Effective-mass renormalization and de Haas–van Alphen effect in heavy-fermion systems

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(Submitted 24 July 1992)
Pis'ma Zh. Eksp. Teor. Fiz. **56**, No. 4, 221–226 (25 August 1992)

The spectrum of the broad conduction band undergoes a pronounced renormalization in the Kondo-lattice model as a result of inelastic scattering by spin excitations which form a system of neutral heavy fermions as $T\to 0$. This renormalization is not universal, however, and the effective electron mass is generally smaller than the thermodynamic mass. The inelastic interaction with the spin liquid, in constrast with phonons, leads to the explicit appearance of a Dingle factor in the amplitude of the de Haas–van Alphen effect. A correlation between the renormalized electron mass as $T\to 0$ and the resistance of the heavy-fermion system at $T\sim T_K$ is analyzed. Experimental aspects of the problem of identifying the nature of the spin correlations at low temperatures are discussed.

1. In Ref. 1 we presented a case for the proposition that heavy fermions arise as neutral excitations of a spin nature in systems with a nearly integer f-shell valence. In a Kondo lattice, the interaction of f electrons with conduction electrons leads to a partial spin screening and to an indirect interaction between spins, giving rise to a quantum spin liquid. Low-temperature excitations of this liquid carry no charge and obey Fermi statistics (cf. Ref. 2, for example). All the excitations of the spin liquid lie in a narrow energy band. The scale size of this band is characterized by the temperature T_S, at which collective interactions in the spin system are disrupted. The thermodynamic properties of the systems (the heat capacity and the magnetic susceptibility) are determined by this branch of excitations.

The Fermi liquid formed by conduction electrons determines the charged branch of excitations which is responsible for the conductivity and for such an effect as the quantum oscillations of the magnetic susceptibility, i.e., the de Haas–van Alphen (dHvA) effect. There is a strong interaction between excitation branches (particularly at energies $\lesssim T_S$), as can be seen in the temperature dependence of the resistance of a heavy-fermion system. This interaction can, in general, lead to a pronounced renormalization of the mass of the conduction electrons, m^*. However, the general analysis carried out in Ref. 1 shows that, at least under the condition $J\ll W$ (J is the energy of the exchange interaction between conduction electrons and localized spins, and W is the width of the conduction band), the carrier mass m^* is much smaller than the effective mass m_H found from thermodynamic measurements. All the experiments which have been carried out on the dHvA effect in Ce-based systems support this assertion. The masses observed in the dHvA effect are often considerably larger than those found in band-theory calculations. We show below that there is a correlation between the renormalized mass as $T\to 0$ and the resistance at $T\sim T_S$ in the picture of a two-component liquid, under some extremely general assumptions regarding the properties of the spin system. Analysis of the experimental results reveals that there is such a correlation.

Theoretical results derived for the case of an interaction with phonons (Ref. 3; see also Ref. 4) have led to the understanding that an inelastic interaction always leads to exclusively a renormalization of the observable mass, that this renormalization persists over a wide temperature range, and that it does not lead to the appearance of a Dingle factor. Actually, the high-temperature behavior of the amplitude of the quantum oscillations is dictated by electron damping in all cases. In the case of phonons, however, the number of excitations increases linearly with T (simulating a preservation of the mass renormalization), while the number of spin excitations approaches a constant value. As a result, the interaction with the spin liquid leads to an increase in the temperature and to the appearance of a constant Dingle factor.

2. In the mode of a two-component liquid, the Hamiltonian of the heavy-fermion system can be written

$$H = H_B + H_{SL} + H_{int}, \qquad (1)$$

where H_B is the band Hamiltonian, H_{SL} is the Hamiltonian of the spin liquid, and $H_{\rm int}$ is the interaction between the two subsystems.

When there are two scale energies, W and T_S, which are sharply different, the adiabatic part of the interaction, associated with the excitations of electrons in the interval between T_S and W, goes into the formation of the spectrum of a narrow band. Thereafter, the nonadiabatic corrections are small, as in the case of an interaction with phonons.[5] The term H_{SL} in Hamiltonian (1) thus describes a spin system with an adiabatic renormalization, and $H_{\rm int}$ contains only the low-frequency part of the interaction. If the interaction constant is small, $\rho J \ll 1$, where ρ is the density of states at the Fermi surface in the conduction band, the renormalization of the vertex is also slight. We assume everywhere below that the intersite interaction dominates the formation of the spin liquid and that this inequality holds.

