Strong Electron-Phonon Coupling and Sizeable Depairing in $MgCNi_3$

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The recently found superconductor $MgCNi_3$ is investigated by specific heat measurements. Strong electron-phonon coupling is derived from the superconducting part. An unusual magnetic field dependent low temperature upturn of the specific heat is analyzed in terms of ferromagnetic spin fluctuations, suggesting suppression of superconductivity from $T_c \approx 20$ K to $T_c \approx 7$ K. The results are discussed within a proposed two-band model, also explaining so far not fully understood transport measurements.

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I. INTRODUCTION

The discovery of superconductivity in the intermetallic perovskite $MgCNi_3$ [1] with a T_c of $\simeq 8$ K is astonishing, since from the high Ni content a magnetic state would be the obvious expectation. Band structure calculations indeed revealed a dominant contribution of the Ni 3*d* orbitals to the electronic density of states, which drives the compound near a ferromagnetic instability [2]. Due to the unknown electron-paramagnon coupling, the question of the electron-phonon coupling is still unsolved [1, 3–6]. In the present investigation, specific heat data were investigated, to analyze the pairing and depairing contributions and possible multi-band character of $MgCNi_3$.

II. EXPERIMENTS AND RESULTS

Polycrystalline samples of $MgCNi_3$ have been prepared by solid state reaction [1]. Specific heat measurements have been performed in fields up to 14 T.

By modeling the specific heat in the normal state, the superconducting part can be separated. The specific heat of a non-magnetic material consists of an electronic and a lattice part. In a first approximation one may treat the electronic part $\gamma_N T$ as constant over temperature, and the lattice part as a composition of $3N - 3 = 12$ vibrations with constant frequency (Einstein-model) and 3 vibrations with linear (Debye-model) frequency

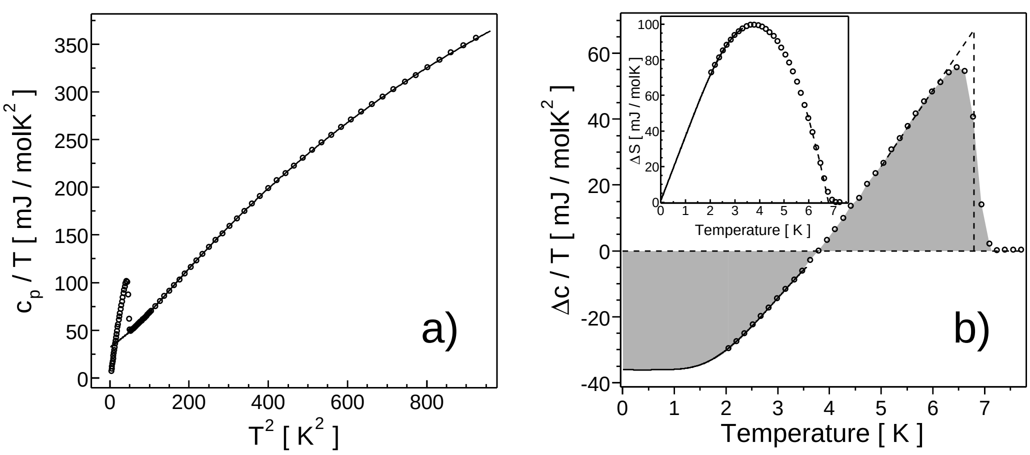

FIG. 1: Specific heat of $MgCNi_3$. Left panel: c_p/T vs T. Solid line: Fit of Eq. (1) to the normal state data. Right panel: Superconducting part $\Delta c/T$ vs. T. Solid line: Fit of Eq. (2). Dashed line: Entropy conserving construction. Inset: Entropy ΔS vs. T.

dispersion:

$$c_p(T) = \gamma_N T + \sum_{i=1}^{3} 3R\left(\frac{T}{\Theta_{Di}}\right)^3 \int_0^{\Theta_{Di}/T} dx \frac{e^x x^4}{(e^x - 1)^2} + \sum_{i=4}^{15} R\left(\frac{\Theta_{Ei}}{T}\right)^2 \frac{e^{\Theta_{Ei}/T}}{\left(e^{\Theta_{Ei}/T} - 1\right)^2}. \quad (1)$$

