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Evolution of Magnetism and its Interplay with Superconductivity in Heavy-Fermion $U(\text{Pt},\text{Pd})_3$

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Appendix I

E-model: sixth order correction

The low-temperature properties of UPT_3 are determined by both the antiferromagnetic and the superconducting order parameters. The total free energy with respect to the normal state consists therefore of three components:

$$F = F_M + F_S + F_{MS} \quad (\text{I.1})$$

Here F_M and F_S describe the antiferromagnetic and the superconducting contributions and F_{MS} is the coupling term of the antiferromagnetic and the superconducting order parameters. In the E-model the free energy of the superconducting state is expanded in terms of a vector order parameter, $\eta = (\eta_x, \eta_y) = (|\eta_x| e^{i\phi_x}, |\eta_y| e^{i\phi_y})$, describing the complex components of a 2-dimensional gap function ($E_{1g}, E_{2g}, E_{1u}, E_{2u}$). The degeneracy of the components of the superconducting vector order parameter is lifted by a symmetry breaking field (ϵ). With the antiferromagnetic order as the symmetry breaking field $\epsilon = \gamma m^2$. In section 3.2.5.2 the fourth order expansion of the free energy is given. There exist four independent sixth-order terms (e.g. $|\eta|^6, |\eta^3|^2, |\eta^2 \eta^*|^2, |\eta^2|^2 |\eta|^2$). We performed calculations adding one sixth order term, $\delta |\eta|^6/3$, to the free energy. In order to minimise the total free energy it is written in the components $|\eta_x|^2$ and $|\eta_y|^2$:

$$F = F_M + \alpha_S \left(|\eta_x|^2 + |\eta_y|^2 \right) + \frac{1}{2} \beta_S \left(|\eta_x|^4 + |\eta_y|^4 \right) + \beta_\phi |\eta_x|^2 |\eta_y|^2 + \frac{\delta}{3} \left(|\eta_x|^6 + |\eta_y|^6 \right) + \delta |\eta_x|^2 |\eta_y|^2 \left(|\eta_x|^2 + |\eta_y|^2 \right) - \epsilon \left(|\eta_x|^2 - |\eta_y|^2 \right) \quad (\text{I.2})$$

Here $\alpha_S = \alpha_{S_0} (T - T_c)$, $\beta_S = \beta_1 + \beta_2$, $\beta_\phi = \beta_1 + \beta_2 \cos(2(\phi_x - \phi_y))$ and α_{S_0} , β_1 and β_2 are the Ginzburg-Landau coefficients which are positive in the superconducting state. By minimising the free energy with respect to $|\eta_x|$, $|\eta_y|$, m and $\phi_x - \phi_y$, one obtains four coupled equations for the equilibrium state. The magnetic term is assumed to be constant in the superconducting state, because the moment is nearly saturated and $\phi_x - \phi_y = \pi/2$. There are two coupled equations for the equilibrium state:

$$\begin{aligned}
2|\eta_x| \left[\alpha_- + \beta_S |\eta_x|^2 + \beta_\phi |\eta_y|^2 + \delta \left(|\eta_x|^4 + |\eta_y|^4 + 2|\eta_x|^2 |\eta_y|^2 \right) \right] &= 0 \\
2|\eta_y| \left[\alpha_+ + \beta_S |\eta_y|^2 + \beta_\phi |\eta_x|^2 + \delta \left(|\eta_x|^4 + |\eta_y|^4 + 2|\eta_x|^2 |\eta_y|^2 \right) \right] &= 0
\end{aligned} \tag{I.3}$$

Here $\alpha_{\pm} = \alpha_S \pm \epsilon$. The two superconducting phases are expressed through normalised order parameter components. The phases are the (1,0) phase with only $|\eta_x|$ different from zero and the (1, α i) phase where both amplitudes are nonzero and have a relative phase $\phi_x - \phi_y = \pi/2$. A double superconducting transition is found for $\beta_1, \beta_2, \gamma > 0$ with the following solutions:

$$(1,0) \text{ phase: } T_c^+ = T_c + \frac{\epsilon}{\alpha_{S_0}} \tag{I.4}$$

$$\left. \begin{aligned}
|\eta_x|^2 &= \frac{-\beta_S + \sqrt{\beta_S^2 - 4\delta\alpha_-}}{2\delta} \\
|\eta_y|^2 &= 0
\end{aligned} \right\} T_c^- < T < T_c^+ \tag{I.5}$$

$$(1,\alpha i) \text{ phase: } T_c^- = T_c - \frac{\beta_1}{\beta_2} \frac{\epsilon}{\alpha_{S_0}} - \frac{\epsilon^2 \delta}{\alpha_{S_0} \beta_2^2} \tag{I.6}$$

$$\left. \begin{aligned}
|\eta_x|^2 &= \left(\frac{\epsilon}{2\beta_2} - \frac{\beta_1}{4\delta} \right) + \frac{1}{4\delta} \sqrt{\beta_1^2 - 4\delta\alpha_S} \\
|\eta_y|^2 &= -\left(\frac{\epsilon}{2\beta_2} + \frac{\beta_1}{4\delta} \right) + \frac{1}{4\delta} \sqrt{\beta_1^2 - 4\delta\alpha_S}
\end{aligned} \right\} T < T_c^- \tag{I.7}$$

$$\Delta T_c = T_c^+ - T_c^- = \frac{\epsilon}{\alpha_{S_0}} \left(1 + \frac{\beta_1}{\beta_2} + \frac{\epsilon\delta}{\beta_2^2} \right) \tag{I.8}$$

In the limit of $\delta \rightarrow 0$, all equations are the same as in the fourth order E-model. The temperature dependence of the specific heat divided by temperature is derived from the free energy by $c/T = -\partial^2 F / \partial T^2$. The results for some reasonable values of the coefficients are plotted in section 3.2.5.2 figure 3.2. The analytical calculation of c/T from the free energy is straight forward, but tedious. As a check we performed the calculation both analytically and numerically. The analytical expression is given by:

$$\begin{aligned}
\Delta_{NA} c(T) / T &= \frac{\alpha_{S_0}^2}{\sqrt{\beta_S^2 - 4\delta\alpha_-}} \\
\Delta_{NB} c(T) / T &= \frac{\alpha_{S_0}^2}{\sqrt{\beta_1^2 - 4\delta\alpha_S}}
\end{aligned} \tag{I.9}$$