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Magnetism and superconductivity in heavy-fermion superconductors with a partially gapped Fermi surface

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Abstract. A large-degeneracy model is applied to study antiferromagnetic order and superconductivity in heavy-fermion superconductors with a partially gapped Fermi surface. An antiferromagnetic order opens a gap on those parts of the Fermi surface where nesting takes place. Below the Néel temperature, antiferromagnetic moments of f atoms are anomalously small ($\sim 10^{-2}\,\mu_B$). The rest of the Fermi surface becomes gapped due to superconductivity stimulated by the long-range antiferromagnetic order. The superconducting gap is anisotropic and vanishes on lines. A satisfactory agreement with experimental data for URu_2Si_2 is obtained.

1. Introduction

At present there are a lot of experimental data on a profound relation between magnetism and superconductivity in heavy-fermion compounds such as URu_2Si_2, UPt_3, $CeCu_2Si_2$ and UBe_{13} (see reviews [1–5] and references therein). In these compounds the superconductivity follows an antiferromagnetic transition. Direct evidence for an antiferromagnetic order has been given by neutron-scattering measurements in URu_2Si_2 [6, 7] and UPt_3 (see the review paper of Aeppli *et al* [8] and references therein), x-ray magnetic scattering in URu_2Si_2 [9], muon-spin-relaxation measurements [10] and nuclear quadrupole resonance [11] in $CeCu_2Si_2$. While in URu_2Si_2 the antiferromagnetic transition is accompanied by an anomaly in specific heat [12], no anomaly in specific heat at $T = T_N$ has been observed in UPt_3, $CeCu_2Si_2$ and UBe_{13}. Another puzzle of these compounds is in their very small antiferromagnetic moments ($\sim 10^{-2}\,\mu_B$). Moreover, in the superconducting phase, the specific heat demonstrates a power-law temperature dependence contrary to the conventional Bardeen–Cooper–Schrieffer (BCS) theory that predicts a simple exponential law. This fact means that the superconducting gap is anisotropic and vanishes on lines or points on the Fermi surface. A wide experimental study of the superconducting state has led to the conclusion that a superconducting coupling arises between electrons with enhanced mass. The mass enhancement is a result of the Kondo effect, which at temperatures below the Kondo temperature T_K renormalizes the Fermi surface. Unusual properties of the superconducting phase in these compounds have stimulated the search for a non-phonon mechanism of superconductivity (a detailed list of references on the problem may be found in [5] for example).

In previous papers [13–15] I have proposed a microscopic model that may be applied to study magnetism and superconductivity of heavy-fermion compounds. Using the model treated by the mean-field approach, I have found that an antiferromagnetic order arising in the heavy-fermion state at the Néel temperature T_N is characterized by small antiferromagnetic moments even at zero temperature. The magnitude of these moments is proportional to the ratio T_N/T_0 where T_0 is the low-temperature Kondo scale. In the case $T_N \sim 0.1T_0$ the moments are of order $10^{-2}\,\mu_B$, in agreement with experimental data. In [14, 15] I have assumed that nesting takes place on the whole Fermi surface. This assumption results in a non-zero spin-density-wave (SDW) gap on the whole Fermi surface for the half-filled band. However the heavy-fermion compound URu_2Si_2 clearly demonstrates that an SDW transition opens a gap over a portion of the Fermi surface [12]. In the present paper I take this fact into account and consider a model with a partially gapped Fermi surface. It enables us to make a more accurate estimation of the antiferromagnetic moments. For URu_2Si_2 my theoretical result 0.035 μ_B is in good agreement with experimental data 0.04 μ_B [6, 7]. Moreover, I calculate the jump in the electronic specific heat at the Néel temperature T_N and find that the jump is proportional to the portion of the gapped part of the Fermi surface. If the portion is small, then the jump is also small. This result gives a qualitative explanation of the absence of an anomaly at T_N in the specific heat of some heavy-fermion superconductors.

The next problem that I shall be concerned with is a study of the superconducting state arising in the antiferromagnetic heavy-fermion state ($T_c < T_N < T_K$). In my previous paper [14] I have shown that a long-range antiferromagnetic order formed in the heavy-fermion state can change an exchange interaction between conduction electrons and localized f electrons in such a way that this exchange interaction becomes attractive for heavy quasiparticles in lower antiferromagnetic bands. In the present paper I shall show that this mechanism of superconductivity leads to a superconducting state with an anisotropic gap. This gap is equal to zero along lines on the Fermi surface.

2. Mean-field approach

I shall study magnetic and superconducting properties of heavy-fermion compounds by using the following Hamiltonian [13–15]:

$$H = H_0 + H_m + H_{cf} \tag{2.1}$$

where H_0 is either the Coqblin–Schrieffer Hamiltonian [16]

$$H_0 = \sum_{\sigma k} \epsilon_k c^+_{\sigma k} c_{\sigma k} - \frac{J}{N} \sum_{\sigma\eta i} f^+_{\sigma i} c_{\sigma i} c^+_{\eta i} f_{\eta i} \tag{2.2}$$

or the slave-boson Hamiltonian [17–19]

$$H_0 = \sum_{\sigma k} \epsilon_k c^+_{\sigma k} c_{\sigma k} + \sum_{\sigma i} \epsilon_f f^+_{\sigma i} f_{\sigma i} - N^{-1/2} \sum_{\sigma i} V(b_i f^+_{\sigma i} c_{\sigma i} + \mathrm{HC}). \tag{2.3}$$

Here the pseudospin quantum numbers σ and η run from $-j$ to j, and $N = 2j+1$ is the spin degeneracy. Operators $c^+_{\sigma k}$, $c_{\sigma k}$ and $f^+_{\sigma i}$, $f_{\sigma i}$ are related to conduction electrons with wavevector $\boldsymbol{k}$ and f electrons localized at sites $\boldsymbol{R}_i$. In terms of the slave-boson method the constraints

$$b^+_i b_i + \sum_{\sigma} f^+_{\sigma i} f_{\sigma i} = q_0 N \tag{2.4}$$

are imposed on each site $\boldsymbol{R}_i$. The interaction between c and f electrons described by Hamiltonian (2.2) or (2.3) results in the formation of the heavy-fermion state at temperatures T lower than the Kondo temperature T_K [17–19].

