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New details of the Fermi surface of 2H-$NbSe_2$ revealed by quantum oscillations in the magnetostriction

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Abstract. The layered charge-density wave (CDW) superconductor 2H-$NbSe_2$ (T_S=7.2 K) is the very first material in which quantum oscillations have been observed in the mixed state by means of magnetization and magnetostriction measurements. The magnetostriction technique offers the advantage that quantum oscillations are particularly pronounced, which is due to pressure sensitivity of the relevant cross-section of the Fermi surface. Moreover, measurements can be performed for a field oriented along the crystallographic axis in contrast to the torque technique that is routinely used. Here we present magnetostriction measurement on a high-quality single-crystalline sample for temperatures 0.25-8.0 K using a sensitive capacitance dilatometer. Two oscillation frequencies are observed at the lowest temperatures for the in-plane orientation of the applied magnetic field. These new data reveal that the Fermi-surface sheet in the first Brillouin zone has two cross-sections, rather than the conventional pan-cake shape.

1. Introduction

The layered transition-metal dichalcogenide 2H-$NbSe_2$ has attracted particular attention because of the inhomogeneous ground state apt to coexistence of charge density wave instabilities (CDW) and superconducting phase. So far, however, a conclusive picture of the topology of the three-dimensional Fermi surface (FS) and its relation to the observed CDW has not yet been achieved. Early band structure calculations [1,2] and magnetothermal quantum oscillations measurements [3] indicated the presence of several hole-like sheets on FS including the Γ-centered thin pan-cake [3] with the slight, about 3%, in-plane anisotropy. Since then, various techniques were applied to study this compound in a CDW regime, however, a conclusive picture of the FS topology and its relation to the observed CDW has not yet been achieved so far. Here we report the results of phase and frequency analysis of quantum magnetostriction oscillations measurements on 2H-$NbSe_2$ indicative of new FS features below the CDW and superconducting transition temperatures.

2. Experimental details and results

The magnetostriction measurements were performed in a sensitive capacitance dilatometer in the applied field up to 14 T oriented in the basal plane (normal to the hexagonal c-axis) of the high-quality single crystal. The typical magnetostriction measurements along the c-axis are presented in figure 1.

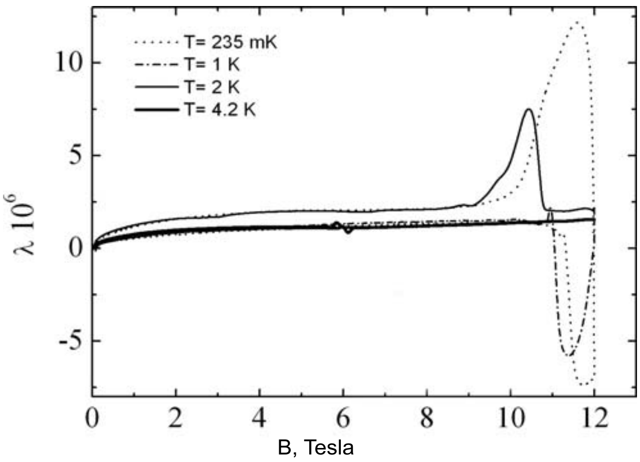

Figure 1. The measured magnetostriction curves.

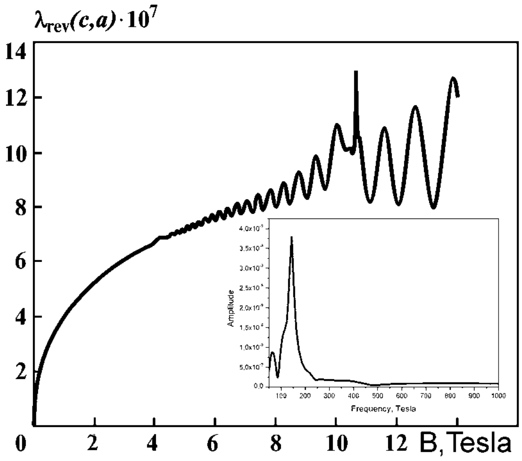

Figure 2. Reversible part of magnetostriction.

A routine procedure [4] was used to derive the reversible part of magnetostriction (figure 2) which clearly demonstrates the presence of quantum oscillations.

2.1. Analysis of oscillations frequency

In order to find the harmonic components of the dependence $\lambda_{rev} = f(1/B)$ and their frequencies, the smooth part of the measured dependences was extracted beforehand by the gliding average technique. The frequencies of the derived harmonic components were determined from the plotted frequency dependence of the oscillation amplitude A(F). The amplitudes were calculated from the Euler-Fourie formula:

$$A_F = \sqrt{a_F^2 + b_F^2}$$

$$a_F = \frac{1}{N}\sum_{i=1}^{N}\lambda_i Cos\left(2\pi F_u\left(\frac{1}{B_i}-\frac{1}{B_1}\right)\right) \qquad b_F = \frac{1}{N}\sum_{i=1}^{N}\lambda_i Sin\left(2\pi F_u\left(\frac{1}{B_i}-\frac{1}{B_1}\right)\right),$$

where F_u is the sequence of oscillation frequencies.

As only the positions of local maxima on the A(F) dependence are of importance here, the calculations of the a_F and b_F values were performed with accuracy to constant multiplier. Two harmonic components are thus revealed (inset in figure 2). The high frequency (F=144 T) was reported before [5] and prevails in high magnetic fields. The lower frequency (F=60 T at 1.5 K) is reported for the first time. It is slightly dependent on temperature and exists in a wide range of lower fields. In the intermediate field range both frequencies are present. This result was also confirmed for the revisited data from the reference [4].