The mass operator for the electrons is determined by the diagram

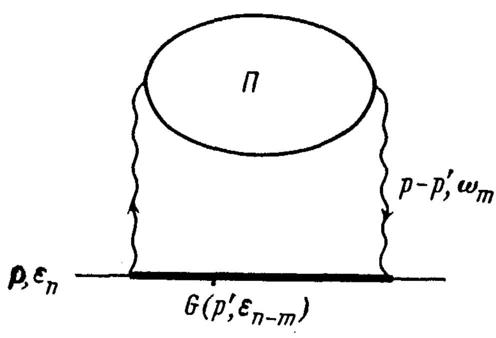

FIG. 1.

$$\Sigma_n(\mathrm{p}) = J^2T\sum_m \int \frac{d\mathrm{p}'}{(2\pi)^3} \frac{\Pi(\mathrm{p}-\mathrm{p}',\omega_m)}{i\epsilon_{n-m} - \xi_{\mathrm{p}'} - \Sigma_{n-m}(\mathrm{p}')}. \tag{2}$$

Here $\epsilon_n = \pi T(2n+1)$, $\omega_m = 2\pi Tm$ are the Matsubara frequencies, and $\xi_{\mathbf{p}} = \epsilon_{\mathbf{p}} - \mu$ is the energy of the electron excitations. For the polarization operator we have the expression

$$\Pi(\mathrm{q},\omega_m) = \int_0^\infty dEP(\mathrm{q},E)\frac{2E^2}{\omega_m^2 + E^2};$$

$$P(\mathrm{q},E) = \sum_{\mathbf{kk}'}(n_{\mathbf{k}} - n_{\mathbf{k}'})\delta(E_{\mathbf{k}} - E_{\mathbf{k}'} - E)\delta_{\mathbf{k}+\mathrm{q},\mathbf{k}'}. \tag{3}$$

We are interested in the renormalization of the electron spectrum at energies and temperatures $\sim T_S$. Expression (2) is dominated by the integration over small values of ξ. In this case the integrations over the direction of the momentum $\mathbf{p}'$ and over the energy ξ can be separated. Ignoring terms on the order of $(pJ)^2$ and T_K/W, we have the following universal expressions for the mass operator:

$$\Sigma_n = -i\pi\rho J^2T\sum_m \Pi_m \,\mathrm{sgn}(\epsilon_{n-m}) \equiv -i\pi\rho J^2T\sum_{m=-n}^{n}\Pi_m\ , \tag{4}$$

$$\Pi_m = < \Pi(\mathrm{p}-\mathrm{p}',\omega_m) >, \tag{5}$$

where $\langle ... \rangle$ means an average over the angle between the vector $\mathbf{p}$ and $\mathbf{p}'$ on the Fermi surface. The mass operator is thus determined exclusively by the expectation value of the polarizability of the spin liquid.

Let us consider two limiting cases. As $T\to 0$ we have

$$\Sigma_n = -i\epsilon_n\rho J^2\Pi_0\ , \tag{6}$$

and for the renormalization of the mass of the conduction electrons we have

$$m^* = m_B(1+\lambda); \tag{7}$$

$$\lambda = \rho J^2\Pi_0(T=0). \tag{8}$$

At $T > T_S$, we can restrict the sum over the frequencies ω_m in (4) to the term with $m = 0$. In this temperature region the polarization operator in (3) is given approximately by

$$\Pi_0(T) \approx \alpha\frac{1}{T}, \tag{9}$$

where α is a numerical factor on the order of one. In this case the mass operator becomes

$$\Sigma_n = -i/2\tau \mathrm{sgn}(n); \qquad 1/\tau = \alpha 2\pi\rho J^2. \tag{10}$$

At $T \ll T_S$, the inelastic interaction thus determines a renormalization of the effective mass, while at $T \gtrsim T_S$ it leads to simply a damping of electron excitations which is independent of the temperature (cf. Ref. 8). This result is important for the dHvA effect.

