Scaling of spin-density-wave effects in the quantum critical (Cr$_{86}$Ru$_{14}$)$_{1-x}$V$_x$ alloy system

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Abstract. An analysis of experimental data on the electrical resistivity, Hall coefficient and electronic specific heat coefficient of a quantum critical (Cr$_{86}$Ru$_{14}$)$_{1-x}$V$_x$ alloy system, is reported. The results give information on the role of spin-density-wave effects on the zero temperature relationships between these physical properties.

1. Introduction

We recently reported [1] experimental data on the electrical resistivity ($\rho$), Hall coefficient ($R_H$) and electronic specific heat coefficient ($\gamma$) of a (Cr$_{86}$Ru$_{14}$)$_{1-x}$V$_x$ alloy system, having $x$ in the range 0 to 0.144. The results were used to classify the $T = 0$ K critical point at $x_c = 0.104$ on the ($x-T$) magnetic phase diagram of this antiferromagnetic (AFM) system, as a commensurate spin-density-wave (CSDW) type of quantum critical point (QCP). In this paper we investigate relationships between the zero-temperature spin-density-wave (SDW) components, $\Delta \rho(x)$, $\Delta \gamma(x)$ and $\Delta R_H(x)$, of these physical properties for $x < x_c$. The superscript refers to the case $T = 0$ K.

2. Analysis

Figure 1(a) shows $R_H(T)$ data for a (Cr$_{86}$Ru$_{14}$)$_{0.926}$V$_{0.074}$ alloy, which is representative of the general behaviour observed for the AFM alloys ($x < 0.104$), except for two alloys with $x = 0.032$ and 0.064 for which a “hump”, as in figure 1(b), is superimposed on the curve in the vicinity of the Néel temperature ($T_N$). The origin thereof is presently unknown. The solid line in figure 1(a) is a polynomial fit through the data points. Also shown in figure 1(a) is the $R_H(T)$ curve (broken curve, open circle data points) for a paramagnetic (PM) (Cr$_{86}$Ru$_{14}$)$_{0.879}$V$_{0.121}$ alloy. This alloy is assumed to represent the PM component of $R_H(T)$ in the absence of SDW effects for all the AFM alloys down to 0 K, after it was moved slightly downwards in order to get coincidence of the two curves at $T > T_N$. The SDW component of $R_H(T)$, $\Delta R_H(T) = [R_H(T)]_{\text{AFM}} - [R_H(T)]_{\text{PM}}$, is then given by the difference between the two curves as in figure 1(a). A similar procedure was followed to obtain $\Delta R_H(T)$ for the other AFM alloys, ignoring the “hump” in the vicinity of $T_N$ for the cases of $x = 0.032$ and 0.064. Behaviour quite similar to that shown in figure 1(a) and (b), except for the humps, were previously also observed [2] for AFM and PM alloys of the binary Cr$_{1-y}$Ru$_y$ system.
Figure 1 Hall coefficient $R_H$ as a function of temperature for $(\text{Cr}_{98}\text{Ru}_{14})_{1-x}V_x$ with (a) $x = 0.074$ and (b) $x = 0.064$. The lines and the symbols are discussed in the text.

Figure 2 The Sommerfeld coefficient $\gamma$ as a function of $e/a$ for: (a) the $(\text{Cr}_{98}\text{Ru}_{14})_{1-x}V_x$ system (○) and (b) an updated compilation of ref. [4] of existing data for Cr-Re (●), Cr-Ru (▼), Cr-V (○, △ and ○), Cr-Os (■) and for the present $(\text{Cr}_{98}\text{Ru}_{14})_{1-x}V_x$ alloy system (●). The lines are discussed in the text. The experimental error in $\gamma$ of figure 2(a) is within the size of the experimental points.

Figure 2(a) shows our previous [1] data for the Sommerfeld electronic specific heat coefficient, $\gamma$, for the $(\text{Cr}_{98}\text{Ru}_{14})_{1-x}V_x$ alloy system, plotted as a function of the electron-to-atom ratio $(e/a)$. The solid line is a guide to the eye through the data points for the AFM alloys.

