Quasiparticle effective mass in the superconducting phase of heavy-fermion systems

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Quasiparticles with an anomalously large effective mass ($m^*=\gamma m_e$) become superconducting in the heavy-fermion systems. Since the phase transition is a second-order transition, the quasiparticle just below T_c must still have the large m^*. Using a simple model, we show that the m^* $[=(1-\partial\Sigma/\partial\omega)_{\omega=0}m]$ in the superconducting phase decreases with decreasing temperature from T_c. Furthermore, it is predicted that $d\gamma/dT$ at T_c is proportional to an initial slope of a critical magnetic field $-dH_c/dT$.

I. INTRODUCTION

In heavy-fermion systems, quasiparticles with anomalously large effective mass m^* ($=\gamma m_e$) become superconducting.[1] In the normal phase of these systems, the m^* is caused by the scattering of the quasiparticles, and it increases with decreasing temperature. Normally, this large m^* is deduced from the conduction-electron specific heat.

When the temperature passes through T_c, properties of the system change drastically. However, since the phase transition is a second-order transition, it is likely that the quasiparticles just below T_c still have anomalously large m^*. (If the quasiparticle participates in the condensate, its m^* reduces to the free electron mass.) In the superconducting phase, since the specific heat is strongly influenced by the temperature dependence of the order parameter, no information on m^* can be obtained from the specific heat.

Recently, de Haas–van Alphen (dHvA) oscillations have been observed in the vortex state of the superconducting phase as well as the normal phase.[2] It is natural to inquire what occurs in the m^* at $T<T_c$. As the temperature is decreased from T_c, the number of the quasiparticles that participate in the superfluid condensate grows progressively. Since the condensate does not contribute to scattering, the interaction between the quasiparticles will change. This change will suppress the mass enhancement mechanism. Thus, a possible picture is as follows: As the temperature decreases from T_c, the m^* of the quasiparticles decreases progressively. In this paper, we deal with the problem using a simple model.

II. FORMALISM

The heavy-fermion systems are described by the periodic Anderson model. In this paper, for simplicity we consider the model without orbital degeneracy,

$$H=\sum_{\mathbf{k},\sigma}\varepsilon_{\mathbf{k}}c^+_{\mathbf{k},\sigma}c_{\mathbf{k},\sigma}+\varepsilon_f\sum_{\mathbf{k},\sigma}f^+_{\mathbf{k},\sigma}f_{\mathbf{k},\sigma}+V\sum_{\mathbf{k},\sigma}(c^+_{\mathbf{k},\sigma}f_{\mathbf{k},\sigma}+f^+_{\mathbf{k},\sigma}c_{\mathbf{k},\sigma})+U\sum_{\mathbf{k}}\sum_{\mathbf{k}'}\sum_{\mathbf{q}\neq 0}f^+_{\mathbf{k}-\mathbf{q},\uparrow}f^+_{\mathbf{k}'+\mathbf{q},\downarrow}f_{\mathbf{k}',\downarrow}f_{\mathbf{k},\uparrow}\ , \tag{1}$$

where ε_f is an f-electron level.

Above the Kondo temperature ($T>T_K$), this system behaves like a magnetic system, which has itinerant electrons with a conventional mass and well localized f electrons, whereas at $T<T_K$, the conduction electrons and the f electrons are combined into quasiparticles that scatter against one another. The hybridization of the conduction and f electrons yields two new bands with an energy $E^{(\pm)}_{\mathbf{k}}$:[3-5]

$$a_{\mathbf{k},\sigma}=\cos\theta_{\mathbf{k}}c_{\mathbf{k},\sigma}+\sin\theta_{\mathbf{k}}f_{\mathbf{k},\sigma}\ , \tag{2a}$$

$$b_{\mathbf{k},\sigma}=\sin\theta_{\mathbf{k}}c_{\mathbf{k},\sigma}-\cos\theta_{\mathbf{k}}f_{\mathbf{k},\sigma}\ , \tag{2b}$$

where

$$\cot 2\theta_{\mathbf{k}}=\frac{\varepsilon_{\mathbf{k}}-\varepsilon_f}{2V}\ , \tag{2c}$$

$$E^{(\pm)}_k=\frac{\varepsilon_{\mathbf{k}}+\varepsilon_f}{2}\pm\left[\left(\frac{\varepsilon_{\mathbf{k}}-\varepsilon_f}{2}\right)^2+V^2\right]^{1/2}\ . \tag{2d}$$

We assume (1) the Fermi level ε_F falls in the upper or lower bands, and (2) the dominant low-energy excitations occur within the upper band, or within the lower band.[6] Hence, the Cooper pair is composed of two quasiparticles belonging to the upper band, or that belonging to the lower band. Thus, we find, for the upper band,

$$H=\sum_{\mathbf{k},\sigma}E^{(+)}_{\mathbf{k}}a^+_{\mathbf{k},\sigma}a_{\mathbf{k},\sigma}+\sum_{\mathbf{k}}\sum_{\mathbf{k}'}\sum_{\mathbf{q}\neq 0}U_{\mathbf{k},\mathbf{k}-\mathbf{q},\mathbf{k}',\mathbf{k}'+\mathbf{q}}a^+_{\mathbf{k}-\mathbf{q},\uparrow}a^+_{\mathbf{k}'+\mathbf{q},\downarrow}a_{\mathbf{k}',\downarrow}a_{\mathbf{k},\uparrow}\ , \tag{3a}$$

$$U_{\mathbf{k},\mathbf{k}-\mathbf{q},\mathbf{k}',\mathbf{k}'+\mathbf{q}}=U\sin\theta_{\mathbf{k}-\mathbf{q}}\sin\theta_{\mathbf{k}'+\mathbf{q}}\sin\theta_{\mathbf{k}'}\sin\theta_{\mathbf{k}}\ , \tag{3b}$$