3. The general expression for the amplitude of the quantum oscillations of the magnetic susceptibility is[3]

$$A_r = \sum_{n=0}^{\infty} \exp\left\{-\frac{2\pi r}{\omega_C}(\epsilon_n + i\Sigma_n)\right\}, \tag{11}$$

where r is the index of the harmonic, and $\omega_C = EH/m_B C$ is the cyclotron frequency in the magnetic field H. The argument of the exponential function with $n=0$ is usually considerably greater than one under experimental conditions, and expression (11) can be restricted to the first term, at an exponential accuracy. Substituting the expression found above for Σ, (4), we find

$$-\ln A_1 \approx \frac{2\pi^2 T}{\omega_C}(1 + \rho J^2 \Pi_0(T)) , \tag{12}$$

$$\Pi_0(T) = 2\int dEP(E)/E; \qquad P(E) = \langle P(\mathrm{p} - \mathrm{p}', E) \rangle . \tag{13}$$

At $T \ll T_S$ the temperature dependence of the amplitude determines m^*. With increasing temperature, the effective mass becomes undressed, and a temperature-independent Dingle factor appears at the same time.

Here we see a fundamental distinction from the case of the electron–phonon interaction. In the latter case we would have[6]

$$\Sigma_0 = -i\pi T\lambda_{ph}, \tag{14}$$

where λ_{ph} is independent of the temperature. The constant value of Σ_0/T created the illusion that inelastic scattering was unimportant at all T and that the only factor of importance was a change in the effective mass. Actually, there is a continuous transition from a leading role of mass renormalization to a pure damping again in this case. At temperatures above the Debye temperature, the electron mass is close to its seed value, but here the Dingle factor is a linear function of T, since the number of phonons itself increases linearly with T in the classical temperature range. In the case of the spin subsystem, the number of excitations is limited by the number of spins, so τ^{-1} reaches a plateau as the temperature is raised.

In the intermediate temperature region, the amplitude of the dHvA effect reflects simply the scale of the inelastic interaction, not the mass renormalization or the lifetime of excitations separately.

It is important to note that the result found for a two-component Fermi liquid is a general result, which applies to an arbitrary interaction of a broad conduction band with *any* band of excitations in a crystal which are concentrated in a narrow energy interval $T_S \ll W$. The fact that the spin liquid unavoidably transforms into a system of quasi-independent spins at $T \sim T_S$ causes no change in the limiting results which we have found.

The sensitivity to the nature of the excitations in the spin liquid is seen in the temperature dependence $\Pi_0(T)$ at intermediate temperatures $T < T_S$. Accordingly, it may prove informative to study the amplitude of the dHvA effect for moderately heavy masses (but under the condition $m^* \gg m_B$), in order to cover a temperature range as broad as possible. The temperature dependence of the difference $\Pi_0(T) - \Pi_0(0)$ in (12) and (13) actually reflects internal properties of the spin liquid. If the low-temperature excitations obey Fermi statistics, in accordance with (3), this difference is proportional to $(T/T_S)^2$. The detection of an early deviation from this law might shed some light on manner in which the restructing of the properties of collective excitations change. Such a change may be associated with an early deviation of the temperature dependence of the resistance from the quadratic Fermi-liquid law.

4. The scale of the mass renormalization at $T=0$ is determined by the value of the parameter λ in (8). Since we have $\Pi_0 \sim 1/T_S$, we also have