Figure 2(b) shows a compilation by Heiniger et al. [4] of published $\gamma$-data, updated here with new results of Tacheuchi et al. [3], for other AFM SDW and PM Cr alloys; that of Cr-V, Cr-Re, Cr-Ru and Cr-Os, Os being isoelectronic with Ru. Data for the current $(\text{Cr}_{98}\text{Ru}_{14})_{1-x}V_x$ alloy system are also presented in this figure. The binary alloys in figure 2(b) having $e/a \leq 5.95$ or $e/a \geq 6.30$, are PM and the two dotted curves in this figure represent smooth interpolations (polynomial fits up to the cubic term) between these two PM regions for the cases of the Cr-Re and Cr-Os systems. The interpolations can be considered [4] as representative of the PM component ($\gamma_{PM}$) of the AFM alloys with $5.95 \leq e/a \leq 6.30$. Values of $\gamma$ for the AFM alloys in figure 2(b) are seen to be significantly reduced to below the $\gamma_{PM}$ dotted line curves. This is ascribed to a reduction of the density of states at the Fermi surface due to annihilation of nesting portions of the electron and hole Fermi surface sheets on SDW formation. The jump at $e/a \approx 6.18$ in figures 2(a) and (b) on tuning the $(\text{Cr}_{98}\text{Ru}_{14})_{1-x}V_x$ system through the QCP, using decreasing $e/a$, is then understood qualitatively with reference to the general behaviour in figure 2(b).

Guided by the behaviour of $\gamma_{PM}$ in figure 2(b), the broken line in figure 2(a) was constructed through the data points for $e/a < 6.17$ by polynomial curve fitting up to the cubic term (a dotted
straight line fit is also shown for comparison) to represent the PM component of $\gamma_{\text{AFM}}$ for (Cr$_{66}$Ru$_{14}$)$_{1-x}$V$_x$ with $e/a > 6.17$. The SDW AFM component of $\gamma$ is then obtained by subtraction of the experimental data from corresponding values on the polynomial fitted curve of figure 2(a).

### 3. Discussion and Conclusion

The SDW components $\Delta \rho_0^\gamma$, $\Delta \gamma$ and $\Delta R_0^H$ in Cr alloys all result from a reduction in the density of states, described above, and the accompanying loss of charge carriers on SDW formation. These components are thus connected by a common origin, and in the following we investigate such relationships.

Figure 3(a) shows a plot of $\Delta \rho_0^\gamma/\rho_{\text{AFM}}^0$ as a function of $\Delta \gamma/\gamma_{\text{PM}}$ for the (Cr$_{66}$Ru$_{14}$)$_{1-x}$V$_x$ alloy system, using our [1] previous data for $\Delta \rho_0^\gamma/\rho_{\text{AFM}}^0$ and that of $\Delta \gamma/\gamma_{\text{PM}}$ obtained from the polynomial fit in figure 2(a). Although it is difficult to set an error on $\Delta \gamma/\gamma_{\text{PM}}$, a least-squares linear fit, $\Delta \rho_0^\gamma/\rho_{\text{AFM}}^0 = (0.31 \pm 0.02) - (1.0 \pm 0.3) \Delta \gamma/\gamma_{\text{PM}}$, through the data points is nevertheless shown in figure 3(a). The negative coefficient of $\Delta \gamma/\gamma_{\text{PM}}$ in this equation differs from the positive coefficient in the direct relationship, $\Delta \rho_0^\gamma/\rho_{\text{AFM}}^0 = +0.8 \Delta \gamma/\gamma_{\text{PM}}$, obtained by applying similar methods to data [3] for the quantum critical Cr$_{1-z}$V$_z$ system. The difference in sign is empirically related to the fact that $d(\Delta \gamma)/d(e/a)<0$ for $e/a > 6.1$ (as for (Cr$_{66}$Ru$_{14}$)$_{1-x}$V$_x$) in figure 2(b), while the derivative is positive for $e/a < 6.1$ (as for Cr$_{1-z}$V$_z$). The alloys of figure 2(b) show a similar change of sign in $dT_N/d(e/a)$ at $e/a = 6.1$, which was ascribed [2] in the case of Cr$_{1-z}$Ru$_y$, to a suppression of SDW antiferromagnetism for $e/a > 6.1$, possibly through a partial breakdown of the SDW band picture in this system as $e/a$ is increased to above 6.1. The same mechanism is probably responsible for the change in sign of $d(\Delta \gamma)/d(e/a)$.