and for the lower band,

$$H=\sum_{\mathbf{k},\sigma} E_{\mathbf{k}}^{(-)} b_{\mathbf{k},\sigma}^{+} b_{\mathbf{k},\sigma}+\sum_{\mathbf{k}}\sum_{\mathbf{k}'}\sum_{\mathbf{q}\neq 0} U_{\mathbf{k},\mathbf{k}-\mathbf{q},\mathbf{k}',\mathbf{k}'+\mathbf{q}} b_{\mathbf{k}-\mathbf{q},\uparrow}^{+} b_{\mathbf{k}'+\mathbf{q},\downarrow}^{+} b_{\mathbf{k}',\downarrow} b_{\mathbf{k},\uparrow} \, , \tag{4a}$$

$$U_{\mathbf{k},\mathbf{k}-\mathbf{q},\mathbf{k}',\mathbf{k}'+\mathbf{q}}=U\cos\theta_{\mathbf{k}-\mathbf{q}}\cos\theta_{\mathbf{k}'+\mathbf{q}}\cos\theta_{\mathbf{k}'}\cos\theta_{\mathbf{k}} \, , \tag{4b}$$

where

$$\sin^2\theta_{\mathbf{k}}=\frac{V^2}{V^2+(E_{\mathbf{k}}^{(+)}-\varepsilon_f)^2} \, . \tag{5}$$

Experimental results suggest (1) antiferromagnetic spin fluctuations play an important role,[7] and (2) the pairing is of an unusual kind with a line of zeros of the gap functions on the Fermi level. From these results, it is likely that the attractive force responsible for the pairing is strongly dominated by the spin fluctuations.[8]

Let us obtain gap and self-energy equations for the quasiparticles. We assume (1) the spin-fluctuation interaction is responsible for the pairing of the quasiparticles,[9] and (2) the pairing is a d-wave spin singlet. (Experimentally, there still remain uncertainties in the symmetry type: d-wave spin singlet or p-wave spin triplet. To describe a relevant physics for the effective mass simply, the d-wave spin singlet is appropriate. An extension to the spin-triplet pairing is straightforward.) Although the attractive interaction due to the spin fluctuation depends strongly on the model structure, we assume for simplicity (3) isotropy of the system, (4) electron-hole symmetry with a cutoff frequency ω_c (we set $\varepsilon=0$ at the Fermi level on the upper or lower band), and (5) constant density of states N.

We study a leading-order term. Thus, we find,

$$\Sigma(p)=\frac{1}{\beta}\sum_q\left[-U_{\mathbf{p},\mathbf{p}+\mathbf{q},\mathbf{p},\mathbf{p}+\mathbf{q}}+\frac{1}{\beta}\sum_k U^2_{\mathbf{k},\mathbf{k}+\mathbf{q},\mathbf{p},\mathbf{p}+\mathbf{q}}[G(k+q)G(k)+F^*(k+q)F(k)]\right]G(p+q) \, , \tag{6a}$$

$$\phi(p)=\frac{1}{\beta}\sum_q\left[-U_{\mathbf{p},\mathbf{p}+\mathbf{q},\mathbf{p},\mathbf{p}+\mathbf{q}}+\frac{1}{\beta}\sum_k U^2_{\mathbf{k},\mathbf{k}+\mathbf{q},\mathbf{p},\mathbf{p}+\mathbf{q}}[G(k+q)G(k)+F^*(k+q)F(k)]\right]F(p+q) \, , \tag{6b}$$

where

$$\begin{aligned} G(p)&=-\frac{i\omega_n+\varepsilon_p+\Sigma(-p)}{|i\omega_n-\varepsilon_p-\Sigma(p)||i\omega_n+\varepsilon_p+\Sigma(-p)|-|\phi(p)|^2} \, , \\ F(p)&=-\frac{\phi(p)}{|i\omega_n-\varepsilon_p-\Sigma(p)||i\omega_n+\varepsilon_p+\Sigma(-p)|-|\phi(p)|^2} \, , \end{aligned} \tag{6c}$$

and $p=(i\omega_n,\mathbf{p})$ for fermions and $q=(i\varepsilon_m,\mathbf{q})$ for bosons.

In applying the Bardeen-Cooper-Schrieffer (BCS) theory to the Fermi-liquid theory, one usually makes the problem simpler by treating the mass enhancement process and the formation of the off-diagonal long-range order separately. However, Eqs. (6) say that both processes depend on each other, and that they manifest themselves in a complicated manner as illustrated in Fig. 1: The formation of the superfluid state modifies the pairing interaction between the quasiparticle, and this pairing interaction determines the superfluid state, leading to a feedback effect.[10] The self-consistency scheme beyond the Gor'kov decoupling is needed.[11,12]

Let us study the effective mass m^* $(=[1-\partial\Sigma(\omega)/\partial\omega]_{\omega=0}m)$ at $T<T_c$. From now on, we focus on the behavior of the system near T_c, and obtain the Ginzburg-Landau (GL) theory. The interaction between the quasiparticles, Eqs. (3b) and (4b), depends strongly on the particle momentum. However, the fact that Eq. (3b) and (4b) are written as the product of the different momentum components allows us to treat it simply. We redefine new Green's functions $G'(p)$ and $F'(p)$ by multiplying $G(p)$ and $F(p)$ by a factor with a same momentum: $\sin^2\theta_{\mathbf{p}}$ for the upper band, and $\cos^2\theta_{\mathbf{p}}$ for the lower band. Hence, Eq. (6a) is rewritten for the upper hand,

$$\Sigma(p)=\sin^2\theta_{\mathbf{p}}\frac{1}{\beta}\sum_q\left[-U+U^2\frac{1}{\beta}\sum_k[G'(k+q)G'(k)+F'^*(k+q)F'(k)]\right]G'(p+q) \tag{7}$$

and for the lower band, $\sin^2\theta_{\mathbf{p}}$ must be replaced by $\cos^2\theta_{\mathbf{p}}$.

