Kinks: Fingerprints of strong electronic correlations

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Abstract. The textbook knowledge of solid state physics is that the electronic specific heat shows a linear temperature dependence with the leading corrections being a cubic term due to phonons and a cubic-logarithmic term due to the interaction of electrons with bosons. We have shown that this longstanding conception needs to be supplemented since the generic behavior of the low-temperature electronic specific heat includes a kink if the electrons are sufficiently strongly correlated.

1. Introduction

Landau’s Fermi liquid theory [1] can be considered as the “standard theory” of solid state physics. It predicts that the electronic properties of a (normal) metal follow, in the presence of Coulomb correlations, a renormalized (quasiparticle) version of those for non-interacting electrons. Among the most fundamental physical properties is the heat capacity which, at low temperatures, is predominated by the electronic degrees of freedom. For a normal metal, Landau’s Fermi liquid theory [1] predicts a linear increase of the specific heat capacity with temperature \( c_V = \gamma_{FL} T \) and a cubic term, more precisely a term \( \sim T^3 \log(1/T) \), as the leading correction [2, 3]. For free electrons, the prefactor \( \gamma_0 \) is directly proportional to the electronic density of states at the Fermi level since, due to the Pauli principle, only these electrons contribute. In the case of a Fermi liquid, we merely need to introduce a quasiparticle renormalization factor \( 0 < Z_{FL} < 1 \) to account for the Coulomb interaction, which enhances the specific heat of a correlated metal by \( \gamma_{FL} = \gamma_0 / Z_{FL} \). However, this electronic contribution prevails only at temperatures much lower than the Debye temperature. Otherwise the cubic phononic term, which has a much higher prefactor because of its bosonic nature, dominates.

As we have shown in a recent letter [4], this longstanding conception needs to be supplemented: For strongly correlated electrons, a clear kink in the temperature dependence of the specific heat appears, marking the abrupt change from one linear behavior to a second one with a reduced slope at higher temperatures. This can be shown numerically solving the Hubbard model [5] within dynamical mean field theory [6], using exact diagonalization as an impurity solver. Quantitatively the same results can also been obtained analytically, following the derivation by Abrikosov et al. [2] for the specific heat, taking the recently observed kinks in the self energy as a starting point [7, 8].

The experimental confirmation of these theoretical results is somewhat problematic since typically, at the kink temperature, the phononic contribution to the specific heat is already dominating. An exception in this respect is LiV₂O₄ [9, 10], the first heavy Fermion system
with $d$-electrons, since the kink temperature is here particularly low. And, indeed, the precise inspection of the experimental data shows a kink in the correct temperature range [4]. In this Proceeding, we will review the previous theoretical results and include additional data.

2. **Kinks in the self energy**

In the presence of strong electronic correlations, the $\mathbf{k}$-integrated spectral function $A(\omega)$ shows a typical three peak structure with a lower and an upper Hubbard band and a quasiparticle peak in between. Using the DMFT formula

$$\Sigma(\omega) = \omega + \mu - 1/G(\omega) - \Delta(G(\omega))$$

which relates Green function and self energy at frequency $\omega$, one can show [8] that such a strongly correlated three peak structure necessarily entails a kink. Note that the hybridization function $\Delta(G(\omega))$ in Eq. (1) is for a simple semi-circular density of states just $\Delta(G(\omega)) = D^2/4G(\omega)$ ($D$: half the bandwidth). For other lattices, $\Delta(G(\omega))$ depends on the moments of the non-interacting density of states with a similar term proportional $G(\omega)$ dominating.

The kink argument is now as follows [8]: The first three terms of the r.h.s of Eq. (1) yield an almost linear frequency dependence for the real part of the self energy over the entire region of the central quasiparticle peak. The derivative hence gives a quasiparticle renormalization factor

$$Z_{QP} = \left[1 - \frac{\partial \text{Re} \Sigma(\omega)}{\partial \omega} \right]_{\omega=0}^{-1}$$

The last (hybridization) term however yields an additional contribution to $\text{Re} \Sigma(\omega)$ which basically is proportional to $\text{Re} G(\omega)$. This real part can be directly obtained from the spectral function of the central quasiparticle peak $A(\omega) = -\frac{1}{\pi} \text{Im} G(\omega)$ via a Kramers-Kronig transformation. Inside the overall width of the quasiparticle peak, there is a turning point in $A(\omega)$. Hence, $\text{Re} G(\omega)$ has a linear frequency dependence up to an maximum at the turning point $A(\omega)$. After this maximum changes in $\text{Re} G(\omega)$ are minor. Altogether this means that at low frequencies we have to add the slope obtained from the $\Delta(G(\omega))$ in Eq. (2) yielding an altogether smaller Fermi liquid renormalization factor $Z_{FL}$ at low energies. In between the two regimes $Z_{FL}$ and $Z_{QP}$, there is a kink at a frequency $\omega^*$. In summary we hence have:

$$\text{Re} \Sigma(\omega) = \begin{cases} (1 - \frac{1}{Z_{FL}})\omega & \omega < \omega^* \\ (1 - \frac{1}{Z_{QP}})\omega - b & \omega > \omega^* \end{cases}$$

with the constant $-b = (\frac{1}{Z_{QP}} - \frac{1}{Z_{FL}})\omega^*$ providing for a continuous function.

