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L-K Treatment of the SdH Oscillations in the SDW state of Q1D Materials

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Abstract

We have applied Lifshitz-Kosevich theory to directly fit the high field oscillatory magnetoresistance in the Q-1-dimensional Bechgaard salts in $(TMTSF)_2X$ ($X = AsF_6$ or ClO_4[Q-state]) in their spin density wave states. Values of m*, Dingle temperature, and SdH frequencies are obtained, and the anomalous temperature dependence of the oscillation amplitudes are discussed.

Keywords: organic charge transfer salts, high field magnetotransport, quantum oscillations

Bechgaard salts which form a spin density wave (SDW) state under ambient conditions can exhibit oscillations in their magnetoresistance at high magnetic fields. These include $(TMTSF)_2X$, where $X = PF_6$, AsF_6, and NO_3 [1, 2], and $X = Q\text{-}ClO_4$ [3], that is for the thermally quenched state where the ClO_4 anions do not order. Generally, below the ordering temperature T_{SDW} the original quasi-one-dimensional Fermi surface nests, thereby creating electron and hole pockets in the case where the nesting is incomplete. The origin of the oscillations may be described semiclassically if we consider that these pockets, which lie on the along the contours of the reconstructed Q-1-D Fermi surface, provide a magnetic breakdown path with Bragg reflection points at the reconstructed Brillouin zone [4]. Hence oscillations in the range of 180 to 265 T in frequency, which correspond to about 3% of the original Brillouin zone, can arise. Following this semiclassical picture, below T_{SDW} the amplitude of the oscillations may be described by the standard Lifshitz-Kosevich description of quantum oscillations[5] with the inclusion of the magnetic breakdown probabilities and the evolution of the SDW order parameter[4]. In this model the amplitudes increase with lower temperature, and the correspondence with experiment is reasonably close.

Anomalous in the behavior of these oscillations is their amplitudes, which are non-monotonic with decreasing temperature, and which have a maximum at a characteristic temperature T* below T_{SDW}. It is important to quantify this behavior in terms of the parameters of the problem, i.e. the effective mass, the Dingle temperature, and the oscillation frequency. For pulsed magnetic field measurements at low Landau level index (< 10), it is necessary to consider analysis of sometimes very few oscillations which are small with respect to the background magnetoresistance. To determine these parameters we have applied a single or multiple frequency fit of a simplified form of the LK formula to the normalized oscillatory data: $R_{osc} = \frac{\sigma}{B^{1/2}} f\, Cos(F/B + \Phi) + \rho(B)$. Here $f = \exp(-Y)X/Sinh(X)$, $X = 14.69Tm^*/B$, $Y = 14.69T_D m^*/B$, $\rho(B)$ is a residual background term, and m*, T_D, F, and Φ are the effective mass, Dingle temperature, oscillation frequency, and phase factor. σ is normally a temperature independent pre-factor.

Shown in Figure 1 is a study of the oscillatory magnetoresistance of $(TMTSF)_2AsF_6$ *vs.* temperature. Here the total magnetoresistance has been divided by a low order polynomial fit (which represents the average magnetoresistance). This eliminates that part of the oscillatory amplitude which is dependent on the background resistance. The non-monotonic dependence of the amplitudes with temperature is clear from the data. To address this anomalous behavior, we first applied the LK relationship to the data with all parameters variable in the fit, including the pre-factor σ_n. From these results yield average values for the effective mass (typically about $0.5\ m_0$ for $X = AsF_6$ and PF_6 and $1.2\ m_0$ for $X = ClO_4$ [3]) and the other parameters. We then fixed m* to its average value and also fixed σ_n based on the high temperature region of the data. A second iteration of the fits are then performed where T_D is allowed to change with temperature (See concluding section for relation to m*). This specific assignment of fixed vs. variable parameters places the temperature dependence of the amplitudes on the LK reduction factors. Below T*≈3.5 K, some new mechanism starts to quickly attenuate the oscillations, although their frequency remains essentially constant. This means that the orbital paths remain unchanged, but either the conventional LK factors or some new reduction factor takes on a temperature dependence below T*.

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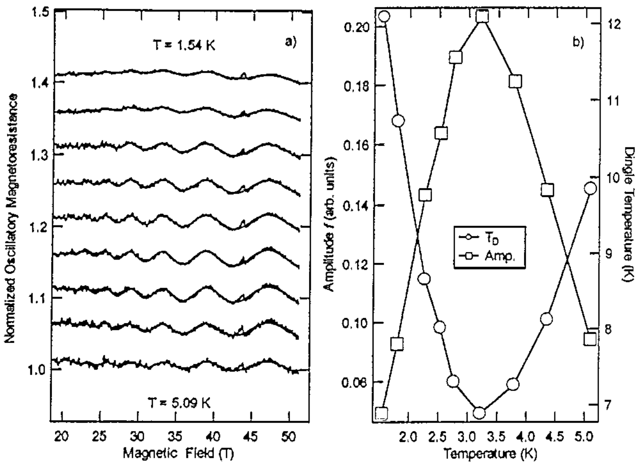

Fig. 1. a) Oscillatory Magnetoresistance for X = AsF_6 for different temperatures. Smooth curves are the LK fits. b) Variation of T_D and LK reduction factor f for fixed mass ($m^* = 0.6\ m_0$) and pre-factor σ_n. The oscillation frequency is 220 T. Here I//c-axis and B//c-axis.