The Hamiltonian

$$H_{\mathrm{m}} = \frac{J_1}{N^3} \sum_i S^z_{\mathrm{c}i} S^z_{\mathrm{f}i} \tag{2.5}$$

describes an anisotropic local exchange interaction where the spin operators S^z are

$$S^z_{\mathrm{f}i} = \sum_\sigma \sigma f^+_{\sigma i} f_{\sigma i} \qquad S^z_{\mathrm{c}i} = \sum_\sigma \sigma c^+_{\sigma i} c_{\sigma i}. \tag{2.6}$$

Below, this interaction is supposed to be antiferromagnetic ($J_1 > 0$). Because in the limit $N \gg 1$ the numbers of c and f electrons per orbital (n_{c} and n_{f} correspondingly) are of order O(1), the local moments $\langle S^z_{\mathrm{f}i}\rangle$ and $\langle S^z_{\mathrm{c}i}\rangle$ are of order $\mathrm{O}(N^2)$. Owing to the factor N^{-3}, the energy of magnetic interaction (2.5) is of order $\mathrm{O}(N)$, while the Hamiltonian (2.2) (or (2.3)) gives a contribution of order O(1) to the energy of Ruderman–Kittel–Kasuya–Yoshida (RKKY) interactions. Therefore, in the framework of the model (2.1) at $N \gg 1$, it is the interaction (2.5) that is responsible for a magnetic phase transition.

The Hamiltonian

$$H_{\mathrm{cf}} = -J_2 N^{-1} \sum_{\sigma\eta i} f^+_{\sigma i} c^+_{-\sigma i} c_{-\eta i} f_{\eta i} \tag{2.7}$$

describes an additional local exchange interaction between c and f electrons. It has been shown that, at positive J_2 and temperatures T lower than the Néel temperature T_{N} ($T_{\mathrm{N}} < T_{\mathrm{K}}$), interaction (2.7) generates an attraction between heavy quasiparticles [14]. It is this attraction that brings about the superconducting transition ($T_{\mathrm{c}} < T_{\mathrm{N}}$).

Temperature properties of the system described by Hamiltonian (2.1) are determined by the ratio of the parameters J, J_1 and J_2 to each other, the topology of the Fermi surface and the total number of electrons $n_{\mathrm{t}} = n_{\mathrm{c}} + n_{\mathrm{f}}$. Phase diagrams of the model (2.1) have been presented in [15] for some cases. Below, I shall only consider the case $T_{\mathrm{K}} > T_{\mathrm{N}} > T_{\mathrm{c}}$, which is typical for heavy-fermion superconductors.

In the mean-field approach the Hamiltonian (2.1) may be written in the form [14, 15]

$$H_{\mathrm{MF}} = \sum_{\sigma k} \epsilon_k c^+_{\sigma k} c_{\sigma k} + \sum_{\sigma i} [\epsilon^*_{\mathrm{f}i} f^+_{\sigma i} f_{\sigma i} - V(r_{0i} f^+_{\sigma i} c_{\sigma i} + \mathrm{HC}) + \sigma J_1 N^{-1} \\ \times (M_{\mathrm{c}i} f^+_{\sigma i} f_{\sigma i} + M_{\mathrm{f}i} c^+_{\sigma i} c_{\sigma i}) - J_2(\Delta_i f^+_{\sigma i} c^+_{-\sigma i} + \mathrm{HC})]. \tag{2.8}$$

Here the following order parameters are introduced:

$$\begin{aligned} M_{\mathrm{f}i} &= N^{-2} \langle S^z_{\mathrm{f}i}\rangle_{\mathrm{MF}} \qquad & M_{\mathrm{c}i} &= N^{-2} \langle S^z_{\mathrm{c}i}\rangle_{\mathrm{MF}} \\ r_{0i} &= \frac{V}{N\lambda} \sum_\sigma \langle c^+_{\sigma i} f_{\sigma i}\rangle_{\mathrm{MF}} \qquad & \Delta_i &= N^{-1} \sum_\sigma \langle c_{-\sigma i} f_{\sigma i}\rangle_{\mathrm{MF}}. \end{aligned} \tag{2.9}$$

$\lambda \equiv \epsilon^*_f - \epsilon_{\mathrm{f}}$; ϵ^*_{f} is the renormalized energy of the f level and may be determined from the equation

$$\sum_\sigma \langle f^+_{\sigma i} f_{\sigma i}\rangle_{\mathrm{MF}} = N(q_0 - r^2_{0i}) \equiv N n_{\mathrm{f}} \tag{2.10}$$

where $N_{\mathrm{f}} = N n_{\mathrm{f}}$ is the occupancy of the f level. In equations (2.9) and (2.10) the designation $\langle A\rangle_{\mathrm{MF}}$ means

$$\langle A\rangle_{\mathrm{MF}} \equiv Z^{-1}\,\mathrm{Sp}\exp(-\beta H_{\mathrm{MF}})A. \tag{2.11}$$

The free energy of the model under consideration is

$$F_{\mathrm{MF}} = -N \sum_i [J_1 M_{ci} M_{fi} - J_2 \Delta_i^* \Delta_i + (q_0 - r_{0i}^2)\lambda] + \Phi \tag{2.12}$$

where

$$\Phi = -T \ln \mathrm{Sp} \exp[-\beta(H_{\mathrm{MF}} - \mu \hat{N}_t)]$$
$$\hat{N}_t = \sum_{\sigma k} c_{\sigma k}^+ c_{\sigma k} + \sum_{\sigma i} f_{\sigma i}^+ f_{\sigma i}.$$

The chemical potential μ depends on the total number of c and f electrons. A minimization of free energy (2.12) relative to M_{ci}, M_{fi}, r_{0i}, ϵ_f^* and the complex order parameter Δ_i gives equations (2.9) and (2.10).