Normally, $G(p)$ and $F(p)$ are expanded in powers of the order parameter and are integrated along a radial direction as follows:[10]

$$G(\omega_n)=iN\pi\,\mathrm{sgn}(\omega_n)\left[1-\frac{1}{2\omega_n^2}|\Delta(\hat{\mathbf{p}})|^2+\frac{3}{8\omega_n^4}|\Delta(\hat{\mathbf{p}})|^4\right] \, , \tag{8a}$$

$$F(\omega_n)=N\pi\,\mathrm{sgn}(\omega_n)\left[\frac{1}{\omega_n}\Delta(\hat{\mathbf{p}})-\frac{1}{2\omega_n^3}|\Delta(\hat{\mathbf{p}})|^2\Delta(\hat{\mathbf{p}})\right] \, . \tag{8b}$$

$\Delta(\hat{\mathbf{p}})$ $[=\Delta(T)f_\alpha(\Omega)]$ is a renormalized and frequency-averaged d-wave order parameter $Z^{-1}\phi(p)$. $[f_\alpha(\Omega)$ is a normalized basis function in d-wave symmetry. $\hat{\mathbf{p}}$ is a unit vector, and Δ is assumed to depend only on the direction of $\hat{\mathbf{p}}$.]

In this paper, we assume that the cutoff frequency of the spin fluctuation ω_c is small compared with ε_f and V. Thus $\sin^2\theta$'s or $\cos^2\theta$'s in Eq. (7) can be approximated by a value at the Fermi level ($\varepsilon=0$). Corresponding formulas for the $G'(p)$ and $F'(p)$ are given by

$$G'(\omega_n)=iN\pi\,\mathrm{sgn}(\omega_n)\left[1-\frac{1}{2\omega_n^2}|\Delta(\hat{\mathbf{p}})|^2+\frac{3}{8\omega_n^4}|\Delta(\hat{\mathbf{p}})|^4\right]w(\varepsilon_f,V)\,, \tag{9a}$$

$$F'(\omega_n)=N\pi\,\mathrm{sgn}(\omega_n)\left[\frac{1}{\omega_n}\Delta(\hat{\mathbf{p}})-\frac{1}{2\omega_n^3}|\Delta(\hat{\mathbf{p}})|^2\Delta(\hat{\mathbf{p}})\right]w(\varepsilon_f,V)\,, \tag{9b}$$

where parameters in the periodic Anderson model appear in the factor,

$$w(\varepsilon_f,V)=\begin{cases}\dfrac{V^2}{V^2+\varepsilon_f^2} & \text{(the upper band)}\\[2mm] \dfrac{\varepsilon_f^2}{V^2+\varepsilon_f^2} & \text{(the lower band)}\,.\end{cases} \tag{9c}$$

[See Appendix A. If ω_c is not small, extra terms that have complicated the ω_n dependence appear in Eqs. (9a) and (9b). These terms will be discussed in a future paper.]

Since we focus on the ω dependence of $\Sigma(p)$, the spin-fluctuation interaction $U^2\chi_s(\mathbf{q},i\varepsilon_m)$ in Eq. (7) where

$$\chi_s(\mathbf{q},i\varepsilon_m)=\frac{1}{\beta}\sum_{\mathbf{k},n}[G'(\mathbf{k}+\mathbf{q},i\omega_n+i\varepsilon_m)G'(\mathbf{k},i\omega_n)+F'^*(\mathbf{k}+\mathbf{q},i\omega_n+i\varepsilon_m)F'(\mathbf{k},i\omega_n)]\,, \tag{10}$$

is spatially averaged. Substituting Eqs. (9) into it yields the following Ginzburg-Landau expression (Appendix B):

$$\chi_s(\varepsilon_m)=\frac{\pi^2}{2}N^2\left[-D_0(m)k_BT+\frac{D_1(m)}{(2\pi)^2k_BT}|\Delta(T)|^2-\frac{D_2(m)}{(2\pi)^4(k_BT)^3}|\Delta(T)|^4\right]w^2(\varepsilon_f,V)\,, \tag{11a}$$

where

$$D_0(m)=\begin{cases}2X-3|m| & (|m|\le X)\\ -X+|m| & (X\le|m|\le 2X),\end{cases}\quad\left[X=\frac{\omega_c}{2\pi k_BT}\right]. \tag{11b}$$

$$D_1(m)=\begin{cases}2c_2\Psi^{(1)}(\tfrac12+m)+\dfrac{4c_1^*c_1}{m}[\Psi(\tfrac12+m)-\Psi(\tfrac12)] & (m>0)\,,\\ (2c_1^*c_1+2c_2)\Psi^{(1)}(\tfrac12) & (m=0)\,,\\ D_1(-m) & (m<0)\,.\end{cases} \tag{11c}$$

$$D_2(m)=\begin{cases}\dfrac{c_4}{4}\Psi^{(3)}(\tfrac12+m)+\dfrac{(c_1^*c_3+c_1c_3^*)}{m}[\Psi^{(2)}(\tfrac12+m)-\Psi^{(2)}(\tfrac12)]\\ \quad+\dfrac{(c_2^2-2c_1^*c_3-2c_1c_3^*)}{m^2}\Psi^{(1)}(\tfrac12+m)+\dfrac{2(2c_1^*c_3+2c_1c_3^*-c_2^2)}{m^3}[\Psi(\tfrac12+m)-\Psi(\tfrac12)], & (m>0)\,,\\ \dfrac{(3c_4+2c_1^*c_3+2c_1c_3^*+c_2^2)}{12}\Psi^{(3)}(\tfrac12) & (m=0)\,,\\ D_2(-m) & (m<0)\,.\end{cases} \tag{11d}$$

