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Canted phase of an antiferromagnetic Anderson lattice

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Abstract

On the basis of extended periodic Anderson model with antiferromagnetic (AFM) exchange and s–f exchange interactions the energy spectrum of heavy-fermion (HF) AFM metals is calculated. The quasiparticle band structure in collinear AFM phase is described by four splitted bands one of which is very narrow (order of exchange interaction constant) and lies in the vicinity of a localized level. Application of an external magnetic field causes a canting of the sublattice magnetization and due to s–f exchange interaction strongly modifies the HF band picture. Thus eight different quasiparticle bands appear. Their evolution when temperature and magnetic field change is studied.

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Ground state structure and low-temperature properties of heavy-fermion (HF) systems keep on to be the object of intensive experimental and theoretical investigations. These systems are believed to be well described by the periodic Anderson model (PAM), which comprises lattice of strongly correlated localized f-levels, hybridizing with a delocalized s–p electron band. HF state at low temperatures often coexists with the long-range antiferromagnetic (AFM) order. By now the fermion quasiparticle spectrum in AFM phase was studied only for zero magnetic fields H [1,2], when collinear structure of magnetic sublattices is formed. Switching on the magnetic field causes canting of magnetic sublattices. For HF systems with metallic type of the ground state (localized level embedded into conduction band) strong influence of magnetic field on fundamental thermodynamic characteristics was found (magnetoresistance [3], heat capacity [4], susceptibility [5]). That is why to interpret the experimental results it is necessary to go beyond the scope of collinear geometry.

In the present work on the basis of extended PAM the energy spectrum problem of a conducting HF—antiferromagnet in canting phase is considered.

Our starting point is the Anderson lattice model. The corresponding Hamiltonian is given by

$$\hat{H} = \sum_{k\sigma}(\varepsilon_{k\sigma}-\mu)c^{+}_{k\sigma}c_{k\sigma} + \sum_{f\sigma}(E_{\sigma}-\mu)d^{+}_{f\sigma}d_{f\sigma} + \frac{1}{\sqrt{N}}\sum_{kf\sigma}[V_k e^{-ikf}c^{+}_{k\sigma}d_{k\sigma} + \text{h.c.}] + U\sum_{f}\hat{n}_{f\uparrow}\hat{n}_{f\downarrow}. \quad (1)$$

Here $\varepsilon_{k\sigma} = \varepsilon_k - 2\sigma\mu_B H$ and $E_\sigma = E_0 - g\sigma\mu_B H$. The other notations are conventional. In the limit of the strong electron correlations ($U \to \infty$) Hamiltonian (1) can be reduced to the effective one that acts on the basis with no double states. The effective Hamiltonian in the second order of V/U contains s–f exchange interaction and in the fourth order there appear exchange interactions that are supposed to result in long-range magnetic order. Thus our effective PAM Hamiltonian in Hubbard operator

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representation reads

$$\hat{H} = \sum_{k\sigma}(\varepsilon_{k\sigma}-\mu)c^{+}_{k\sigma}c_{k\sigma} + \sum_{f\sigma}(E_{\sigma}-\mu)X^{\sigma\sigma}_{f} + \frac{1}{\sqrt{N}}\sum_{kf\sigma}[V_{k}\mathrm{e}^{-\mathrm{i}kf}c^{+}_{k\sigma}X^{0\sigma}_{f} + \mathrm{h.c.}] + \sum_{fg}J_{fg}(\mathbf{S}_{f}\boldsymbol{\sigma}_{g}) - \frac{1}{2}\sum_{fg}I_{fg}(\mathbf{S}_{f}\mathbf{S}_{g}). \quad (2)$$

In order to study AFM canted phase we introduced lattice with two interpenetrating F- and G-sublattices. Since external magnetic field courses canting of the sublattice magnetization $\mathbf{R}$, it is convenient to go over the new local coordinates so that the equilibrium $\mathbf{R}$ was aligned along the new z-axis in each sublattice. For this purpose, we apply the unitary transformation

$$U(\theta) = \prod_{f}\prod_{g}\mathrm{e}^{\{\mathrm{i}\theta(S^{y}_{f}+\sigma^{y}_{f})\}}\mathrm{e}^{\{-\mathrm{i}\theta(S^{y}_{g}+\sigma^{y}_{g})\}}, \quad (3)$$

to the Hamiltonian (2).

Tackling the transformed Hamiltonian within the slave boson approach in the mean field approximation we arrive at a closed system of eight equations for retarded Green's functions. The corresponding determinant of eighth order can be factorized $\Delta^{(8)}_{k}(\omega) = \Delta^{(4)}_{k\uparrow}(\omega)\Delta^{(4)}_{k\downarrow}(\omega)$, and dispersion equation is

$$\Delta^{(4)}_{k\sigma}(\omega) = (\omega^{2}_{E} - \tilde{H}^{2}/4)\Big(\omega^{2}_{t} - \Gamma^{2}_{k} + 2\sigma\Gamma_{k} \times(2h\sin\theta + \tilde{H}\cos\theta) - h^{2} - \frac{\tilde{H}^{2}}{4}\Big) + 2\omega_{E}(u^{2}_{k}(2\sigma h\sin\theta + \sigma\tilde{H}\cos\theta - \Gamma_{k}) - \omega_{t}v^{2}_{k}) + 2\sigma\tilde{H}(u^{2}_{k}\omega_{t}\cos\theta + v^{2}_{k}(\Gamma_{k}\cos\theta - \sigma\tilde{H})) + \tilde{H}|\tilde{W}_{k}|^{2}(\sin^{2}\theta\tilde{H} - h\sin 2\theta) + v^{4}_{k} - u^{4}_{k} = 0, \quad (4)$$

