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FERMI SURFACE MODIFICATIONS AND MAGNETIC BREAKDOWN

CONNECTED TO CHARGE-DENSITY WAVES IN NbSe_3 ^{*}

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Fermi Surface Modifications and Magnetic Breakdown Connected to Charge-Density Waves in NbSe_3 *

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The magnetoquantum oscillations in NbSe_3 show frequency shifts and beat structures due to interaction with the pinned charge-density-wave (CDW) configuration. Measurements in magnetic fields up to 220 kG indicate that local deformations of the pinned CDW cause extremal area changes in small lens-shaped sections of normal Fermi surface (FS). Calculations of magnetic breakdown (MB) to the open nested sections of FS with a distribution of areas at the MB junctions can explain the data.

1. INTRODUCTION

The Fermi surface (FS) of NbSe_3 at helium temperatures reflects both the band structure of the quasi-one-dimensional crystal structure and the presence of two charge-density-waves (CDWs) which form below 144 and 59K respectively [1]. The high temperature Fermi surface as calculated by Shima and Kamimura [2] consists of four large quasi-parallel sheets approximately perpendicular to the b -axis which can nest in pairs to form the CDWs. In addition a 5th band crosses the Fermi level at several points in the Brillouin zone (BZ) and can contribute small hole or electron pockets to the low temperature FS. The imperfect nesting associated with the 59K CDW transition can also generate hole and electron pockets which remain at low temperature.

In magnetotransport experiments these small lens-shaped pockets can be connected to the open sheets of the nested FS by magnetic breakdown (MB) across the CDW gaps resulting in an open-orbit network. The presence of this type of FS topology and the existence of critical MB fields at relatively low values of magnetic field can produce major contributions to the magnetoquantum oscillations observed in the transverse magnetoresistance.

In this paper we report observations of the magnetoquantum resistance oscillations in NbSe_3 which provide evidence of such an open-orbit network in NbSe_3 . In addition, the experiments show that the magnetoquantum oscillation frequencies and amplitudes are perturbed by changes in the pinned CDW configuration due to a transfer of electrons between the CDW condensate and the normal electron FS.

The proposed MB mechanisms involving an open-orbit network provide a consistent explanation for the unusual changes associated with the pinned CDW structure. Deformation of the CDW can shift the local Fermi level changing both the extremal FS area and the MB gaps.

2. EXPERIMENTAL RESULTS

The magnetoquantum oscillations in NbSe_3 at 1.2K are dominated by a few low frequency oscillations representing an extremum FS area that corresponds to approximately 10^{-3} of the BZ cross-sectional area. For transverse magnetic fields parallel to $\hat{c}$ the frequency of the dominant oscillation is measured in the range 0.30 to 0.31 MG when the crystal is in the as-cooled CDW state. By depinning

and repinning the CDW, or by reversing the magnetic field, or by reversing the current it is possible to shift the frequency down to a range of 0.28 to 0.29 MG. This shift is also accompanied by large changes in the amplitude of the oscillation. Both the frequency shift and the amplitude are sensitive functions of the specific crystal residual resistance ratio (RRR) and the impurity pinned CDW configuration.

For a fixed CDW configuration and a fixed magnetic field direction the magnetic field dependence of the amplitude can also show strong modulations corresponding to beats that suggest the presence of two closely spaced frequencies. However, both the

Fig. 1. (a) Oscillatory transverse magnetoresistance, 0-70 kG at 1.2K. $\hat{H}||(\hat{c}+10^\circ)$, $\hat{I}||\hat{b}$, RRR=258. (b) MB model calculations of magnetoresistance, $\rho_{11}/\rho_s \equiv (m\omega_c/ne^2)$. $F_{AV}=0.31$ MG, $\Delta F=0.022$ MG.

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spacing and the magnitude of the frequencies can be changed by reconfiguring the CDW either by warming and recooling the crystal or by depinning and repinning the CDW at 1.2K. This behavior has been observed for most magnetic field directions lying in the $\bar{a}$ - $\bar{c}$ plane, but it varies considerably from crystal to crystal or for different runs on the same crystal indicating a high sensitivity to the detailed pinned configuration of the CDW.

Fig. 1(a) shows a typical field sweep using ac second harmonic detection in the range 0 to 70 kG. A strong beat is observed and the Fourier transform shows a clear frequency split with $\Delta F = 0.022$ MG with the midpoint frequency equal to 0.31 MG for $\bar{H}||(\bar{c}+10^\circ)$. The same crystal has been rerun many times to test the variation in frequency splitting and amplitude modulation. A second magnetic field sweep in the range 0 to 220 kG is shown in Fig. 2(a). In this case the frequency split is greater, $\Delta F = 0.042$ MG, with a midpoint frequency of 0.34 MG for $\bar{H}||(\bar{c}+25^\circ)$. The beats have fewer oscillations between nodes consistent with a greater ΔF and the Fourier transform shows a high harmonic content. This is partially due to the spin splitting at high fields, but can also arise from the MB mechanisms to be discussed in 3.

3. MAGNETIC BREAKDOWN MECHANISMS

Assuming that the quantum oscillations in NbSe_3 are dominated by a MB network and that the pinned CDW structure interacts with the local FS through local variations of the CDW phase deformation, then MB models can explain the results. The major new feature required takes into account dephasing effects in MB caused by small changes in the critical cross sections of the FS caused by deformation of the CDW around impurity sites. The calculational framework required in this model was developed by Sowa and Falicov [3] using a one-dimensional open-orbit network incorporating MB junctions [4]. This model consists of a FS intersecting the BZ such that a vanishingly small closed lens orbit results connected across a gap to open sections which form one-dimensional open-orbits. No scattering occurs on the lens-shaped orbits but small-angle scattering completely destroys phase coherence from one end to the other of the open arm. In this case the network reduces to a semiclassical set of "touching" circles -- in which only wave packet intensity is relevant -- connected by "quantum" nodes with modulated transmission and reflection coefficients governing the topology. The FS area distribution is represented by a phase with a rectangular probability distribution between two limiting values determined by the minimum and maximum k-space cross-sectional areas of the lens orbit.

The calculated magnetoresistance curves using this model with $\omega_0\tau = 1$ ($\omega_0 = eH_0/mc = \text{MB cyclotron frequency}$) give good fits to the data as shown in Figs. 1(b) and 2(b). The spread in frequencies of the lens orbits required to fit the data represent a variation of 10-15% in the fundamental frequency. The critical MB field has been taken to be 10 kG so that $\omega_0 = 0.1 H_0$ and the units $10\omega_c/\omega_0$ in Figs. 1(b) and 2(b) correspond to the experimental magnetic field ranges used for the data although the model does not uniquely determine H_0 .

Fig. 2. (a) Oscillatory transverse magnetoresistance, 0-220 kG at 1.2K. $\bar{H}||(\bar{c}+25^\circ)$, $\bar{I}||\bar{b}$. RRR=258. (b) MB model calculation of magnetoresistance, $\rho_s \equiv (m\omega_0/ne^2)$. $F_{AV} = 0.34$ MG, $\Delta F = 0.042$ MG.

4. CONCLUSIONS

Phase deformations of the pinned CDW can introduce significant changes in the local Fermi level, the CDW gap and the extremal FS areas. In the presence of an open-orbit network with MB junctions this spatial variation in local FS area introduces a coherent beat modulation in the quantum oscillatory magnetoresistance. Fits of the data to a calculated MB model provide a good determination of the frequency spread and corresponding area variation of the local FS.

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