Spin and Magnetic Field Dependences of Quasiparticle Mass in Ferromagnetic State of Heavy Fermions

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Abstract. We investigate the mechanism underlying the suppression of heavy-fermion mass enhancement in the presence of a magnetic field. In the framework of statistically consistent Gutzwiller method (SGA) we study the periodic Anderson model in the strong correlation limit. The finite-$U$ corrections are included systematically allowing to describe the coexistence of Kondo compensation effect and ferromagnetic ordering, as well as weak delocalization of the f-electrons. In particular, we observe that the resulting mass enhancement factor of spin-up electrons and that of spin-down are not equal in ferromagnetic phases and depend strongly on the applied field and the f-level occupancy. We predict that mass enhancement for the spin-up quasiparticles is larger then that of spin-down and both of them decrease in the applied magnetic field. We argue that above features, as well as a nonmonotonic variation of the quasiparticle effective masses observed in our model are in good agreement with earlier experimental measurements for $Ce_xLa_{1-x}B_6$.

1. Introduction

Heavy-fermion (HF) metals are customarily regarded as lattice of strongly correlated f-electrons and coupled to them conduction (band) electrons via an antiferromagnetic Kondo exchange interaction. The f-electrons are associated with the rare-earth or actinides ions. The f-f on-site Coulomb repulsion is strong and the f-electrons behave often in a solid as localized (or almost localized) magnetic moments, even in the presence of the interband hybridization.

One of characteristic properties of the HF compounds is the metamagnetic behavior, i.e. a sudden magnetization increase at a critical value of the applied magnetic field, and observed in HF compounds such as $CeRu_2Si_2$ [1], $CeCoGe_3$ [2], $UPd_2Al_3$, $URu_2Si_2$, and $UPT_3$ [3]. Moreover, de Haas-van Alphen (dHvA) oscillation measurements [4, 5, 6] show that the spin-direction dependent effective masses and their field dependences are observed in a number of HF compounds. These features of HF electron systems makes the applied magnetic field a useful experimental probe of observing the strong correlation behavior. In particular, it is crucial to understand the field dependence of the mass enhancement.

We present a scenario in which the heavy itinerant f-electron quasiparticles tend to localize at metamagnetic transition (MMT), with a concomitant suppression of the HF state at that
critical field. This can be visualized as a gradual decrease of effective mass with the increasing applied field.

To account for the interplay between the localized- and the itinerant-type behavior of f-electrons we start from the periodic Anderson model (PAM) in an external magnetic field included via the Zeeman term. We also use the large, but finite $U$ version of PAM formulated before [7, 8], in which both residual hybridization and the Kondo-type coupling are accounted for in a systematic manner. Additionally, we utilize the so-called statistically-consistent extension of the Gutzwiller-type approach (SGA) [9, 10]. Such formulation allows for a consistent mean-field discussion of correlated states.

2. Model and method

The starting point of our investigation is periodic Anderson model subjected to canonical perturbation expansion [11, 8] in the strong-correlation and mixed-valence limits. We use this transformation in order to include large (but finite) $U$ effects within the Anderson lattice model, with both the effective hybridization and the Kondo interaction effects incorporated in a systematic manner. Explicitly, we start from effective two-orbital Hamiltonian of the form

\[
\mathcal{H} = \mathcal{P}\left\{ \sum_{im\sigma} t_{im}\sigma c_{m\sigma}^{\dagger} c_{n\sigma} + \sum_{im\sigma} \frac{V_{im}^{\sigma} V_{in}^{\sigma}}{4(U + \epsilon_f)} \nu_{if}\sigma c_{m\sigma}^{\dagger} c_{n\sigma} + \sum_{im\sigma} (1 - \hat{N}_{i\sigma})(V_{im}\sigma^{\dagger} c_{m\sigma} + h.c.) \right\} \mathcal{P} \\
+ \mathcal{P}\left\{ \sum_{im\sigma} \frac{2|V_{im}|^2}{U + \epsilon_f} \left( \hat{S}_{i\sigma} \cdot \hat{\sigma}_{m\sigma} - \frac{\nu_{if}\sigma c_{m\sigma}^{\dagger} c_{n\sigma}}{4} \right) + \sum_{i\sigma} \epsilon_f \nu_{if}\sigma \right\} \mathcal{P} \\
- \mathcal{P}\left\{ \frac{1}{2} g_{\sigma} H_{\mu B} \sum_{i\sigma} \sigma \hat{N}_{i\sigma} - \frac{1}{2} g_{\sigma} H_{\mu B} \sum_{m\sigma} \sigma \hat{n}_{m\sigma} \right\} \mathcal{P},
\]

