{(P_1 - P_2)(P_1 + P_2)}. \quad (31)$$

A more complicated situation arises in the case where Fermi quasiparticles occupy subbands with opposite polarizations in the spin angular momentum. For example, let electrons occupy both spin subbands, while holes, as before, lie only in the lower spin subband. This occurs when the following conditions are satisfied:

$$\frac{4}{3} \frac{(m_e \Delta_e)^{3/2}}{\pi^2 \hbar^3} < n < \frac{4}{3} \frac{(m_h \Delta_h)^{3/2}}{\pi^2 \hbar^3}, \quad (32)$$

then it is easy to find expressions for the temperature dependences of the Fermi energies for the two electron and one hole bands by solving the equation for electrical neutrality. Calculating the temperature phase shifts in the usual way, we obtain the three periods in T^2 for the oscillations:

$$P_+^e = \left(\frac{2 \sin \theta}{g} \right) \left(\frac{m_0}{m_e} \right) \left(\frac{12SK_0(g_+^e + g_-^e + g_h)}{2g_-^e |J_e| + g^h (|J_e| + |J_h|)} \right) \left(\frac{K_0 S}{k_B} \right)^2,$$

$$P_-^e = \left(\frac{2 \sin \theta}{g} \right) \left(\frac{m_0}{m_e} \right) \left(\frac{12SK_0(g_+^e + g_-^e + g_h)}{2g_+^e |J_e| - g^h (|J_h| - |J_e|)} \right) \left(\frac{K_0 S}{k_B} \right)^2,$$

$$P^h = \left(\frac{2 \sin \theta}{g} \right) \left(\frac{m_0}{m_h} \right) \left(\frac{12SK_0(g_+^e + g_-^e + g_h)}{g_+^e (|J_e| + |J_h|) + g_-^e (|J_h| - |J_e|)} \right) \times \left(\frac{K_0 S}{k_B} \right)^2, \quad (33)$$

where g_+^e and g_-^e are the densities of electronic states on the Fermi surface for the two spin subbands and g^h is the density of hole states on the Fermi surface for $T=0$. When the difference in effective masses is relatively small, the amplitudes of the oscillations will be of the same order of magnitude for the electrons and holes. In this case, the resulting magnetization M_- is obtained by adding three periodic functions and, therefore, is generally periodic in T^2 . This is illustrated in Fig. 4. In these calculations the effective masses of the electrons and holes were chosen to be different, with $m_e = m_0/2$ and $m_h = m_0$. The concentration of electrons (and holes) per lattice site was chosen to be 0.06. The remaining parameters were the same as in the calculation of the quantum temperature fluctuations shown in Fig. 3. Curves *a-c* are quantum temperature fluctuations that are periodic with respect to T^2 and originate from the two electron- and one hole-spin subbands. The total fluctuating part of the magnetization is shown in the lowest curve of this figure. It is this form of quantum temperature fluctuations that is observed experimentally. Thus, the method proposed here for analyzing the experimental data and based on the above results, is of special importance. In fact, plotting the M_- curve as a function of T^2 and then Fourier analyzing it makes it possible to isolate the periodic contributions from quasiparticles in the different spin subbands. After determining the periods of the oscillations for the different components and comparing them with the values obtained from Eq. (33), we obtain numerical relations for the electronic structure parameters.

Analogous results can be obtained easily even when both electrons and holes occupy both spin subbands. Then the

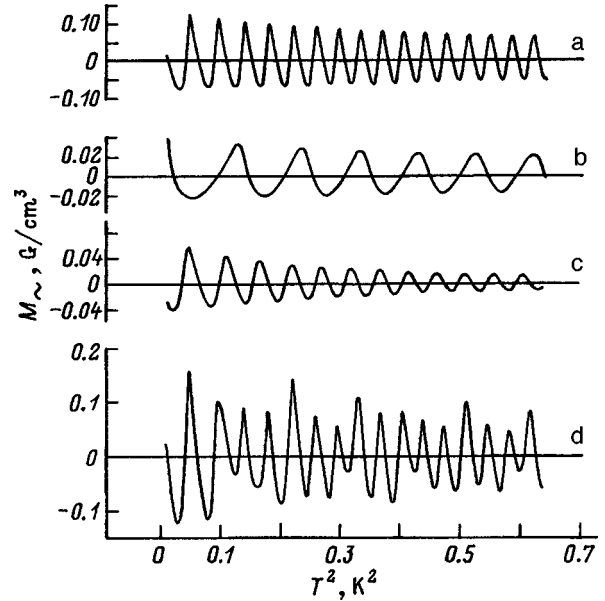


FIG. 4. Quantum temperature fluctuations of an antiferromagnetic semimetal. Two electron subbands and one hole subband are occupied. (a-c) Contributions of the electron and hole subbands; (d) total fluctuating part of the magnetization.

oscillating magnetization is made up, in general, of four functions that are periodic in T^2 . The proposed method for analyzing the experimental data is effective in this case, as well. We do not give concrete expressions for the four periods of the oscillations here in order to save space.

In conclusion, we summarize the main results of this study. The main conclusion of this work is a proof of the possible existence of a new type of oscillations, quantum temperature fluctuations, in antiferromagnetic semimetals. The conditions for a distinct experimental observation of quantum temperature fluctuations are: (a) relatively low Neel temperatures ($T_n \leq 1-10$ K); (b) the existence of an exchange coupling between the spin angular momenta of the current carriers and localized electrons; and, (c) samples of sufficiently good quality. At present, choosing solid-state compounds which satisfy these requirements presents no difficulties. As an example, we note the already-mentioned cerium monopnictides. These compensated semimetals have antiferromagnetic order with a Neel temperature $T_N \sim 5-7$ K. The high quality of the single crystals is confirmed, in particular, by the intense signals from the de Haas-van Alphen effect¹⁹ in CeAs. Given that the order of magnitude of the amplitude of the quantum temperature fluctuations is the same as that of the de Haas-van Alphen effect, we may hope for good observations of quantum temperature fluctuations in these antiferromagnetic materials.

It should be noted that studies of quantum temperature fluctuations are of interest, both from the standpoint of observing the effect itself and in order to obtain additional information on the electronic structure. The predicted contributions from the individual spin subbands to the quantum temperature fluctuations periodic in T^2 provide a large information input to studies on quantum temperature fluctuations, which is, to a substantial extent, similar in its possibilities to

the usual de Haas-van Alphen effect. It is important that the period of the quantum temperature fluctuations, as opposed to the period of the de Haas-van Alphen oscillations, is easily changed by an external magnetic field. This offers additional experimental means for testing the electronic structure with the aid of quantum temperature fluctuations.

This work was supported by the Russian Fund for Fundamental Research (Grant No. 96-02-16075) and by the Krasnoyarsk Regional Science Foundation (Grant No. 6F0150).

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Translated by D. H. McNeill