3. Antiferromagnetic phase transition

In this section I shall study the properties of an antiferromagnetic state in the case when the Néel temperature is lower than the Kondo temperature. For simplicity I consider a simple cubic lattice with f atoms at lattice sites. At temperatures $T < T_K$ the coherent Kondo state is formed. In this state the energy spectrum consists of two hybridized bands [19]

$$\begin{aligned} E_{1k} &= \tfrac{1}{2}\{\epsilon_k + \epsilon_f^* - [(\epsilon_k - \epsilon_f^*)^2 + 4V^2 r_0^2]^{1/2}\} \\ E_{2k} &= \tfrac{1}{2}\{\epsilon_k + \epsilon_f^* + [(\epsilon_k - \epsilon_f^*)^2 + 4V^2 r_0^2]^{1/2}\}. \end{aligned} \tag{3.1}$$

Annihilation operators $b_{\nu\sigma k}$ for quasiparticles in these bands are related to the operators $c_{\sigma k}$ and $f_{\sigma k}$ by the Bogliubov transformation

$$\begin{aligned} &c_{\sigma k} = \sum_{\nu=1,2} u_{\nu k} b_{\nu\sigma k} \qquad f_{\sigma k} = \sum_{\nu=1,2} v_{\nu k} b_{\nu\sigma k} \\ &u_{1k} = v_{2k} = \cos\alpha_k \qquad u_{2k} = -v_{1k} = \sin\alpha_k \\ &\cot\alpha_k = (\epsilon_f^* - E_{1k})/V r_0. \end{aligned} \tag{3.2}$$

At low temperatures quasiparticles with wavevector $\boldsymbol{k}$ near the Fermi surface have the enhanced mass

$$m^*/m_0 = \rho^*/\rho_0 = \cos^{-2}\alpha_F = 1 + n_f/\rho_0 T_0 \gg 1 \tag{3.3}$$

$$T_0 = \epsilon_f^* - \mu = n_c \rho_0^{-1} \exp(-1/\rho_0 J) \tag{3.4}$$

where ρ_0 and m_0 are the density of states and electron mass on the Fermi surface in the conduction band ϵ_k, and $T_0 = \epsilon_f^* - \mu$ is the low-temperature scale. In the case $n_t < 1/2$ the lower band E_{1k} is partially full. The Fermi surface is determined by the equation

$$E_{1k} = \mu. \tag{3.5}$$

Let us suppose that a portion (ν) of the Fermi surface satisfies the nesting condition

$$E_{1k} - \mu = \mu - E_{1k-Q} \tag{3.6}$$

for wavevectors $\boldsymbol{Q} = (\pm\pi, \pm\pi, \pm\pi)$. If $\nu = 1$, then nesting takes place on the whole Fermi surface. If ν is not too small, then the system under consideration is unstable against antiferromagnetic ordering with the wavevector $\boldsymbol{Q}$. At T below the Néel temperature T_N an SDW arises:

$$M_{f(c)i} = M_{f(c)} \cos(\boldsymbol{Q}\boldsymbol{R}_i). \tag{3.7}$$

According to (3.7) the local magnetic moment M_{fi} changes its sign from site to site. The Néel temperature T_N is determined by the equation [14]

$$[1 + J_1 N^{-3} F(\boldsymbol{Q})]^2 = J_1^2 N^{-6} \chi_f(\boldsymbol{Q}) \chi_c(\boldsymbol{Q}) \tag{3.8}$$

where

$$\begin{aligned} \chi_{f(c)}(\boldsymbol{Q}) &= \beta \langle\langle S^z_{f(c)}(\boldsymbol{Q}) S^z_{f(c)}(-\boldsymbol{Q}) \rangle\rangle_{MF} \\ F(\boldsymbol{Q}) &= \beta \langle\langle S^z_f(\boldsymbol{Q}) S^z_c(-\boldsymbol{Q}) \rangle\rangle_{MF}. \end{aligned} \tag{3.9}$$

In the case $T_N \ll T_0$ the correlation functions (3.9) may be found by assuming that the main contribution is given by those parts of the Fermi surface where nesting (3.6) takes place. Thus one obtains

$$\begin{aligned} \chi_c(\boldsymbol{Q}) &= N^3 \alpha \rho_0 [(\nu m_0/m^*) \ln(T_0/T) + A] \\ \chi_f(\boldsymbol{Q}) &= N^3 \alpha \rho_0 [(\nu m^*/m_0) \ln(T_0/T) + A'] \\ F(\boldsymbol{Q}) &= N^3 \alpha \rho_0 [\nu \ln(T_0/T) + A'']. \end{aligned} \tag{3.10}$$