where energies of conduction and f-electrons are referenced against the chemical potential. Also, in this Hamiltonian we have projected out completely (with the help of projector $\mathcal{P}$) the double occupancies of f states, as well as have defined the following projected quantities for f electrons $\nu_{if}\sigma \equiv \hat{N}_{i\sigma}(1 - \hat{N}_{i\sigma})$, $\nu_{if} \equiv \sum_{i\sigma} \nu_{if}\sigma$, $\hat{S}_{i\sigma} \equiv (\hat{S}_{i\sigma}^x, \hat{S}_{i\sigma}^y) = [f_{i\sigma}\sigma, 1/2(\hat{N}_{i\sigma} - \hat{N}_{i\sigma}^\dagger)]$, and the corresponding (non-projected) quantities for the conducting band electrons are $\hat{n}_{m\sigma} = c_{m\sigma}^{\dagger} c_{m\sigma}$, $\hat{n}_{m\sigma} = \sum_{i\sigma} \hat{n}_{m\sigma}$ and $\hat{\sigma}_{m\sigma} \equiv (\sigma^x_{m\sigma}, \sigma^y_{m\sigma}) = [c_{m\sigma}^{\dagger} c_{m\sigma}, 1/2(\hat{n}_{m\sigma} - \hat{n}_{m\sigma}^\dagger)]$. Additionally, as we assume that $g_{\sigma} = g_f = g = 2$, the applied field is defined as $h = \frac{1}{2} g_{\mu B} H$.

We construct a mean-field Hamiltonian using the Gutzwiller type approach. Proper ground variation state can be represented in the form $|\Psi\rangle = \mathcal{P}|\Psi_0\rangle$, where $|\Psi\rangle$ indicates the correlated state and $|\Psi_0\rangle$ is an eigenstate of the effective single-particle Hamiltonian. Then the expectation value of any operator can be in principle calculated as $\langle \hat{O} \rangle = \frac{\langle \Psi|\hat{O}|\Psi\rangle}{\langle \Psi|\Psi\rangle} = \frac{\langle \Psi_0|\hat{O}\mathcal{P}|\Psi_0\rangle}{\langle \Psi_0|\mathcal{P}|\Psi_0\rangle} = \frac{\langle \mathcal{P}\hat{O}\mathcal{P}|\Psi_0\rangle}{\langle \mathcal{P}|\Psi_0\rangle} = \langle \mathcal{P}\hat{O}\mathcal{P}|\Psi_0\rangle$.

In the subsequent analysis, we use projector in more general form $\mathcal{P} = \prod_{i\sigma} \lambda_{i\sigma}^{\hat{N}_{i\sigma}/2} \lambda_{i\sigma}^{\hat{N}_{i\sigma}^\dagger/2} (1 - \hat{N}_{i\sigma}^\dagger\hat{N}_{i\sigma})$, which eliminates the double occupancies of f-electrons in real space and conserves average number of f-electrons at each site before and after projection; the latter is accomplished by fixing the fugacity factors $\lambda_{\sigma} = \frac{1 - n_{i\sigma} / f}{1 - n_{i\sigma} / f}$ [12].

In effect, this kind of Gutzwiller approximation gives us possibility to calculate the mean value $\langle \mathcal{H} \rangle$ of the Hamiltonian. We have additionally assumed, that all the mean fields appearing in our model represent spatially homogeneous quantities, namely, $n_{if} \equiv \sum_{\sigma, \gamma, \delta} \langle \hat{N}_{i\sigma} \rangle \equiv n_f$, $n_{mc} \equiv \sum_{\sigma, \gamma, \delta} \langle \hat{n}_{m\sigma} \rangle \equiv n_c$, $m_{\sigma} \equiv \frac{1}{2} \sum_{\gamma, \delta} \langle \sigma \hat{N}_{i\sigma} \rangle \equiv m_f$, $\gamma_{i\sigma} \equiv \langle \sigma f_{i\sigma} c_{m\sigma} \rangle \equiv \gamma_{\sigma}$, $m_{mc} \equiv \frac{1}{2} \sum_{\gamma, \delta} \langle \sigma \hat{n}_{m\sigma} \rangle \equiv m_c$, $\xi_{i\sigma} \equiv \langle \sigma c_{m\sigma} c_{n\sigma} \rangle \equiv \xi$. In order to provide a statistically-consistent mean-field approximation we supply the expectation value of Hamiltonian $\langle \mathcal{H} \rangle$ with a number of constrains containing appropriate
Figure 1: (Color online) (a): Phase diagram on $n_e - h$ plane displaying transition from WFM (weakly ferromagnetic) phase to SFM (strongly ferromagnetic) phase. The phase diagram is drawn for $U = 4.5$, $\epsilon_f = -0.75$, $|V| = 0.3$ and $t = -1/8$, all in units of the conduction electron bandwidth $W = 1$. The insets visualize the density-of-states for both WFM and SFM phases. (b): The spin-resolved quasiparticle effective masses on the $n_e - h$ plane. Also, $h \equiv (1/2)g\mu_B H$. Note the relatively low values of the effective mass enhancements, $m^*_\sigma \equiv m^*/m$.