Here Ψ is the digamma function, and $\Psi^{(1)}$, $\Psi^{(2)}$, and $\Psi^{(3)}$ are its derivatives, and

$$c_{2n}=\int|f_\alpha(\Omega)|^{2n}\frac{d\Omega}{4\pi}\,,\qquad c_{2n+1}=\int|f_\alpha(\Omega)|^{2n}f_\alpha(\Omega)\frac{d\Omega}{4\pi}\,. \tag{11e}$$

A Ginzburg-Landau form of the mass enhancement factor $\gamma(T)$ [$=1-\partial\Sigma(\omega)/\partial\omega|_{\omega=0}$] is obtained using Eqs. (7), (9a), and (11a) (Appendix B),

$$\gamma(T)=\gamma(T_c)-2N\omega_cw^4(\varepsilon_f,V)\frac{(NU)^2N}{k_BT_c}g\left[\frac{\omega_c}{\pi k_BT_c}\right]|\Delta(T)|^2\,, \tag{12a}$$

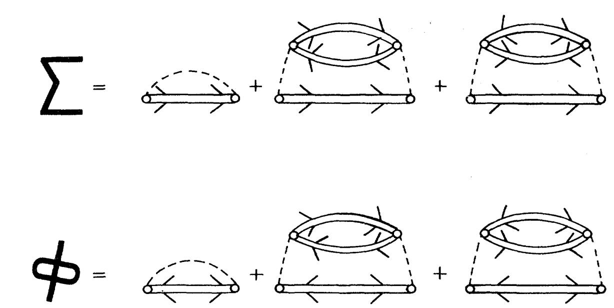

FIG. 1. The self-consistency scheme in Eqs. (6). The lines with two parallel arrows represent the normal Green's function G and that with two opposite arrows the anomalous Green's function F, themselves being under the influence of the self-energy Σ and the order parameter ϕ.

where

$$g(x)=\frac{1}{8}\sum_{n=1}^{x}\left[\frac{a_n}{(n-0.5)^2}-\left[\frac{dD_1(y)}{dy}\right]_{y=n}\right] \quad (12b)$$

($a_n=1.5$ for $n<X/2$, and $a_n=-0.5$ for $n>X/2$). $g(x)$ is a positive monotonically increasing function: As an example, $g(x)$ for a d-wave basis function of one-dimensional representation of D_4,[13]

$$f_\alpha(\Omega)=\hat{\mathbf{k}}_x^2-\hat{\mathbf{k}}_y^2 \quad (c_1=0,\ c_2=\tfrac{4}{15},\ c_3=0,\ c_4=\tfrac{16}{105}),$$

is depicted in Fig. 2.

Equation (12a) says that, as the temperature is decreased from T_c, the quasiparticle effective mass progressively decreases. Figure 3 illustrates this schematically. The solid curve at $T<T_c$ in Fig. 3(b) represents $\gamma(T)$ in Eq. (12a). For reference, $\gamma(T)$ extrapolated naively from $T>T_c$ to $T<T_c$ is depicted as a dotted curve. The prediction in Sec. I is confirmed in this model.[14]

Once the GL-type expression of $\gamma(T)$ is obtained, $d\gamma/dT$ can be combined with temperature dependence of other thermodynamic quantities such as the critical magnetic field H_c. For this, the Ginzburg-Landau free energy must be obtained. The self-consistency mechanism in Eqs. (6) involves the effect beyond the Gor'kov decoupling, which leads to a strong-coupling effect δ in the GL free energy. To the fourth order of Δ, the free energy is

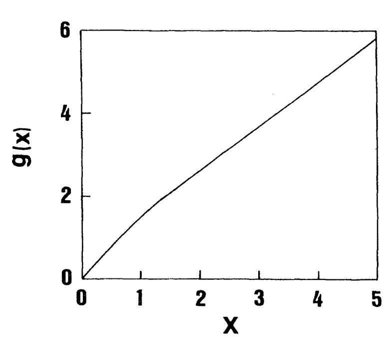

FIG. 2. Plot of $g(x)$ for $k_x^2-k_y^2$ vs x. [$g(x)$ is depicted as if it is a continuous function of x.]

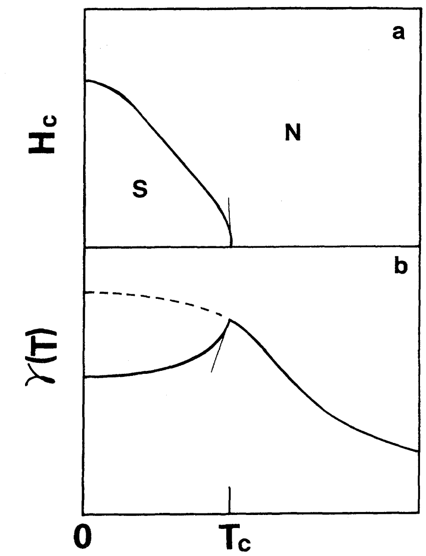

FIG. 3. Schematic picture of the temperature dependence of (a) the critical magnetic field H_c and (b) the mass enhancement factor γ $(=1-\partial\Sigma/\partial\omega|_{\omega=0})$. A solid curve at $T<T_c$ in (b) represents $\gamma(T)$, predicted by Eq. (11a), and a dotted curve at $T<T_c$ represents $\gamma(T)$ extrapolated naively from $T>T_c$ to $T<T_c$. The initial slope of H_c at T_c [a thin straight line in (a)], and that of γ [a thin straight line in (b)], are related by Eq. (14).

