Evolution of Magnetism and its Interplay with Superconductivity in Heavy-Fermion U(Pt,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:

$$F = F_{\mathrm{M}} + F_{\mathrm{S}} + F_{\mathrm{MS}} \tag{I.1}$$

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). Whith the antiferromagnetic order as the symmetry breaking field $\varepsilon = \gamma m^2$. 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 $|\eta_y|^2$:

$$\begin{aligned} F = F_{\mathrm{M}} &+ \alpha_{\mathrm{S}}\left(|\eta_x|^2 + |\eta_y|^2\right) + \frac{1}{2}\beta_{\mathrm{S}}\left(|\eta_x|^4 + |\eta_y|^4\right) + \beta_\phi |\eta_x|^2 |\eta_y|^2 + \\ &\frac{\delta}{3}\left(|\eta_x|^6 + |\eta_y|^6\right) + \delta |\eta_x|^2 |\eta_y|^2 \left(|\eta_x|^2 + |\eta_y|^2\right) - \varepsilon\left(|\eta_x|^2 - |\eta_y|^2\right) \end{aligned} \tag{I.2}$$

Here $\alpha_{\mathrm{S}} = \alpha_{\mathrm{S}_0}(T - T_{\mathrm{c}})$, $\beta_{\mathrm{S}} = \beta_1 + \beta_2$, $\beta_\phi = \beta_1 + \beta_2 \cos(2(\phi_x - \phi_y))$ 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 $\alpha_\pm = \alpha_S \pm \varepsilon$. 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 $(1,\alpha i)$ phase where both amplitudes are nonzero and have a relative phase $\phi_x - \phi_y = \pi/2$. A double superconducting transition is found for β_1, β_2, $\gamma > 0$ with the following solutions:

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

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

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

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

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

In the limit of $\delta \to 0$, 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:

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