It is found, that 9 phonons are sufficient to describe the specific heat up to $T = 30$ K. The fit result is shown in Fig. 1a). The Sommerfeld parameter converged to $\gamma_N = 31.4$ mJ/molK^2. From Fig. 2a) it is seen, that the low temperature field data are not described by this model. This strongly indicates the influence of paramagnons, particularly since a small field dependence is observed. Using the bare electron parameter $\gamma_0 = 11.0$ mJ/molK^2, $\gamma_N = 31.4$ mJ/molK^2 and $\gamma_{diff} \approx 5$ mJ/molK^2 due to paramagnons, the mass enhancement relation $\gamma_N + \gamma_{diff} = \gamma_0 (1 + \lambda_{ph} + \lambda_{sf})$ results in strong electron-phonon coupling of $\lambda_{ph} \approx 1.85$ and sizeable electron-paramagnon coupling of $\lambda_{sf} \approx 0.43$.

The superconducting transition temperature is determined by an entropy conserving construction (inset and dashed line in main-panel of Fig. 1b)), resulting in $T_c = 6.8$ K. The superconducting jump height amounts $\Delta c/(\gamma_N T_c) = 2.09$ indicating significant strong coupling influence (weak-coupling BCS : 1.43). To analyze the gap, a BCS expression valid for 1 K $< T <$ 3.4 K is used:

$$\Delta c(T) = 8.5\gamma_N T_c \exp\left(-0.82\frac{\Delta_{BCS}(0)}{k_B T}\right) - \gamma_N T. \quad (2)$$

For a strong coupling material the gap opens faster than predicted by the weak-coupling BCS theory. As expected, the fitted phenomenological gap $2\Delta_{exp}/k_B T_c = 3.75$ exceeds the BCS weak coupling prediction $2\Delta_{BCS}(0)/k_B T_c = 3.52$ (see Fig. 1b)). The extent of strong coupling corrections to the gap $\Delta_{\mathrm{exp}} \approx 1.10$ meV can be analyzed, using an approximative formula derived from Eliashberg theory [7]:

$$\frac{2\Delta(0)}{k_{\mathrm{B}}T_{\mathrm{c}}} = 3.52\left[1 + 12.5\left(\frac{T_{\mathrm{c}}}{\omega_{\mathrm{ln}}}\right)^2 \ln\left(\frac{\omega_{\mathrm{ln}}}{2T_{\mathrm{c}}}\right)\right].$$

Using $T_{\mathrm{c}} = 6.8$ K, the logarithmically averaged phonon frequency amounts $\omega_{\mathrm{ln}} = 149$ K. The derived coupling parameters and ω_{ln} can now be rechecked, using a refined McMillan formula:

$$T_{\mathrm{c}} \approx \frac{\omega_{\mathrm{ln}}}{1.2}\exp\left[-\frac{1 + \lambda_{\mathrm{ph}} + \lambda_{\mathrm{sf}}}{\lambda_{\mathrm{ph}} - \lambda_{\mathrm{sf}} - \mu^{\star}\left[1 + 0.6\left(\lambda_{\mathrm{ph}} + \lambda_{\mathrm{sf}}\right)\right]}\right]. \tag{3}$$

With $\omega_{\mathrm{ln}} = 149$ K and $\lambda_{\mathrm{ph}} \approx 1.85$, $\lambda_{\mathrm{sf}} \approx 0.43$ and an usual value of $\mu^{\star} = 0.13$, the superconducting transition temperature of $MgCNi_3$ amounts $T_{\mathrm{c}} \approx 6.5$ K. With $\lambda_{\mathrm{sf}} = 0$ (ignoring the low-temperature specific heat upturn), one arrives at a much higher $T_{\mathrm{c}} \approx 20$ K.