given by

$$F_s-F_n=Nw(\varepsilon_f,V)\left[c_2\left[\frac{T}{T_c}-1\right]|\Delta(T)|^2+b_{\rm BCS}(1-\delta)|\Delta(T)|^4\right], \quad (13a)$$

where T_c must be determined using higher-order diagrams in the random-phase approximation (RPA),[15] and

$$b_{\rm BCS}=\frac{7\zeta(3)c_4}{(4\pi k_B T_c)^2}, \quad (13b)$$

$$\delta=\frac{\pi^2}{7\zeta(3)}w^3(\varepsilon_f,V)(NU)^2Nk_BT_c h\left[\frac{\omega_c}{\pi k_B T_c}\right] \quad (13c)$$

[$h(x)$ is a positive monotonically increasing function. For $k_x^2-k_y^2$, it is depicted in Fig. 4. See Appendix C.]

A combination of Eqs. (12a) and (13a) leads to a simple relationship between $d\gamma/dT$ and dH_c/dT at T_c. Substituting $\Delta(T)$, which is obtained by Eq. (13a), into Eqs. (13a) and (12a), we find at T_c,

$$\frac{d\gamma}{dT}=-\frac{2N\omega_c w^{3.5}(\varepsilon_f,V)}{\sqrt{8\pi b_{\rm BCS}(1-\delta)}}\frac{(NU)^2\sqrt{N}}{k_BT_c}g\left[\frac{\omega_c}{\pi k_B T_c}\right]\frac{dH_c}{dT}. \quad (14)$$

This means that the temperature dependence of the m^* at $T<T_c$ manifest itself through the initial slope of the H_c as illustrated in Fig. 3. dH_c/dT at T_c [a thin straight line in Fig. 3(a)] is related to $d\gamma/dT$ at T_c [a thin straight line in Fig. 3(b)] by Eq. (14). This dependence is detect-

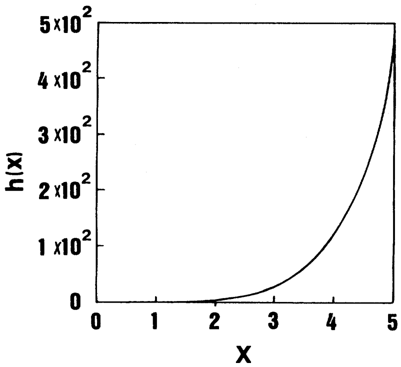

FIG. 4. Plot of $h(x)$ for $k_x^2-k_y^2$ vs x. [$h(x)$ is depicted as if it is a continuous function of x.].

able especially in materials with an enormous initial slope of the upper critical magnetic field H_{c2}.[16] To test Eq. (14), the measurement of the m^* at $T<T_c$ by the dHvA effect is expected especially in materials such as UBe_{13}.[17] (If the spin-triplet pairing is assumed, the coefficient in Eq. (14) is slightly modified, but its sign is not changed.)

III. DISCUSSION

The heavy-fermion superconductors exhibit two remarkable features: (1) The quasiparticles with anomalously large effective mass m^* in the normal phase (several hundred times m_e) become superconducting. (2) In spite of relatively low T_c (<1 K), they show an enormous initial slope of the upper critical magnetic field dH_{c2}/dT. Since the BCS theory is based on the free-fermion picture, the first feature seems strange. To explain the second feature within the BCS theory, unnatural adjustment of the model parameters is needed. In this sense, this superconductivity is unusual.

Experiments such as inelastic neutron scattering suggests that the spin fluctuation plays an important role both for the pairing and the large effective mass, which gives a clue to clear understanding. Thus, an effective interaction Hamiltonian is

$$H_{\text{int}}=\tfrac{1}{2}\sum_{\mathbf{k}}\sum_{\mathbf{k}'} J(\mathbf{k}-\mathbf{k}')\sigma_{\alpha\beta}\sigma_{\gamma\delta}a^{+}_{\mathbf{k},\alpha}a^{+}_{-\mathbf{k},\gamma}a_{-\mathbf{k}',\delta}a_{\mathbf{k}',\beta}\ . \quad (15)$$

$J(\mathbf{q})$ is a quantity determined by the dynamics of the quasiparticles at $T>T_c$, and by that of the Cooper pairs at $T<T_c$. If $J(\mathbf{q})$ is assumed to be a phenomenological parameter, the mass enhancement mechanism and the superconductivity are treated separately. To gain an insight into a relationship between them, it is necessary to begin with a microscopic model, which underlies Eq. (15), and to incorporate the mass enhancement and the superconductivity into a new self-consistency scheme. In this paper, an attempt is made along this line.

This paper predicts decreasing m^* at $T<T_c$. The large m^* comes from (1) the band structure and (2) the many-body effect. The influence of the superconductivity on m^* must appear through the latter process. If this prediction is confirmed experimentally, it is worth examining the validity of the assumptions in this paper using more rigorous theories.

The most important assumptions in this paper are as follows: (1) The quasiparticles made of the conduction electron and the f electron interact with each other through the Coulomb repulsion, and (2) the antiferromagnetic spin fluctuation plays an important role in the quasiparticle interaction. It is worth examining the behavior of m^* at $T<T_c$ using theories that start from the $U=\infty$ periodic Anderson model such as variational theories and slave-boson theories. In contrast to the above assumptions, other assumptions in this paper are made to avoid complications, not affecting the conclusions qualitatively. However, to explain the variety of heavy-fermion compounds, careful calculations without such assumptions will be needed.