2.2. Phase analysis of oscillations

Phase analysis was performed for high-frequency harmonic component using the Shoenberg plot (figure 3). Notwithstanding numerous studies of quantum oscillations of various physical characteristics of niobium diselenide [3-9], their detailed phase analysis has not been performed so far.

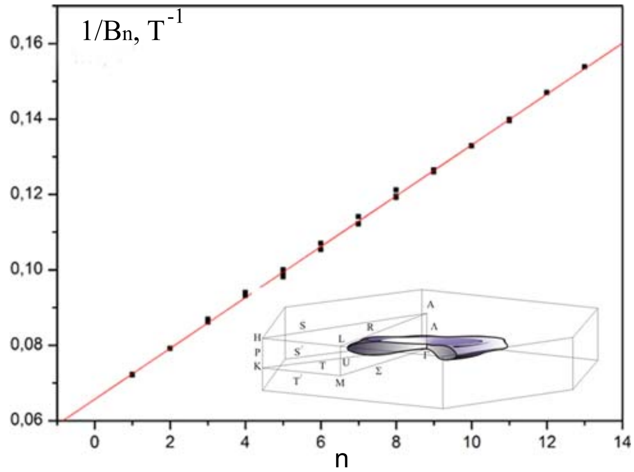

Figure 3. The Shoenberg plot for high frequency component ofmagnetostriction oscillations in the single crystal 2H-$NbSe_2$ with the in-plane orientation of the applied magnetic field (*n* being the number of oscillation peak). Inset shows a corresponding modification of the pan-cake sheet of the Fermi surface.

3. Discussion

3.1. FS topology

The pancake sheet of FS is acknowledged to be responsible for quantum oscillations in the hexagonal modification of the layered niobium dichalcogenide. At the same time, account of the anisotropy of oscillations frequency when the orientation of the in-plane applied magnetic field is changed [3] on the one hand, and two frequencies for in-plane field orientation from present investigation on the other, suggest a more complicated form of this sheet as is shown in the inset of figure 3.

3.1.1. Oscillation phase

Within accuracy of experiment (±0.02, as the accuracy of field measurement is 1%) the Shoenberg plot (figure 3) yields intersection of $1/B_n$ with axis *n* at 0.35. In the reverse field region ($0.07 < 1/B_n < 0.20$) only the high-frequency oscillation is observed and therefore the Kosevich - Lifshits formula [10] is simplified for 2*H*-$NbSe_2$:

$$M \sim M_1 \sin\left(\frac{\hbar c S_{ex}}{|e| B} + \Phi\right),$$

as well as Chandrasekhar formula for magnetostriction [11].

Here, $\Phi = -2\pi\gamma+\delta+\pi$, where γ is relevant to the so-called geometrical phase (Berry phase [12]):

$\gamma = 1/2 - \Phi_B/2\pi$,

where Φ_B refers to the Berry phase and δ labels an ordinary phase. In three dimensions (which is the case of 2*H*-$NbSe_2$, despite its high anysotropy), the δ phase becomes [13]:

$\delta = -\pi/4$ for the maximum cross section of Fermi surface, S_{max}

$\delta = +\pi/4$ for S_{min}

A condition of maximum **M** reads:

$$\frac{\hbar c S_{ex}}{|e| B_{\max,n}} + \Phi = \frac{\pi}{2} + 2\pi n$$

or:

$$\frac{A}{B_{\max,n}} = n + \underbrace{\gamma - \frac{1}{4} - \frac{\delta}{2\pi}}_{\gamma_1}$$

Taking a notation $\gamma_1 = \gamma - 1/4 - \delta/2\pi$, we obtain $\gamma = 1/2$ for $\Phi_B = 0$, and $\gamma_1 = 3/8$ (or -5/8) for the case of S_{max}, $\gamma_1 = 1/8$ (or -7/8) for the case of S_{min}. If $\Phi_B = \pi$, then $\gamma = 0$ [13] and, which is the same $\gamma_1 = 7/8$ (or -1/8) for the case of S_{max} and $\gamma_1 = 5/8$ (or -3/8) for the case of S_{min}. The phase Φ_B emerges after seminal Berry's work [10] if the Hamiltonian of quantum system is parameter dependent and the relevant parameters experience adiabatic change in such a way that they gradually approach their initial values. It is sufficient for us that this phase Φ_B occurs when trajectory of the system in a parametric space is localized in the vicinity of the degeneracy point (line) [10].

Electrons relevant to quantum oscillations in 2H-$NbSe_2$ pertain to the $\Gamma(000)$ point of the Brillouin zone (the so-called "pancake"). The symmetry space group of 2H-$NbSe_2$ is D_{6h}^4 [8]. The table of characters of irreducible representation of the symmetry group corresponding to Γ point shows that among irreducible representations both the non-degenerated (Γ_1 Γ_2 Γ_3 Γ_4) and double degenerated (Γ_5 Γ_6) states are present. Therefore, the symmetry analysis does not allow us to determine unambiguously if the electronic space responsible for magnetic oscillations in 2H-$NbSe_2$ are degenerated. Below we will try to answer this question using analysis of the phase of quantum oscillations. Our measurements are obtained at the in-plane orientation of applied field and their linear approximation yields the value $\gamma_1 = -0.34\pm0.04$. The theoretical values of γ_1 for S_{max} in both degenerate ($\Phi_B = \pi$) and non-degenerate ($\Phi_B = 0$) case differ sufficiently from the measured γ_1. Surprisingly, the measured value $\gamma_1 = -0.34$ is close to the derived theoretically for the case of S_{min} and $\Phi_B = \pi$, $\gamma_1 = -0.375$. The complicated shape of the FS sheet responsible for magnetic oscillations derived with account of the recent measurements and data of [3] (inset in figure 3) allows both cases (S_{max} and S_{min}). Therefore, the question of the Berry phase occurrence in 2H-$NbSe_2$ is still open.

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