The electron-phonon coupling constant is usually analyzed by the deviation function $D(t) = H_{\mathrm{c}}(T)/H_{\mathrm{c}}(0) - (1 - t^2)$ with $t = T/T_{\mathrm{c}}$, giving the deviation of the thermodynamic critical field $H_{\mathrm{c}}(T)$ from the two-fluid model. $H_{\mathrm{c}}(T)$ is calculated from the Gibbs free energy using $H_{\mathrm{c}}(T) = \sqrt{-8\pi\Delta F}$ and $\Delta c(T) = -T\mathrm{d}^2\left(\Delta F\right)/\mathrm{d}T^2$. Weak-coupling superconductors are described by the BCS model (see Fig. 2b)), whereas strong coupling superconductors like Pb have a pronounced maximum in $D(t)$. But $D(t)$ for $MgCNi_3$ closely resembles that of niobium (with $\lambda_{\mathrm{ph}} \approx 1.0$). This seemingly contradiction to the derived value of $\lambda_{\mathrm{ph}} \approx 1.85$ for $MgCNi_3$ can be resolved within a two-band model of superconductivity, which can mask strong-coupling behavior of the deviation function [6]. Band structure calculations revealed a 90 % contribution of a slow hole band (with a Fermi velocity of $\overline{v}_{\mathrm{F}} \approx 1.2 \times 10^5$ m/s) and 10 % contribution of a fast electron band ($\overline{v}_{\mathrm{F}} \approx 3.9 \times 10^5$ m/s). Two-band superconductivity would also naturally explain tunnel spectroscopy and Hall experiments, which are both much more sensitive to the faster charge carriers [5, 8, 9]. Thus the effective charge carriers measured by Hall experiments are electrons, despite the much lower partial density of states. The gap of $2\Delta/\left(k_{\mathrm{B}}T_{\mathrm{c}}\right) > 4$, measured in tunnel spectroscopy experiments is also mainly influenced by the faster electrons. Specific heat measurements average over both bands and the measured gap is mainly influenced by the hole band due to the much higher partial density of states. Therefore the gap as well as the electron-phonon coupling constant in the electron band is expected to be larger than in the hole band [6].

III. CONCLUSIONS

The present analysis revealed a highly interesting interplay of competing effects. The strong mass enhancement found from the specific heat analysis and the correspondingly much too low T_{c} can be understood by the presence of ferromagnetic spin fluctuations. It was shown, that superconductivity in $MgCNi_3$ is indeed suppressed by these paramagnons

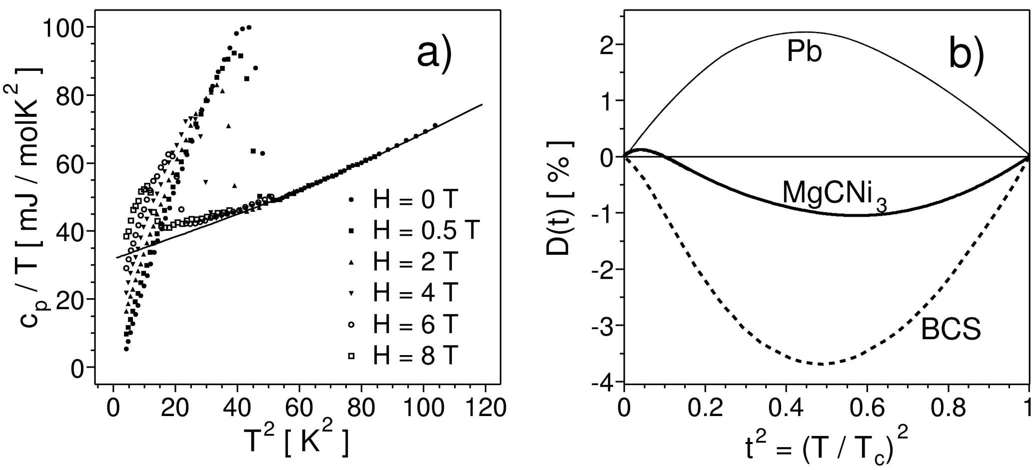

FIG. 2: Field dependent specific heat and deviation function $D(t)$ of $MgCNi_3$. Left panel: c_p/T vs. T. Solid line: Fit of Eq. (1) to the zero field normal state data. Right panel: $D(t)$ vs. $t^2 = (T/T_c)^2$, giving the deviation of $H_c(T)$ from the two-fluid model prediction.

from $T_c \approx 20$ K down to $T_c \approx 7$ K. The possibility of multi-band superconductivity in accord with the theoretical proposed multiple Fermi surface sheets, a van Hove singularity and possible phonon softening and anharmonic effects highly motivate further experimental and theoretical studies.

Acknowledgments

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