Norman et al. [5] proposed two possible scenarios for a relationship between $R_0^H$ and $\rho_0^\gamma$ for quantum critical Cr alloys, based on a model that assumes flat nesting portions of the electron and hole Fermi surface sheets. In the one scenario where the system is tuned through the QCP using a parameter $(e)$, like pressure, that does not affect the electron elastic scattering, the relation is:

$$\left[ R_0^H(e) / R_{\text{AFM}}^0(e) \right]_{\text{PM}} = \left[ \rho_{\text{PM}}^0(e) / \rho_{\text{AFM}}^0(e) \right]_{\text{PM}}^2 .$$

The second scenario allows for $x$-dependent elastic scattering effects on tuning the system by doping:
Equation (2) was applied successfully [5] to experimental data for the quantum critical $\text{Cr}_{1-x}V_x$ alloy system. Unexpectedly, application of this equation to the present data on the $(\text{Cr}_{56}\text{Ru}_{14})_{1-x}V_x$ system, using curve fitting to obtain the derivatives from the $\rho$-data, gave unsatisfactory results. Instead, applying equation (1), using $x$ as the tuning parameter, gives a good fit to the present data.

Equation (1) with $c = x$ is easily transformed to one rather relating the SDW components $\Delta R_H^0(x)$ and $\Delta \rho^0(x)$, by using the definitions for these two quantities. The transformation gives:

$$\Delta R_H^0(x)/[R_H^0(x)]_{\text{AFM}} = 2g(x) - [g(x)]^2,$$

where $g(x) = \Delta \rho^0(x)/\rho_{\text{PM}}^0$ represents [3] the fraction of the electron and hole Fermi surface sheets that is annihilated due to the presence of the SDW in the AFM state. Figure 3(b) shows the fit of equation (3), which is reasonable, taking the experimental error into account. The point marked by an open square in figure 3(b) was obtained by applying similar procedures, as described above, to data [2] of the $\text{Cr}_{1-x}\text{Ru}_x$ system. It gives some credence to the present results.

Our results [1] show a linear $x$-dependence of $\rho_{\text{PM}}^0$, indicative of $x$-dependent elastic scattering, contrary to the condition required in equation (1). The failure of equation (2) and the success of equation (1), in the form of equation (3), for the present system are then surprising. It may furthermore be mentioned that $[R_H^0(x)]_{\text{PM}}$ in the present study remains nearly independent of $x$, leaving the $x$-dependence of the LHS of equation (3) to originate mainly from the SDW component, $[R_H^0(x)]_{\text{AFM}}$. The $x$-dependence of the RHS of equation (3), on the other hand, is only related to the $x$-dependence of $g(x)$. Doping presumably has no influence on either $g(x)$ or $[R_H^0(x)]_{\text{AFM}}$.

The methods used to approximate the SDW contributions to $\gamma$ and $R_H$ in this study are, to the best of our knowledge, the only ones presently available. Although these methods seem to be appropriate, there are experimental limitations. It is nevertheless concluded that the experimentally obtained relationships between $\Delta \rho^0(x)$, $\Delta \gamma(x)$ and $\Delta R_H^0(x)$ for the quantum critical $(\text{Cr}_{56}\text{Ru}_{14})_{1-x}V_x$ and $\text{Cr}_{1-x}V_x$ alloy systems differ markedly. The exact reason for this difference is presently unknown. It is, however, suggested that the restriction of flat Fermi surface nesting sheets in equations (1) and (2) and the validity of the rigid band picture for the SDW state, that work well for the $\text{Cr}_{1-x}V_x$ system, probably break down partly in the present $(\text{Cr}_{56}\text{Ru}_{14})_{1-x}V_x$ system.

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