$$\lambda \sim \frac{\rho J^2}{T_S} \approx \frac{1}{2\pi\tau T_S}. \tag{15}$$

The relaxation time τ in (10), which was determined for $T \gtrsim T_S$, can be estimated from the value of the resistance at its maximum, $\rho_{\max}(T)$. This maximum occurs at $T \sim T_S$. Using experimental results (see Ref. 7, for example), we can easily show that the relation $\lambda \gg 1$ holds. This result means that aa $T \to 0$, the mass of the conduction electrons at the Fermi surface satisfies $m^* \gg m_B$. This result was first derived by Éliashberg,[8] who introduced a model description of the spin subsystem in the form of a set of two-level systems. The universal nature of the behavior of the mass operator in interactions with excitations which lie in a narrow energy band, as mentioned above, suggests that it is reasonable to find a qualitative agreement of the results for the renormalization of the effective mass. Éliashberg assumed that the mass of the conduction electrons was increased by those heavy fermions which determine the thermodynamic properties of the system. In general, however, that is definitely not the case. Any model which assumes a narrow energy band of spin excitations automatically leads to the conclusion that this band makes a universal and governing contribution to the thermodynamics of the system (with an entropy $s \approx \ln 2$ at $T \gtrsim T_S$). On the other hand, the renormalization of the electron mass depends on (in addition to T_S) the parameter ρJ, and in this sense the renormalization is not universal. It may differ significantly for different sheets of the Fermi surface. Furthermore, in assuming $\rho J \ll 1$ we will always have $m^* \ll m_H$. It is for this reason that the mass of the charge carriers in Ce-based systems with a nearly integer valence should be smaller than the heavy-fermion thermodynamic mass m_H.

In this version of the theory, the value of the resistance at $T \sim T_S$ and the value of m^* at $T=0$ are correlated. Adopting some typical values for $T > T_S$—$\rho(T_S) m_B / ne^2\tau = 100$ $\mu\Omega\cdot$cm, $T_S = 10$ K, $n = 10^{22}$ cm^{-3}, and $m_B = m_e$—we find

$m^* = (1+\lambda)m_B \approx 40 m_e$. This estimate turns out to be on the order of the largest effective masses which have been observed to date in Ce-based systems.[9,10]

Along the adiabatic approach, the corrections to the spin-excitation spectrum are small, despite the large value of the parameter λ. However, the question of a self-consistent microscopic calculation of T_S and ρJ^2 lies outside the scope of the model which we are discussing here. One might suggest that the scale of T_S is determined to a large extent by intersite correlations of spins and that it depends on the distance between the f atoms, the structure of the lattice, and so forth, while $H_{\rm int}$ is dominated by the one-site scattering. A partial screening of the spin due to the Kondo effect leads to an increase in λ, suppressing the intersite interaction and strengthening the one-site interaction of electrons with spins. Under these conditions, the inequality $T_S \ll \rho J^2$ may hold.

5. At $T \ll T_S$ the temperature dependence of the resistance is determined by the imaginary part of mass operator (4), continued analytically to the real axis:

$$\mathrm{Im}\Sigma(\omega) = -\pi\rho J^2 \int dE P(E)[2N_E + n_{E+\omega} + n_{E-\omega}]\mathrm{sgn}\,\omega, \tag{16}$$

where N_E and n_E are Bose and Fermi distribution functions, respectively. The static resistance depends on the properties of the spin subsystem exclusively through the function $P(E)$. If the low-frequency spin excitations are neutral fermions,[1] we have $P(E) \sim E$ and $\rho \sim T^2$. The heat capacity of this fermion component, which determines the heat capacity of the overall system, has the standard temperature dependence $C \propto T$. In many heavy-fermion systems, the temperature interval in which the $\rho \propto T^2$ law holds is far narrower than the interval in which the heat capacity is a linear function of T. This important experimental result is apparently a consequence of a change in the nature of the excitations in the spin liquid. Interestingly, the model of two-level systems with a uniform distribution of the difference between energy levels leads to a linear heat capacity, but at the same time it leads to $P(E) = \tanh(E/2T)$const and thus $\rho \propto T$. However, this dependence usually replaces the quadratic dependence; it frequently holds over a broad temperature range (Ref. 10, for example). It is clear from general considerations that at intermediate values of T the statistics of the excitations will cease to be Fermi statistics, since at $T \gtrsim T_S$ we are dealing with a system of quasi-independent spins. Whether this agreement is simply fortuitous or whether this model reflects a real restructuring of the spin system remains an open question.

The analysis above was carried out for systems with a nearly integer valence of the f shell, but all the results concerning the renormalization of the broad conduction band remain valid at an intermediate valence if there is a narrow energy band of heavy charged fermions (U-based compounds). The parameter ρJ may be appreciable in this case, and the seed renormalization of the electrons of the broad band may be very pronounced.

We wish to thank M. Springford and J. Franse for critical discussions.

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Translated by D. Parsons