ACKNOWLEDGMENT

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APPENDIX A

The self-energy $\Sigma(p)$ in Eq. (6c) is renormalized into a renormalization factor Z. Isotropy of the system allows us to integrate Eq. (6c) along a radial direction, leading to $G(\omega_n)$ and $F(\omega_n)$.

(a) The Ginzburg-Landau form of $G(\omega_n)$, Eqs. (8), is obtained by expanding it in powers of ϕ^2 as follows:

$$G(\omega_n)=N\int_{-\omega_c}^{\omega_c} d\varepsilon[G_0(\omega_n,\varepsilon)-G_2(\omega_n,\varepsilon)|\phi(\hat{\mathbf{p}})|^2+G_4(\omega_n,\varepsilon)|\phi(\hat{\mathbf{p}})|^4]\ , \quad (A1)$$

$$G_0(\omega_n,\varepsilon)=\frac{iZ\omega_n+\varepsilon}{(Z\omega_n)^2+\varepsilon^2}\ ,$$

$$G_2(\omega_n,\varepsilon)=\frac{iZ\omega_n+\varepsilon}{[(Z\omega_n)^2+\varepsilon^2]^2}\ ,$$

$$G_4(\omega_n,\varepsilon)=\frac{iZ\omega_n+\varepsilon}{[(Z\omega_n)^2+\varepsilon^2]^3}\ . \quad (A2)$$

(b) A similar formula for the new Green's function $G'(\omega_n)$ is given by

$$G'(\omega_n)=N\int_{-\omega_c}^{\omega_c} d\varepsilon\, f(\varepsilon)[G_0(\omega_n,\varepsilon)-G_2(\omega_n,\varepsilon)|\phi(\hat{\mathbf{p}})|^2+G_4(\omega_n,\varepsilon)|\phi(\hat{\mathbf{p}})|^4]\ , \quad (A3)$$

where

$$f(\varepsilon)=\begin{cases}\dfrac{V^2}{V^2+(\varepsilon-\varepsilon_f)^2} & \text{(the upper band)}\\[2ex] \dfrac{(\varepsilon-\varepsilon_f)^2}{V^2+(\varepsilon-\varepsilon_f)^2} & \text{(the lower band)}\ .\end{cases} \quad (A4)$$

For a small ω_c, $f(\varepsilon)$ in Eq. (A3) can be approximated by $f(0)$. Substituting

$$\int_{-\omega_c}^{\omega_c} G_0(\omega_n,\varepsilon)d\varepsilon = 2i\tan^{-1}\left[\frac{\omega_c}{Z\omega_n}\right], \tag{A5}$$

$$\int_{-\omega_c}^{\omega_c} G_2(\omega_n,\varepsilon)d\varepsilon \to \frac{i}{(Z\omega_n)^2}\tan^{-1}\left[\frac{\omega_c}{Z\omega_n}\right], \tag{A6}$$

$$\int_{-\omega_c}^{\omega_c} G_4(\omega_n,\varepsilon)d\varepsilon \to \frac{3i}{4(Z\omega_n)^4}\tan^{-1}\left[\frac{\omega_c}{Z\omega_n}\right], \tag{A7}$$

into Eq. (A3), and using $\Delta = Z^{-1}\phi$ yields Eq. (9a). [$\tan^{-1}(1/x)$ is approximated by $\mathrm{sgn}(x)\pi/2$ for a small x.] For the $F'(\omega)$, Eq. (9b) is obtained similarly.

APPENDIX B

(a) Integration along a radial direction in Eq. (10) yields $\chi_s(\mathbf{q},\varepsilon_m)$. Substituting Eqs. (9a) and (9b) into it results in a GL-type expression of $\chi_s(\varepsilon_m)$ as follows:

$$\chi_s(\varepsilon_m) = \frac{\pi^2}{2}N^2w^2(\varepsilon_f,V)\left[-\frac{1}{\beta}\sum_n \mathrm{sgn}[\omega_n(\omega_n+\varepsilon_m)]\right.$$
$$+\frac{1}{\beta}\sum_n \mathrm{sgn}[\omega_n(\omega_n+\varepsilon_m)]\left\{\left[\frac{c_1^*c_1}{\omega_n(\omega_n+\varepsilon_m)}+\frac{c_2}{2}\left[\frac{1}{\omega_n^2}+\frac{1}{(\omega_n+\varepsilon_m)^2}\right]\right]|\Delta(T)|^2\right.$$
$$\left.\left.-\left[\frac{3c_4}{8}\left[\frac{1}{\omega_n^4}+\frac{1}{(\omega_n+\varepsilon_m)^4}\right]+\frac{1}{2}\left[\frac{c_1c_3^*}{\omega_n(\omega_n+\varepsilon_m)^3}+\frac{c_1^*c_3}{\omega_n^3(\omega_n+\varepsilon_m)}\right]+\frac{c_2^2}{4}\frac{1}{\omega_n^2(\omega_n+\varepsilon_m)^2}\right]|\Delta(T)|^4\right\}\right], \tag{B1}$$

where integrating $f_\alpha(\Omega)$ over the direction of $\hat{\mathbf{k}}+\hat{\mathbf{q}}$ or $\hat{\mathbf{k}}$ yields the c_n's.