The parameter A is related to the susceptibility of non-interacting electrons in the band $\epsilon_{\boldsymbol{k}}$: $\chi_{0c} \approx N^3 \alpha \rho_0 A$. The number parameter α is

$$\alpha = N^{-3} \sum_\sigma \sigma^2 = j(j+1)/3N^2. \tag{3.11}$$

If the parameter ν is not too small and $\nu \ln(T_0/T_N) \gg 1$, then the Néel temperature T_N determined from (3.8) is equal to

$$T_N = T_0 \exp[-T_0/(A\alpha^2 n_f \rho_0 J_1^2 \nu)]. \tag{3.12}$$

Denoting $T_{N0} = T_N(\nu = 1)$, equation (3.12) may be written in the form

$$T_{N0} = T_N^\nu T_0^{1-\nu}. \tag{3.13}$$

Now I shall calculate the jump of the specific heat at T_N and the temperature dependence of the antiferromagnetic moment (M_f) of f atoms at T near T_N. With that end in view, I expand the free energy (2.12) in M_f and M_c and keep terms up to order $O(M^4)$ inclusive. The free energy (2.12) per f atom is given by

$$\begin{aligned} f = f_0 - N J_1 M_c M_f - \tfrac{1}{2} N^{-2} J_1^2 \chi_f(\boldsymbol{Q}) M_c^2 - \tfrac{1}{2} N^{-2} J_1^2 \chi_c(\boldsymbol{Q}) M_f^2 - N^{-2} J_1^2 F(\boldsymbol{Q}) M_c M_f \\ + (\nu B \alpha_4 \rho_0 m^* J_1^4 N/32 T^2 m_0)[M_c + (m_0/m^*) M_f]^4 \end{aligned} \tag{3.14}$$

where

$$\alpha_4 \equiv N^{-5}\sum_{\sigma}\sigma^4 \qquad B \equiv \int_0^{\infty} \frac{\sinh x\,dx}{x\cosh^3 x} \approx 0.85. \tag{3.15}$$

When calculating the term of order $O(M^4)$ I have neglected the contribution of those parts of the Fermi surface where nesting (3.6) does not take place. For the case $T_N \ll T_0$ the effect of antiferromagnetic order on the parameters r_0 and ϵ_f^* may be neglected. Then the moments M_f and M_c may be found by minimizing the free energy (3.14) relative to these moments. Assuming

$$N^{-3}J_1 F(Q) \approx \alpha\nu\rho_0 J_1 \ln(T_0/T_N) \ll 1 \tag{3.16}$$

I obtain

$$\begin{aligned} M_f(T) &= M_f(0)(8\alpha\tau/B\alpha_4)^{1/2} \\ M_c(T) &= -T_N J_1^{-1}(8\alpha\tau/B\alpha_4)^{1/2} \\ M_f(0) &= \alpha\nu n_f(T_N/T_0)\ln(T_0/T_N) \end{aligned} \tag{3.17}$$

where $\tau \equiv 1 - T/T_N$. It should be noted that at $J_1 \gg T_0$ the antiferromagnetic moment M_f of an f ion is much larger than the amplitude (M_c) of the SDW formed by c electrons. At zero temperature one obtains $M_f(T=0) = M_f(0)$ and $M_c(T=0) = -T_N/J_1$ [14, 15]. According to (2.9) at $T = 0$ the total antiferromagnetic moment of f ions is equal to

$$M_a = g_j\mu_B|\langle S_f^z\rangle| = g_j\mu_B N^2 M_f(0) = [j(j+1)/3N]g_j\mu_B N_f\nu(T_N/T_0)\ln(T_0/T_N) \tag{3.18}$$

where g_j is the gyromagnetic factor, and μ_B is the Bohr magneton. Substituting (3.17) into (3.14) one obtains the free energy per f ion

$$f = f_0 - 2\alpha^2 N_f\nu T_N^2\tau^2/B\alpha_4 T_0. \tag{3.19}$$

This equation enables us to calculate the jump of the specific heat per f atom at the Néel temperature:

$$\delta C = \frac{4\alpha^2 N_f\nu T_N k_B}{B\alpha_4 T_0} = \left(\frac{12\alpha^2}{B\alpha_4\pi^2}\right)\nu\gamma T_N \tag{3.20}$$

where $\gamma = \pi^2 N_f k_B/3T_0$ is the Sommerfeld coefficient of the electronic specific heat, and k_B is the Boltzmann constant. Using (3.11) and (3.15) at $j = 1/2$ one obtains

$$\delta C/\gamma T_N = 1.43\nu. \tag{3.21}$$

It is interesting to note that the ratio $\delta C/M_a$ does not depend on the f occupancy N_f and parameter ν. At $j = 1/2$ one finds

$$p = \mu_B\delta C/k_B M_a = 19/\ln(T_0/T_N). \tag{3.22}$$

This equation shows that the quantity p depends weakly on the ratio T_0/T_N.

The antiferromagnetic order with the wavevector $Q = (\pm\pi, \pm\pi, \pm\pi)$ leads to a doubling of the unit cell. The first Brillouin zone is reduced by a factor of two correspondingly. In the antiferromagnetic state, $T < T_N$, the mean-field Hamiltonian (2.8) may be written as

$$H = \sum_{\sigma k} \begin{vmatrix} b^+_{1\sigma k} \\ b^+_{1\sigma p} \\ b^+_{2\sigma k} \\ b^+_{2\sigma p} \end{vmatrix} \begin{vmatrix} E_{1k} & A^{11}_{\sigma k} & 0 & A^{12}_{\sigma k} \\ A^{11}_{\sigma k} & E_{1p} & A^{21}_{\sigma k} & 0 \\ 0 & A^{21}_{\sigma k} & E_{2k} & A^{22}_{\sigma k} \\ A^{12}_{\sigma k} & 0 & A^{22}_{\sigma k} & E_{2p} \end{vmatrix} \begin{vmatrix} b_{1\sigma k} \\ b_{1\sigma p} \\ b_{2\sigma k} \\ b_{2\sigma p} \end{vmatrix} \tag{3.23}$$

with

$$A^{\nu\mu}_{\sigma k} = (\sigma/N) J_1 (M_c v_{\nu k} v_{\mu p} + M_f u_{\nu k} u_{\mu p}) \tag{3.24}$$

where $\boldsymbol{k}$ runs over the reduced Brillouin zone, $\boldsymbol{p} = \boldsymbol{k} - \boldsymbol{Q}$. This Hamiltonian may be diagonalized by using the perturbation theory with respect to the parameter $A^{12}_{\sigma k}/(E_{2k} - E_{1k})$. I find that the energy spectrum consists of four families of twofold degenerate bands $\mathcal{E}_{\eta\sigma k}$ [14, 15]:

$$\begin{aligned} \mathcal{E}_{1k\sigma} &= \tfrac{1}{2}\{E_{1p} + E_{1k} - [(E_{1p} - E_{1k})^2 + 4(A^{11}_{\sigma k})^2]^{1/2}\} \\ \mathcal{E}_{2k\sigma} &= \tfrac{1}{2}\{E_{1p} + E_{1k} + [(E_{1p} - E_{1k})^2 + 4(A^{11}_{\sigma k})^2]^{1/2}\} \\ \mathcal{E}_{3k\sigma} &= \tfrac{1}{2}\{E_{2p} + E_{2k} - [(E_{2p} - E_{2k})^2 + 4(A^{22}_{\sigma k})^2]^{1/2}\} \\ \mathcal{E}_{4k\sigma} &= \tfrac{1}{2}\{E_{2p} + E_{2k} + [(E_{2p} - E_{2k})^2 + 4(A^{22}_{\sigma k})^2]^{1/2}\}. \end{aligned} \tag{3.25}$$

If the total number (n_t) of c and f electrons is smaller than 0.5, then the lower band $\mathcal{E}_{1\sigma k}$ is partially full. An SDW gap is open due to the long-range antiferromagnetic order on those parts of the Fermi surface $(E_{1k} = \mu)$ where the nesting (3.6) takes place. This gap is equal to $2|A^{11}_{\sigma k}| \approx 2|\sigma J_1(M_c - m_0 M_f/m^*)/N|$. The portion of the gapped Fermi surface is approximately equal to ν. The rest of the Fermi surface remains ungapped. In the antiferromagnetic state the renormalized Fermi surface is determined by the equation

$$\mathcal{E}_{1\sigma k} = \mu. \tag{3.26}$$

According to (3.20) the jump δC at T_N is proportional to the portion (ν) of the gapped Fermi surface. The lower ν, the lower is δC. This fact may be the reason for the lack of an anomaly in the specific heat at T_N in such heavy-fermion compounds as UPt_3, UBe_{13} and $CeCu_2Si_2$.

4. Antiferromagnetic state of URu_2Si_2

In this section I shall analyse in the framework of the theory an antiferromagnetic state of the heavy-fermion compound URu_2Si_2. This compound has the body-centred tetragonal $ThCr_2Si_2$-type crystal structure. An antiferromagnetic order arises at $T_N = 17.5$ [12]. Figure 1 shows the antiferromagnetic structure of URu_2Si_2 obtained by using neutron-scattering measurements [6]. The magnetic moments of the U atom are directed along the tetragonal c axis. The lattice translational vectors of the crystal structure considered are

$$\boldsymbol{a}_1 = \tfrac{1}{2}(a, a, -c) \qquad \boldsymbol{a}_2 = \tfrac{1}{2}(-a, a, c) \qquad \boldsymbol{a}_3 = \tfrac{1}{2}(a, -a, c). \tag{4.1}$$

A primitive unit cell based on these vectors contain one U atom. The corresponding reciprocal vectors are

$$g_1 = 2\pi(a^{-1}, a^{-1}, 0) \qquad g_2 = 2\pi(0, a^{-1}, c^{-1}) \qquad g_3 = 2\pi(a^{-1}, 0, c^{-1}). \tag{4.2}$$

Introducing eight equivalent vectors

$$Q = \pm\tfrac{1}{2}g_1 \pm \tfrac{1}{2}g_2 \pm \tfrac{1}{2}g_3 \tag{4.3}$$

it is easy to show that an SDW

$$M_i = M\cos(QR_i) \tag{4.4}$$

has the antiferromagnetic structure represented in figure 1. The antiferromagnetic order with the wavevector Q leads to a doubling of the unit cell. At $T < T_N$ the unit cell is shown in figure 1. The first Brillouin zone is reduced by a factor of two correspondingly. The initial first Brillouin zone looks like a truncated octahedron. The reduced Brillouin zone is a rectangular prism with sides $2\pi/a$, $2\pi/a$ and $2\pi/c$ inscribed into the truncated octahedron. The reciprocal vectors of the antiferromagnetic structure are

$$\begin{aligned} g_1^* &= \tfrac{1}{2}(g_1 - g_2 + g_3) = (2\pi/a)x \\ g_2^* &= \tfrac{1}{2}(g_1 + g_2 - g_3) = (2\pi/a)y \\ g_3^* &= \tfrac{1}{2}(-g_1 + g_2 + g_3) = (2\pi/a)z. \end{aligned} \tag{4.5}$$

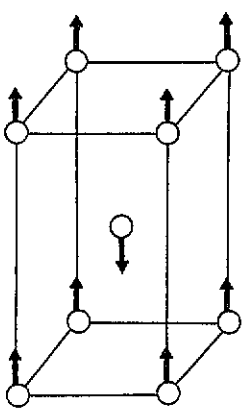

Figure 1. Antiferromagnetic structure of URu_2Si_2 (from [6]).

In order to apply the results obtained above, it is necessary to assume that a part of the Fermi surface of URu_2Si_2 has nesting property (3.6) with respect to the wavevectors (4.3). In other words, I assume that the Fermi surface contains flat parts that are placed near the surface of the reduced Brillouin zone.

Let us compare the theoretical results obtained in section 3 with experimental data for URu_2Si_2.

Maple *et al* [12] have found that the jump of the specific heat in URu_2Si_2 at $T_N = 17.5$ K is $\delta C = 5.82$ J K^{-1} mol^{-1}, $\gamma = 113$ mJ K^{-2} mol^{-1} and, consequently, $\delta C/\gamma T_N = 2.9$.