where $\omega_{E} = \omega - E_{0} + \mu + \lambda$, $\omega_{t} = \omega - t_{k} + \mu$, $\tilde{H} = g\mu_{\mathrm{B}}H\cos\theta - J_{0}m_{\parallel} - L_{0}[m_{\parallel}\cos 2\theta - m_{\perp}\sin 2\theta] - R[K_{0}\cos 2\theta - I_{0}]$, $\tilde{H} = 2\mu_{\mathrm{B}}H\cos\theta - J_{0}R - L_{0}R\cos\theta$, $h = \mu_{\mathrm{B}}H\sin\theta - \frac{1}{2}L_{0}R\sin 2\theta$, $v^{2}_{k} = |\tilde{W}_{k}|^{2} + |\tilde{V}_{k}|^{2}$, $u^{2}_{k} = \tilde{W}^{*}_{k}\tilde{V}_{k} + \tilde{W}_{k}\tilde{V}^{*}_{k}$. Functions Γ_{k}, W_{k}, K_{k}, L_{k} are Fourier transforms of the hopping integral, hybridization, exchange and s–f-exchange interactions between states of different sublattices, and t_{k}, V_{k}, I_{k}, J_{k} are that of the same sublattices. Average number of slave-bosons e^{2} renormalizes hybridization: $\tilde{V}_{k} = eV_{k}$, $\tilde{W}_{k} = eW_{k}$. The Lagrange multiplier λ should hold the constraint $n_{f} + e^{2} = 1$, where $n_{f} = \sum_{\sigma}n_{f\sigma}$ stands for localized electron concentration. Lastly $m_{\parallel}$ ($m_{\perp}$) is parallel (transverse) to the new z-axis component of itinerant electron magnetization.

Thus to derive the HF band structure seven integral equations for parameters e^{2}, μ, R, λ, $m_{\parallel}$, $m_{\perp}$ and angle θ must be selfconsistently solved. Especially, equilibrium angle θ should be found from the equation

$$gH\sin\theta - L_{0}(m_{\perp}\cos 2\theta + m_{\parallel}\sin 2\theta) + J_{0}m_{\perp} - K_{0}R\sin 2\theta = 0. \quad (5)$$

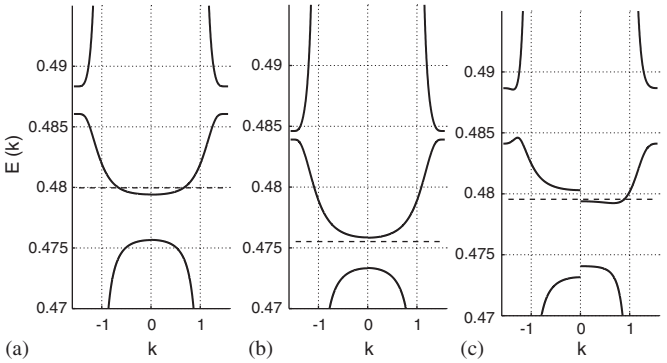

Fig. 1. Quasiparticle band structure in the vicinity of a localized level. Dashed line denotes position of the chemical potential μ. Parameters of the model are: $E_{0} = 0.4\,\mathrm{eV}$, $t_{1} = -0.5\,\mathrm{eV}$, $V = 0.15\,\mathrm{eV}$, $K_{0} = 0.008\,\mathrm{eV}$, $J_{0} = 0.5\,\mathrm{eV}$, $n_{e} = 4.35$. (a) $T = 2\,\mathrm{K}$, $H = 0$; (b) $T = 31\,\mathrm{K}$, $H = 0$; (c) $T = 2\,\mathrm{K}$, $H = 10\,\mathrm{T}$.

Results of numerical calculations are shown on Fig. 1. Fig. 1a shows HF band structure at the very vicinity of a localized level when $H = 0$. In this case the system is in collinear AFM phase and formation of a very narrow HF band, splitted by two gaps, is clearly seen. The width of the band is order of 0.01 eV that is too small when compared with total band width ~8 eV. When temperature rises, the upper gap decreases, as is shown on Fig. 1b where calculations were done at $T = 31\,\mathrm{K}$ and $H = 0$. As temperature, reaches Neel temperature, this gap disappears. Lastly Fig. 1c demonstrates modification of the band structure when magnetic field H is switched on. Now degeneracy on σ is lifted and two narrow HF bands appeared.

Obviously, all these band structure modifications may result in nontrivial magnetic and thermodynamic behavior of the HF-system described by PAM.

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References

[1] V. Dorin, et al., Phys. Rev. B 46 (1992) 10800.
[2] R. Doradzinski, et al., Phys. Rev. B 58 (1998) 3293.
[3] D. Werner, et al., Physica B 259–261 (1999) 10.
[4] K. Heuser, et al., Physica B 259–261 (1999) 392.
[5] S. Raymond, et al., Physica B 259–261 (1999) 48.