Since $\chi_s(\varepsilon_m)$ depends strongly on the cutoff energy ω_c, we perform the ω_n summation in the leading-order term of Eq. (B1) in the range $\leq\omega_c$. For a positive m,

$$\sum_{n=-x}^{x-m}\mathrm{sgn}[\omega_n(\omega_n+\omega_m)] = 2X-3|m| \text{ for } |m|\leq X, \text{ and } -X+|m| \text{ for } X\leq|m|\leq 2X \quad \left[X=\frac{\omega_c}{2\pi k_B T}\right], \tag{B2}$$

which leads to the first term in the right-hand side of Eq. (11a). As for the next order terms in Eq. (B1), we let $x\to\infty$ as in the Gor'kov theory. We decompose Eq. (B1) into following partial fractions,

$$p^{(l)}(n,m) = \begin{cases} \dfrac{1}{\omega_n^l}+\dfrac{1}{(\omega_n+\varepsilon_m)^l}, & \text{for even } l \\[2ex] \dfrac{1}{\omega_n^l}-\dfrac{1}{(\omega_n+\varepsilon_m)^l}, & \text{for odd } l \end{cases} \tag{B3}$$

using

$$\frac{1}{\omega_n(\omega_n+\varepsilon_m)} = \frac{1}{\varepsilon_m}\left[\frac{1}{\omega_n}-\frac{1}{(\omega_n+\varepsilon_m)}\right],$$
$$\frac{1}{\omega_n(\omega_n+\varepsilon_m)^3}+\frac{1}{\omega_n^3(\omega_n+\varepsilon_m)} = \frac{2}{\varepsilon_m^3}\left[\frac{1}{\omega_n}-\frac{1}{(\omega_n+\varepsilon_m)}\right]-\frac{1}{\varepsilon_m^2}\left[\frac{1}{\omega_n^2}+\frac{1}{(\omega_n+\varepsilon_m)^2}\right]+\frac{1}{\varepsilon_m}\left[\frac{1}{\omega_n^3}-\frac{1}{(\omega_n+\varepsilon_m)^3}\right],$$
$$\frac{1}{\omega_n^2(\omega_n+\varepsilon_m)^2} = \frac{1}{\varepsilon_m^2}\left[\frac{1}{\omega_n^2}+\frac{1}{(\omega_n+\varepsilon_m)^2}\right]-\frac{2}{\varepsilon_m^3}\left[\frac{1}{\omega_n}-\frac{1}{(\omega_n+\varepsilon_m)}\right]. \tag{B4}$$

Summation over n in the right-hand side of Eq. (B1) for positive m is

$$\sum_{n=-\infty}^{\infty}\mathrm{sgn}[\omega_n(\omega_n+\varepsilon_m)]p^{(l)}(n,m) = \left[\sum_{n=-\infty}^{-m-1}-\sum_{n=-m}^{-1}+\sum_{n=0}^{\infty}\right]p^{(l)}(n,m) = \left[\sum_{n=-\infty}^{\infty}-2\sum_{n=-m}^{-1}\right]p^{(l)}(n,m). \tag{B5}$$

For even l,

$$\left[\sum_{n=-\infty}^{\infty}-2\sum_{n=-m}^{-1}\right]p^{(l)}(n,m) = 4\left[\sum_{n=0}^{\infty}-\sum_{n=0}^{m-1}\right]\frac{1}{\omega_n^l} = 4\sum_{n=m}^{\infty}\frac{1}{\omega_n^l} = \frac{4}{(2\pi k_B T)^l}\frac{(-1)^l}{(l-1)!}\Psi^{(l-1)}(\tfrac{1}{2}+m), \tag{B6}$$

and for odd l,

$$\left[\sum_{n=-\infty}^{\infty} -2\sum_{n=-m}^{-l}\right] p^{(l)}(n,m) = -2\sum_{n=-m}^{-1} p^{(l)}(n,m)$$
$$= -2\left[\sum_{n=-\infty}^{-1} - \sum_{n=-\infty}^{-m-1}\right]\left[\frac{1}{\omega_n^l} - \frac{1}{(\omega_n+\varepsilon_m)^l}\right]$$
$$= -2\left[\sum_{n=-\infty}^{-1} - \sum_{n=-\infty}^{-m-1} - \left[\sum_{n=-\infty}^{-1} + \sum_{n=0}^{m-1}\right] - \sum_{n=0}^{\infty}\right]\frac{1}{\omega_n^l}$$
$$= \frac{-4}{(2\pi k_B T)^l}\frac{(-1)^l}{(l-1)!}\left[\Psi^{(l-1)}\left[\frac{1}{2}+m\right] - \Psi^{(l-1)}\left[\frac{1}{2}\right]\right] . \tag{B7}$$

As for negative m, similar results are obtained. Using Eqs. (B1)–(B7), D_1 and D_2 in Eqs. (11c) and (11d) are obtained.

(b) Integrating Eq. (7) with respect to **p**, and substituting Eqs. (9a) and (11a) into it yield a GL-type expression of $\Sigma(\omega)$. To second of $|\Delta|$, it is given by

$$\Sigma(\omega_m) = \Sigma_0(\omega_m) + 2N\omega_c w^4(\varepsilon_f, V)\frac{N(NU)^2\pi^3}{2\beta}\sum_n \mathrm{sgn}(\omega_n)\left[\frac{D_0(m-n)}{2\omega_n^2}k_B T + \frac{D_1(|m-n|)}{(2\pi)^2 k_B T}\right]|\Delta(T)|^2 . \tag{B8}$$

To obtain $\gamma(T)$, a component that varies linearly with a small m must be extracted from Eq. (B8). For the first term in the coefficient of $|\Delta|^2$, we find

$$\sum_{n=-x}^{x} \frac{|m-n|}{\omega_n^2}\mathrm{sgn}(\omega_n) \cong \sum_{n=-x}^{x} \frac{(n-m)}{\omega_n^2}, \quad \text{for a small } m . \tag{B9}$$