Moreover, they have estimated the portion of the gapped Fermi surface: $\nu = 0.4$. For $j = 1/2$ and $\nu = 0.4$, equation (3.21) gives the following theoretical estimation: $\delta C_{\rm th}/\gamma T_{\rm N} \approx 0.6$. However, data obtained in [20,21] ($\gamma = 180$ mJ K^{-2} mol^{-1}, $\nu = 2/3$) correspond to $\delta C/\gamma T_{\rm N} \approx 1.8$, while equation (3.21) for $\nu = 2/3$ gives $\delta C_{\rm th}/\gamma T_{\rm N} \approx 0.95$.

The magnitude of the antiferromagnetic moment of U atoms in URu_2Si_2 may be found from equation (3.18). For $j = 1/2$, $T_0 = 70$ K [5], $N_{\rm f} = 1$ and $\nu = 0.4$ [12], one obtains $M_{\rm a} = 0.035\,\mu_{\rm B}$. For $\nu = 2/3$ [21] we have $M_{\rm a} = 0.058\,\mu_{\rm B}$. These theoretical estimations are in satisfactory agreement with neutron-scattering measurements: $M_{\rm a} = (0.03 \pm 0.01)\,\mu_{\rm B}$ [6], $M_{\rm a} = (0.037 \pm 0.005)\,\mu_{\rm B}$ [7]. The x-ray magnetic scattering data $M_{\rm a} = 0.02\,\mu_{\rm B}$ [9] are in slightly worse agreement with the theoretical estimations.

Taking $T_{\rm N} = 17.5$ K and $T_0 = 70$ K, from equation (3.22) one obtains $p_{\rm th} = 14$. For $\delta C = 9.67 \times 10^{-24}$ J K^{-1} per U atom [12] and $M_{\rm a} = 0.037\,\mu_{\rm B}$ [7], the experimental value of the quantity (3.22) is $p \approx 19$. Therefore, the theory is also in satisfactory agreement with experiment relative to the quantity p.

5. Superconducting state

Now I consider peculiarities of a superconducting state arising in the framework of Hamiltonian (2.1). In my previous papers [14, 15] it has been shown that a long-range antiferromagnetic order changes the exchange interaction (2.7) in such a way that this interaction becomes attractive for heavy quasiparticles in the antiferromagnetic bands $\mathcal{E}_{1\sigma k}$. This attraction stimulates a superconducting coupling and brings about the superconducting transition at a critical temperature $T_{\rm c}$. At $T < T_{\rm c}$ the superconducting order parameter Δ_i (2.9) depends on radius vector $\boldsymbol{R}_i$ in the following way [14]:

$$\Delta_i = \Delta \cos(\boldsymbol{Q}\boldsymbol{R}_i) \tag{5.1}$$

where $\boldsymbol{Q}$ is the wavevector of the antiferromagnetic order studied in section 3. In the superconducting state the system under consideration is described by the mean-field Hamiltonian (2.8). In order to diagonalize this Hamiltonian, it is necessary first to diagonalize Hamiltonian (3.23) and find a transformation of the operators $b_{\mu\sigma k}$ to annihilation operators $a_{\eta\sigma k}$ for quasiparticle states in the antiferromagnetic bands $\mathcal{E}_{\eta\sigma k}$. Using the perturbation theory with respect to the off-diagonal elements A^{12} and A^{21} and taking into account terms of order $O(A^{12}_{\sigma k}/(\mathcal{E}_{3\sigma k} - \mathcal{E}_{1\sigma k}))$ I find

$$\begin{aligned} b_{1\sigma k} &= \tau_{1\sigma k} a_{1\sigma k} + \dots \qquad & b_{1\sigma p} &= \tau_{1\sigma p} a_{1\sigma k} + \dots \\ b_{2\sigma k} &= \tau_{2\sigma k} a_{1\sigma k} + \dots \qquad & b_{2\sigma k} &= \tau_{2\sigma p} a_{1\sigma k} + \dots \end{aligned} \tag{5.2}$$

where

$$\begin{aligned} \tau_{1\sigma k} &= \cos\beta \qquad \tau_{1\sigma p} = \sin\beta \\ \tau_{2\sigma k} &= \frac{A^{12}_{\sigma k}\cos\beta \sin(2\gamma)(\mathcal{E}_{3\sigma k} - \mathcal{E}_{4\sigma k})}{2(\mathcal{E}_{1\sigma k} - \mathcal{E}_{4\sigma k})(\mathcal{E}_{1\sigma k} - \mathcal{E}_{3\sigma k})} + A^{21}_{\sigma k}\sin\beta\left(\frac{\cos^2\gamma}{\mathcal{E}_{1\sigma k} - \mathcal{E}_{3\sigma k}} + \frac{\sin^2\gamma}{\mathcal{E}_{1\sigma k} - \mathcal{E}_{4\sigma k}}\right) \\ \tau_{2\sigma p} &= \frac{A^{21}_{\sigma k}\sin\beta \sin(2\gamma)(\mathcal{E}_{3\sigma k} - \mathcal{E}_{4\sigma k})}{2(\mathcal{E}_{1\sigma k} - \mathcal{E}_{4\sigma k})(\mathcal{E}_{1\sigma k} - \mathcal{E}_{3\sigma k})} + A^{12}_{\sigma k}\cos\beta\left(\frac{\cos^2\gamma}{\mathcal{E}_{1\sigma k} - \mathcal{E}_{4\sigma k}} + \frac{\sin^2\gamma}{\mathcal{E}_{1\sigma k} - \mathcal{E}_{3\sigma k}}\right). \end{aligned} \tag{5.3}$$