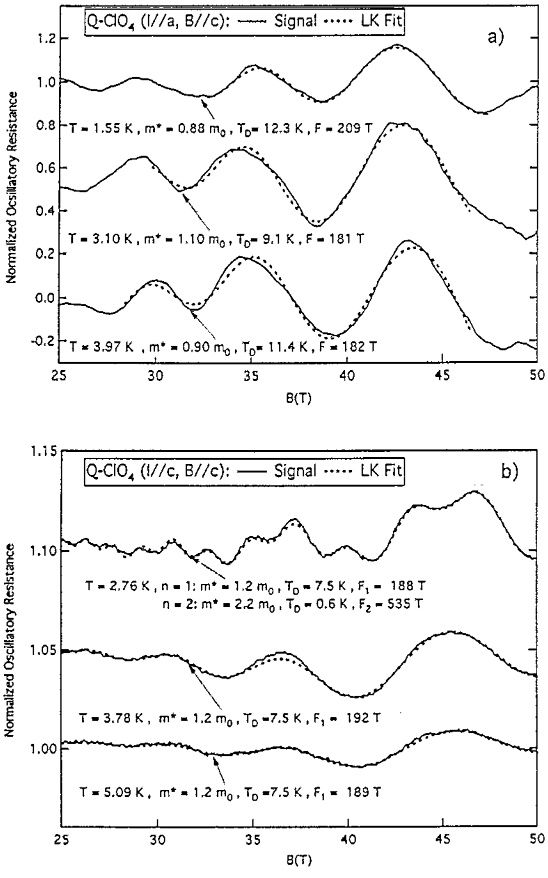

Fig. 2. SdH-like oscillations in thermally quenched $(TMTSF)_2ClO_4$. Parameters of the LK constant are shown. a) a-axis transport (all LK parameters variable). b) panel, c-axis transport (m^* and T_D held fixed for n = 1).

For the traditional LK to remain applicable, this would mean that either m* or T_D become temperature dependent. If m* changes, then many body effects may be important; or, if T_D changes, then scattering processes may come into play. We have recently proposed the opening of a magnetic breakdown gap below T*[3]. Such a gap would have an effect similar to that played by the exponential factor in the LK expression, and would be an alternative to a temperature dependent m* or T_D.

For thermally quenched Q-$(TMTSF)_2ClO_4$, magnetoresistance measurements with B//c*-axis [3] show an orbital frequency at F ≈190 T. This frequency is the result of the nesting of the original Fermi surface by the SDW wave vector Q(1/2,1/4), in contrast to the F ≈ 265 T frequency which appears with anion ordering for Q(0,1/2,0). The 190 T oscillation amplitude in all cases is non-monotonic with a maximum around 3.5 K, very much like AsF_6 in Fig. 1. We show in Fig. 2 results for two different samples. For I//a-axis data only certain regions could be fit with accuracy. Here we let all parameters float in the LK fits as listed in the figure. For the I//c-axis the data was more regular. Here m* and T_D could be replaced by the average values. We note that a second, independent frequency (535 T) was observed at 2.76 K, and both n = 1 and 2 terms were used to fit the data. This second frequency is the second harmonic of the 265 T frequency observed in anion-ordered ClO_4, which indicates that this sample was not totally quenched.

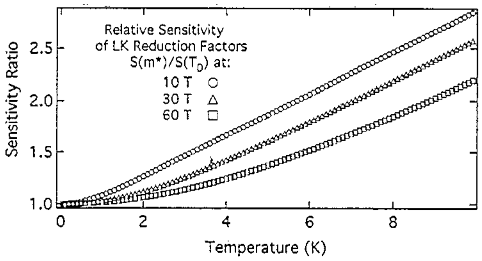

Fig. 3. The sensitivity of the LK reduction factors to the effective mass parameter (relative to the Dingle term). Here the parameters m* = 1 and T_D = 5 K were used for the example.

We conclude by noting that since T_D and m* appear as a product in the exponential term, either term, increasing in the same proportion will cause attenuation. We may determine the relative sensitivity to the effective mass and the Dingle temperature, $S(m^*) \equiv \dfrac{1}{fT_D}\dfrac{\partial f}{\partial m^*}$ and $S(T_D) \equiv \dfrac{1}{fm^*}\dfrac{\partial f}{\partial T_D}$ respectively, to the LK fits through their dimensionless ratio as shown in Fig. 3. Here we see that the most effective separation of the two parameters, based on the LK fits, should be done by fitting data at high temperatures, and at lower fields.

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