For the third term,

$$\sum_{n=-x}^{x} D_1(|m-n|)\mathrm{sgn}(\omega_n) = D_1(|m|) + \sum_{n\geq 1}^{x} D_1(|m-n|) - \sum_{n'\geq 1}^{x} D_1(|m+n'|) . \tag{B10}$$

Since $D_1(|x|)$ is singular at $x=0$, a first term does not contribute to $\gamma(T)$. Thus, for the small m, Eq. (B10) is approximated by a part that varies linearly with m as follows:

$$\sum_{n=-x}^{x} D_1(|m-n|)\mathrm{sgn}(\omega_n) \cong -2\sum_{i=1}^{x}\left[\frac{dD_1(y)}{dy}\right]_{y=i} m . \tag{B11}$$

Substituting Eqs. (B9) and (B11) into Eq. (B8), and differentiating it with respect to ω_m $(=2\pi m k_B T)$, yield Eqs. (12), $\gamma(T)$ $(=[1-\partial\Sigma(\omega)/\partial\omega]_{\omega=0})$.

APPENDIX C

To consider thermodynamic properties, it is appropriate to formulate a thermodynamic functional Ω in such a way that it is stationary if Eqs. (6) are satisfied.[18] Such a functional Ω is obtained by following steps. (In this appendix, we abbreviate $U_{\mathbf{k},\mathbf{p},\mathbf{q},\mathbf{r}}$ by U.)

First, Ω must include a part equivalent to the BCS theory, which was derived by Eliashberg as follows:[19]

$$\Omega_1 = -\frac{1}{\beta}\sum_p \ln[-X(p)] + \frac{2}{\beta}\sum_p[\Sigma(p)G(p)+\phi^*(p)F(p)] + \frac{1}{\beta^2}\sum_p\sum_{p'} U[G(p)G(p')+F^*(p)F(p')] , \tag{C1}$$

where $X(p)=[i\omega_n-\varepsilon_p-\Sigma(p)][i\omega_n+\varepsilon_p+\Sigma(-p)]-|\phi(p)|^2$. An approximation in Eq. (C1) is equivalent to the Gor'kov decoupling. This is reflected by the third term on the right-hand side of Eq. (C1), where a four-operator product is factorized into two Green's functions.

Second, it is necessary to include terms beyond the Gor'kov decoupling. When we calculate the Gor'kov equation one step further than usual, not only an expectation value of the four-operator product but also that of an eight-operator product appears. It is necessary to incorporate this into Ω as well. This expectation value of the eight-operator product must be factorized using that of the four-operator product Γ. There are three possible combinations: (1) one Γ and two G's, (2) one Γ and two F's, and (3) two Γ's.

For the one Γ and two G's, and for the one Γ and two F's, we find a contribution to Ω,

$$\Omega_2 = \frac{1}{\beta^2}\sum_p\sum_{p'} U[G(p)\Gamma(p-p')G(p')+F^*(p)\Gamma(p-p')F(p')] , \tag{C2}$$

and for the two Γ's, we find

$$\Omega_3=\frac{1}{\beta}\sum_q \Gamma(q)\Gamma(-q)\ . \tag{C3}$$

The total potential $\Omega(=\Omega_1+\Omega_2+\Omega_3)$ is a natural extension of the Gor'kov decoupling to the higher-order terms. The Ω is stationary with respect to the variations in $\Sigma(p)$, $\phi(p)$, and $\Gamma(q)$, if these quantities are given by

$$\Sigma(p)=\frac{1}{\beta}\sum_q[-U-U\Gamma(q)]G(p+q)\ , \tag{C4}$$

$$\phi(p)=\frac{1}{\beta}\sum_q[-U-U\Gamma(q)]F(p+q)\ , \tag{C5}$$

$$\Gamma(q)=-\frac{1}{\beta}\sum_k U[G(k+q)G(k)+F^*(k+q)F(k)]\ . \tag{C6}$$

Equations (C4)–(C6) are the same as Eqs. (6).

Substituting Eqs. (9a), (9b), and (11a) into Eqs. (C1)–(C3) yields the Ginzburg-Landau energy Eqs. (13a), where the effect beyond the Gor'kov decoupling, $\Omega_2+\Omega_3$, appears in the T_c and the δ. $h(x)$ in Eq. (13c) is given by the coefficient of the $|\phi|^4$ term in $\Omega_2+\Omega_3$ as follows:

$$\begin{aligned}h(x)=&\frac{1}{16}\sum_{n=-x}^{x}\sum_{n'=-x}^{x}\mathrm{sgn}(\omega_n\omega_{n'})[2c_2^2a(2,2)+3c_4a(4,0)+3c_4a(0,4)+4c_1^*c_3a(1,3)+4c_1c_3^*a(3,1)]D_0(n-n')\\&+\frac{1}{4}\sum_{n=-x}^{x}\sum_{n'=-x}^{x}\mathrm{sgn}(\omega_n\omega_{n'})[c_2a(2,0)+c_2a(0,2)+2c_1^*c_1a(1,1)]D_1(n-n')\\&+\frac{1}{2}\sum_{n=-x}^{x}\sum_{n'=-x}^{x}\mathrm{sgn}(\omega_n\omega_{n'})D_2(n-n')-\frac{1}{4}\sum_{n=0}^{2x}[D_1(n)D_1(-n)+D_0(n)D_2(-n)+D_0(-n)D_2(n)]\ ,\end{aligned} \tag{C7}$$

where

$$a(i,j)=\frac{1}{(n+\frac{1}{2})^i(n'+\frac{1}{2})^j}\ . \tag{C8}$$

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