Here

$$
\begin{aligned}
&\cos\beta = (E_{1p} - \mathcal{E}_{1k\sigma})/D_1 \qquad \sin\beta = -A^{11}_{\sigma k}/D_1 \\
&\cos\gamma = (E_{2p} - \mathcal{E}_{3k\sigma})/D_2 \qquad \sin\gamma = -A^{22}_{\sigma k}/D_2 \\
&D_1 = [(E_{1p} - \mathcal{E}_{1k\sigma})^2 + (A^{11}_{\sigma k})^2]^{1/2} \\
&D_2 = [(E_{2p} - \mathcal{E}_{3k\sigma})^2 + (A^{22}_{\sigma k})^2]^{1/2}.
\end{aligned}
\tag{5.4}
$$

The following important properties may be obtained from equations (5.3) and (5.4):

$$
\begin{aligned}
&\tau_{1,-\sigma,k} = \tau_{1\sigma k} \qquad \tau_{1,-\sigma,p} = -\tau_{1\sigma p} \\
&\tau_{2,-\sigma,k} = \tau_{2\sigma k} \qquad \tau_{2,-\sigma,p} = -\tau_{2\sigma p}.
\end{aligned}
\tag{5.5}
$$

Substituting the Bogoliubov transformations (3.2) and (5.2) into (2.8), one obtains that in the superconducting state the system under consideration is described by the Hamiltonian

$$
H_{\mathrm{SC}} = \sum_{\sigma k} [\mathcal{E}_{1\sigma k} a^+_{1\sigma k} a_{1\sigma k} - \tfrac{1}{2}(\Delta_{\sigma k} a^+_{1\sigma k} a^+_{1,-\sigma,-k} + \mathrm{HC})]
\tag{5.6}
$$

where $\Delta_{\sigma k}$ is an anisotropic superconducting order parameter:

$$
\Delta_{\sigma k} = J_2 \varphi_{\sigma k} \Delta
\tag{5.7}
$$

$$
\varphi_{\sigma k} = \sum_{\mu,\nu=1,2} \phi^{\mu\nu}_{kp} (\tau_{\mu\sigma k} \tau_{\nu,-\sigma,-p} - \tau_{\nu\sigma p} \tau_{\mu,-\sigma,-k})
\tag{5.8}
$$

$$
\phi^{\mu\nu}_{kp} = v_{\mu k} u_{\nu p} - v_{\nu p} u_{\mu k}.
\tag{5.9}
$$

In Hamiltonian (5.6) I omit terms corresponding to the upper antiferromagnetic bands, since at $T < T_c \ll T_N$ these bands are empty and do not participate in superconducting coupling. If wavevectors k and $p = k - Q$ are near the Fermi surface, then the function $\varphi_{\sigma k}$ takes a simpler form [14, 15]

$$
\varphi_{\sigma k} = -2\frac{\sigma}{N} \left(\frac{m_0}{m^*}\right)^{1/2} \frac{J_1(M_f - M_c)\cos(2\beta)}{\mathcal{E}_{3\sigma k} - \mathcal{E}_{1\sigma k}}.
\tag{5.10}
$$

At $T < T_c$ the superconducting gap $|\Delta_{\sigma k}|$ is open over the remaining part of the Fermi surface. The superconducting order parameter Δ is determined by the following equation:

$$
\frac{1}{J_2} = \frac{1}{N} \sum_{\sigma} \int \frac{\mathrm{d}k}{(2\pi)^d} |\varphi_{\sigma k}|^2 \frac{\tanh\{[(\mathcal{E}_{1k\sigma} - \mu)^2 + |\Delta_{\sigma k}|^2]^{1/2}/2T\}}{[(\mathcal{E}_{1\sigma k} - \mu)^2 + |\Delta_{\sigma k}|^2]^{1/2}}.
\tag{5.11}
$$

According to equation (5.7), the k dependence of the superconducting order parameter $\Delta_{\sigma k}$ is determined by the function $\varphi_{\sigma k}$ (5.8). Now I show that $\varphi_{\sigma k}$ is equal to zero along some lines on the Fermi surface. Let us consider an intersection between the renormalized Fermi surface (3.26) and the surface of the reduced Brillouin zone (it is a surface $E_{1k} = E_{1p}$). For k lying on lines of the intersection we have

$$
E_{\nu k} = E_{\nu p} \qquad \mathcal{E}_{1\sigma k} = \mu.
\tag{5.12}
$$

One can prove that for $\boldsymbol{k}$ lying on these lines $\cos(2\beta) = 0$ and, consequently, $\varphi_{\sigma k} = 0$. It means in accordance with (5.7) that the superconducting gap $|\Delta_{\sigma k}|$ vanishes on the lines. It is well known that the existence of lines with zero superconducting gap leads to a T^2 dependence of specific heat at temperatures T lower than T_c [22, 23] while the BCS theory predicts a simple exponential law.

Though the existence of lines of zero gap has been established above for the simple cubic and tetragonal lattices, this result is also valid for lattices with other symmetries (for example, a hexagonal lattice).

If the mechanism of superconductivity considered in the present paper is realized in heavy-fermion superconductors, then it can explain the simple power law observed in the specific heat of these compounds. A good T^2 dependence of the specific heat in the superconducting state has been observed for UPt_3 [24–26] and for URu_2Si_2 [27]. Additional evidence for zeros of the superconducting gap along lines on the Fermi surface has been given by spin–lattice relaxation measurements for UBe_{13} [28], $CeCu_2Si_2$ and UPt_3 [29]. The ultrasonic attenuation measurements in UPt_3 are also consistent with the existence of lines of the zero gap [30].