Lagrange multipliers regarded as effective mean fields induced by the correlations [9, 13]. Finally, the effective MF Hamiltonian takes the form

$$
\mathcal{H}_{MF} = - \sum_{\langle mn \rangle, \sigma} \left( \eta (c^\dag_{m\sigma} c_{n\sigma} - \xi) + H.c. \right) - \lambda_{cm} \sum_{m\sigma} \left( \sigma c^\dag_{m\sigma} c_{m\sigma} - n_e \right) - \mu \sum_{i\sigma} \left( c_{i\sigma}^\dag c_{i\sigma} + f_{i\sigma}^\dag f_{i\sigma} \right) - \sum_{i\sigma} \left( \tau_{i\sigma} (f_{i\sigma}^\dag c_{i\sigma} - \gamma_{i\sigma}) + H.c. \right) - \lambda_f \sum_{i\sigma} \left( f_{i\sigma}^\dag f_{i\sigma} - n_f \right) - \lambda_{fm} \sum_{i\sigma} \left( f_{i\sigma}^\dag f_{i\sigma} - m_f \right) - \lambda \sum_{i\sigma} \left( f_{i\sigma}^\dag f_{i\sigma} + c_{i\sigma}^\dag c_{i\sigma} - n_e \right) + \langle \mathcal{H} \rangle,
$$

(2)

This Hamiltonian can be brought to a particularly simple $2 \times 2$ matrix form in reciprocal space, namely:

$$
\mathcal{H}_{MF} = \sum_{k\sigma} \begin{pmatrix} c_{k\sigma}^\dag & f_{k\sigma}^\dag \end{pmatrix} \begin{pmatrix} \epsilon_{k\sigma} & \tau_{k\sigma} \\ -\tau_{k\sigma} & \epsilon_{f_k\sigma} \end{pmatrix} \begin{pmatrix} c_{k\sigma} \\ f_{k\sigma} \end{pmatrix} + C,
$$

(3)

where $n_e = n_f + n_c$ is the total number of electrons per site and the constant $C$ includes all the wavevector independent quantities: $C \equiv \langle \mathcal{H} \rangle + \Lambda (16\eta + \lambda_{cm} m_e + 2 \sum_{\sigma} \tau_{\sigma} \gamma_{\sigma} + \lambda_f n_f + \lambda_{fm} m_f + \lambda n)$. For example, the band energy of $c$-electrons in a two-dimensional case is represented explicitly by $\epsilon_{k\sigma} \equiv -4\eta (\cos k_x + \cos k_y) - \mu - \lambda - \lambda_{cm} \sigma$ and the energy of the localized $f$-electrons equals $\epsilon_{f\sigma} \equiv -\mu - \lambda - \lambda_f - \lambda_{fm}\sigma$. It is easy to see that the eigenvalues of the Hamiltonian (3) are then $E_{k\sigma}^\alpha = \frac{1}{2} \left( \epsilon_{k\sigma}^c + \epsilon_{f\sigma}^f + \alpha \sqrt{(\epsilon_{k\sigma}^c - \epsilon_{f\sigma}^f)^2 + 4\tau_{k\sigma}^2} \right)$, where $\alpha = \pm 1$ labels the quasiparticle band.
(antibonding and bonding components, respectively). The quasiparticles form two bands with renormalized characteristics.

The mean-field values can be determined in terms of minimizing the free-energy functional $F = F_0 - \frac{1}{\Lambda} \sum_{k\sigma} \ln \left( 1 + e^{-\beta E_n^{\sigma}} \right) + \mu n_e$ with respect to all expectation values and all mean fields.

3. Results

Here we focus on the spin-dependent effective-mass behavior in the applied field; a number of strongly correlated effects such as metamagnetism, or tendency towards localization, are discussed elsewhere [14]. The effective mass enhancement of quasiparticles is defined in a standard manner

$$m^* \equiv \frac{m^*}{m} = \left( \frac{\partial E_n^{\alpha}}{\partial \epsilon_k^{\sigma}} \right)^{-1} \bigg|_{\mu}.$$ 

Applied magnetic field affects strongly the low-energy physics of the system, as shown in Figure 1(a). Depending on the number of electrons $n_e = n_f + n_c$ and the magnetic field, the system can be found in two different spin-polarized phases. In the weakly ferromagnetic (WFM) phase as well as in strongly ferromagnetic (SFM) phase we observe a compensation of localized moments by those coming from the conduction band. This is a clear evidence of the antiferromagnetic Kondo interaction [14]. In the SFM phase, in which the system is close to f-electron localization, both the effective spin-dependent masses (with $\sigma = \pm 1$) decrease in the stronger applied field (cf. Figure 1(b)). The effective mass of quasiparticles depends also on the total number of electrons $n_e$. We believe that obtained behavior can account for the field dependence of the quasiparticle effective mass of Ce$_x$La$_{1-x}$B$_6$ [6, 15] in strong fields. Our claims are based on the fact that our approach reproduce: (i) the field suppression of effective masses in high field, (ii) the non-monotonic $x \equiv n_f$ dependence of $m^*$ for the dominant spin component and its rather small value for this heavy-fermion compound.

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