Before we turn to the specific heat in the next section, let us note that the kink in the self energy directly leads to a kink in the energy-momentum dispersion relation of the correlated electrons. Let us also remark here, that the result of generic kinks in the self energy of strongly correlated systems should be robust beyond DMFT, as similar effects are to be expected in cluster [11] and diagrammatic extensions [12] of DMFT.

3. **Analytical formula for the specific heat**

Based on Eq. (3), we have developed an analytical theory for the specific heat on the basis of a formula by Abrikosov, Gor’kov and Dzyaloshinskii (AGD) for the entropy of a fermionic system at low temperatures [2]:

$$S(T) = \frac{1}{2\pi i} \int_{-\infty}^{\infty} d\epsilon N(\epsilon) \int_{-\infty}^{\infty} dy \frac{e^y}{(e^y + 1)^2} \left[ \log G^{-1}_R(\epsilon, yT) - \log G^{-1}_A(\epsilon, yT) \right]$$

This AGD formula is (through a low-temperature diagrammatic expansion) based on the low frequency behavior of the self energy $\Sigma(\omega)$ at zero temperature [or the corresponding retarded
and advanced Green function in Eq. (4) so that we can directly apply it with \( \Sigma(\omega) \) from Eq. (3). Let us note that \( N(\epsilon) \) is the density of states and the frequency integral has been rewritten through a dimensionless variable \( y = \omega / T \) \((k_B \equiv 1)\). The AGD formula (4) can be easily differentiated w.r.t. \( T \), so that the specific heat \( c_V(T) = T \frac{dS(T)}{dT} \) can be computed directly. With some algebra (see [4] for more details) and substituting \( A(\epsilon, yT) \) by \( \delta \)-functions, we obtain the final result

\[
c_V(T) = T \left[ \frac{1}{Z_{FL}} \int_{|y|<\omega^*} N\left(\frac{yT}{Z_{FL}}\right) \right. + \left. \frac{1}{Z_{QP}} \int_{|y|>\omega^*} N\left(\frac{yT}{Z_{QP}} + b\right) \right] dy \frac{y^2 e^y}{(e^y+1)^2}.
\]

(5)

Knowing the two renormalization factors \( Z_{FL} \) and \( Z_{QP} \) and the kink frequency \( \omega^* \) as well as the non-interacting density of states \( N(\epsilon) \), Eq. (5) allows us to calculate the specific heat through a simple integral. If vice versa, the specific heat is known, e.g., experimentally, we can employ Eq. (5) as a fit formula for obtaining \( Z_{FL} \), \( Z_{QP} \) and \( \omega^* \).

4. Experimental validation

The latter (fit formula) approach had been taken for the experimental validation of the specific heat kinks in LiV\(_2\)O\(_4\) since LDA+DMFT calculations [13] for LiV\(_2\)O\(_4\) [14] could not provide for a fine enough resolution of the low frequency dependence of the self energy, even when using the projective quantum Monte Carlo method [15] which is most appropriate for this purpose. As Fig. 3 of [12] shows the three fitting parameters provide for an excellent agreement of Eq. (5) and the specific heat of [9, 10], including a clearly visible kink. Let us note that we did not subtract a phonon contribution for the specific heat since (i) it does not alter the existence or non-existence of a kink, (ii) it is still an order of magnitude smaller than the electronic contribution at the kink temperature and (iii) there is a considerable arbitrariness depending on the reference system chosen.

5. Numerical results

Fig. 1 shows results of our final equation (5) applied to the Hubbard model with a semi-circular density of states with half bandwidth \( D \equiv 1 \). As an input to Eq. (5), \( Z_{FL}, Z_{QP} \) and \( \omega^* \) have been fitted to the numerical renormalization data for the DMFT self energy from Ref. [16]. Besides, we have also calculated the DMFT specific heat directly, using exact diagonalization (ED) with 7 levels in the impurity bath. Both results agree very well, and the minor deviations can be attributed to the numerical inaccuracy of the exact diagonalization study for which \( c_V \) had to be obtained via a numerical differentiation of the total energy.

In the inset, we show the specific heat over a slightly extended temperature range. As the quasiparticle peak eventually ends, the specific heat has a maximum after the kink temperature. Note that this maximum is not contained in our formula (5) since it would require an extension of the self energy description Eq. (3) to higher energies where \( \text{Re}\Sigma(\omega) \) has a maximum at the frequencies between Hubbard and quasiparticle bands and \( \text{Im}\Sigma(\omega) \) becomes important.

6. Conclusion

Landau’s Fermi liquid theory predicts a linear temperature dependence of the electronic specific heat capacity with temperature. We have shown this longstanding conception needs to be supplemented: For strongly correlated electrons, a clear kink in the temperature dependence appears, marking the abrupt change from one linear behavior to a second one with a reduced slope at higher temperatures. Recent experiments on LiV\(_2\)O\(_4\), an ideal material for studying the electronic specific heat, confirm our theory. A consequence of our findings is that materials
Figure 1. Specific heat as a function of temperature for various values of the Coulomb interaction U obtained via the AGD based equation (5) [solid lines] and numerically by exact diagonalization of the DMFT equations (crosses). Inset: behavior over an extended temperature range which shows a maximum after the kink temperature marking the end of the quasiparticle band.

with correlated electrons are more resistive to cooling at low temperatures (where cooling is particularly difficult) than expected from the behavior at intermediate temperatures.

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