6. Discussion and conclusion

In the present paper I have discussed the magnetic and superconducting properties of heavy-fermion compounds with the simple cubic and body-centred tetragonal structures. It has been shown that the model (2.1) can explain the anomalously small antiferromagnetic moments ($\sim 10^{-2}\,\mu_B$) observed in heavy-fermion superconductors. For URu_2Si_2 the model gives 0.035 μ_B, in good agreement with experimental data 0.04 μ_B [6, 7]. I have also calculated the jump of the specific heat at the Néel temperature and found satisfactory agreement with experimental data for URu_2Si_2. This is additional evidence in favour of the model proposed. The main assumption used in my calculations is in the hypothesis about the Fermi surface topology. I have assumed that at least a part of the Fermi surface obeys nesting properties. In other words, I have assumed that there are flat parts of the Fermi surface placed near the surface of the reduced Brillouin zone. The commensurate antiferromagnetic transition opens a gap on these parts of the Fermi surface. The rest of the surface remains ungapped in the temperature range $T_c < T < T_N$. Below T_N the long-range antiferromagnetic order changes the character of the exchange interaction (2.7) between conduction electrons and localized f electrons. I have shown that this interaction becomes attractive and generates the superconducting coupling between heavy electrons. The superconducting state formed due to this mechanism is characterized by an anisotropic order parameter. The superconducting gap vanishes along lines on the Fermi surface. Such a character of the gap is also in agreement with experimental data obtained for heavy-fermion superconductors by use of specific heat, spin–lattice relaxation and ultrasonic attenuation measurements [24–30]. Unfortunately, so far the problem of the critical temperature in the framework of the model under consideration remains unsolved. For the purpose of calculating T_c it is necessary to know the $\boldsymbol{k}$ dependence of the energy bands formed in the antiferromagnetic state. This problem demands special consideration.

References

[1] Stewart G R 1984 *Rev. Mod. Phys.* **56** 755

[2] Brandt N B and Moshchalkov V V 1984 *Adv. Phys.* **33** 373
[3] Rauchschwalbe U 1987 *Physica* B+C **147** 1
[4] De Visser A, Menovsky A and France J J M 1987 *Physica* B+C **147** 81
[5] Grewe N and Steglich F 1991 *Handbook on the Physics and Chemistry of Rare Earths* vol 14 ed K A Gschneider Jr and L Eyring (Amsterdam: North-Holland) p 343
[6] Broholm C, Kjems J K, Buyers W J L, Matthews P, Palstra T T M, Menovsky A A and Mydosh J A 1987 *Phys. Rev. Lett.* **58** 1467
[7] Mason T E, Gaulin B D, Garrett J D, Tun Z, Buyers W J L and Isaacs E D 1990 *Phys. Rev. Lett.* **65** 3189
[8] Aeppli G, Broholm C, Bucher E and Bishop D J 1991 *Physica* B **171** 278
[9] Isaacs E D, McWhan D B, Kleiman R N, Bishop D J, Ice G E, Zschack P, Gaulin B D, Mason T E, Garrett J D and Buyers W J L 1990 *Phys. Rev. Lett.* **65** 3185
[10] Uemura Y J, Kossler W J, Yu X H, Schone H E, Kempton J R, Stronach C E, Barth S, Gygax F N, Hitti B, Schenck A, Baines C, Lankford W F, Onuki Y and Komatsubara T 1989 *Phys. Rev.* B **39** 4726
[11] Tien C 1991 *Phys. Rev.* B **43** 83
[12] Maple M B, Chen J W, Dalichaouch Y, Kohara T, Rossel C, Torikachvili M S, McElfresh M W and Thompson J D 1986 *Phys. Rev. Lett.* **56** 185
[13] Goltsev A V 1992 *JETP Lett.* **55** 530
[14] Goltsev A V 1992 *J. Phys.: Condens. Matter* **4** L447
[15] Goltsev A V 1993 *Physica* B submitted
[16] Coqblin B and Schrieffer J R 1969 *Phys. Rev.* **185** 847
[17] Coleman P 1985 *J. Magn. Magn. Mater.* **47&48** 323
[18] Coleman P 1987 *Phys. Rev.* B **35** 5072
[19] Newns D M and Read N 1987 *Adv. Phys.* **36** 799
[20] Palstra T T M, Menovsky A A, van den Berg J, Dirkmaat A J, Kes P H, Nieuwehuys G J and Mydosh J A 1985 *Phys. Rev. Lett.* **55** 2727
[21] Ramires A P, Siegrist T, Palstra T T M, Garrett J D, Bruck E, Menovsky A A and Mydosh J A 1991 *Phys. Rev.* B **44** 5392
[22] Volovik G E and Gorkov L P 1985 *Zh. Eksp. Teor. Fiz.* **88** 1412 (*Sov. Phys.–JETP* **61** 843)
[23] Varma C M 1985 *Comments Solid State Phys.* **11** 221
[24] Franse J J M, Menovsky A, de Visser A, Bredl C D, Gottwick U, Lieke W, Mayer H M, Rauchschwalbe U, Sparn G and Steglich F 1985 *Z. Phys.* B **59** 15
[25] Sulpice A, Gandit P, Chaussy J, Flouquet J, Jaccard D, Lejay P and Tholence J L 1986 *J. Low Temp. Phys.* **62** 39
[26] Fisher R A, Kim S, Woodfield B F, Phillips N E, Taillefer L, Hasselbach K, Flouquet J, Giorgi A L and Smith J L 1989 *Phys. Rev. Lett.* **62** 1411
[27] Schlabiz W, Baumann J, Pollit B, Rauchschwalbe U, Mayer H M, Ahlheim U and Bredl C D 1986 *Z. Phys.* B **62** 171
[28] MacLaughlin D E, Tien C, Clark W G, Lan M D, Fisk Z, Smith J L and Ott H R 1984 *Phys. Rev. Lett.* **53** 1833
[29] Asayama K, Kitaoka Y and Kohori Y 1988 *J. Magn. Magn. Mater.* **76&77** 449
[30] Shivaram B S, Jeong Y H, Rosenbaum T F and Hiks D G 1986 *Phys. Rev. Lett.* **56** 1078