Supplementary Material for Generation of strain-induced pseudo-magnetic field in a doped type-II Weyl semimetal

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High quality Re doped MoTe_2 crystals were cleaved by an *in-situ* cleaver at 80 K under ultra-high vacuum (10^{-11} mbar).

Additional STM images:

Figure 1. 60 nm x 60 nm and 200 nm x 200 nm STM topograph of the cleaved surface of Re- MoTe_2 obtained in a “high-strain” region respectively. The periodic modulation due to strain-induced ripples is observed.

Additional STM spectra:

Figure 2. Differential conductance spectrum recorded at 310 mK showing LL oscillations along with a low-bias conductance dip at two additional points in the high strained region.

The 35 nm-periodicity ripples shown in figure 3(a) are at an angle to the atomic rows. The angle can be clearly seen in 30 nm x 30 nm atomic resolution image and 700 nm x 700 nm scan in the following figure. We have not given any rotation to either of them.

Figure 3. (a) 30 nm x 30 nm and (b) 700 nm x 700 nm STM topograph of the cleaved surface of Re-MoTe₂ obtained in same region. The 35 nm periodicity ripples are at an angle to the atomic rows.

The scans over a large area of 700 nm x 700 nm is often affected by intermittent alteration of the tip conditions. We have however, resolved the stripes in the high-strain area several times as shown in Figure 4(a) here. Another area, far from the 700 nm x 700 nm area shown in Figure 1 of our manuscript is shown in Figure 4(d) of this document. This area was reached by a coarse motion of the stage by more than 200 microns. The broadening seen is due to an altered tip-condition. Two representative dI/dV curves with Landau-level oscillations captured at two different points on this area are also shown in Figure 4(e,f). Careful inspection of the oscillations show that the number of peaks within a given energy range does not change beyond 5% as claimed in the paper. On the other hand, in all the low-strain regions (another example is shown in Figure 4(g)), the oscillations are absent while only superconducting gap is seen (please see Figure 4(h,j) of this document).

If we look at the dI/dV curves as shown in fig 5(b) at different points corresponding to fig 5(a), we do not observe a significant change in all those spectra. Fig 5(c) shows the spectra with different energy scale at four other different points given for clarity.

Theoretical study of strain induced Landau levels in Re doped MoTe₂: We start with a specific model for type-II Weyl semimetal phase for MoTe₂ as presented in

Figure 4. (a) Large area STM topograph of the cleaved surface of Re-MoTe₂ obtained in a "high strain" region. (b,c) Two additional spectra obtained at two different points in the high strain region. (d) Another area, far from the 700 nm x 700 nm area shown in Figure 4(a). This area was reached by a coarse motion of the stage by more than 200 microns. The broadening seen is due to an altered tip-condition. (e,f) Two representative dI/dV curves with Landau-level oscillations captured at two different points in the area shown in (d). (g) STM topograph of a large area in a "low-strain" region. (h,j) The oscillations are absent while only superconducting gap is seen at two different points in the region shown in (g).

Ref. [1, 2] as

$$H(\mathbf{k}) = (\omega_1 k_x + \omega_2 k_y - \epsilon_F) I_{2 \times 2} + (a k_x + b k_y) \sigma_y + (c k_x + d k_y) \sigma_z + e k_z \sigma_x, \quad (1)$$

In MoTe₂ system there are four Weyl nodes $\mathbf{Q}$ at (0.1819, 0.1721, 0),

Figure 5. (a) 60 nm x 60 nm STM topograph of the cleaved surface of Re-MoTe₂ obtained in a “high-strain” region. The peaks of two ripples and a valley between them are visible. (b) dI/dV spectra obtained at different points (marked by numbers) in the area shown in 5(a). (c) spectra at points 15, 16, 17 and 18 with different energy scale shown for clarity.

$(0.1300, 0.0793, \pm 0.298)$, $(0.1011, 0.0503, 0)$ where we use the same notation as in Ref. [1] for the expansion parameters and a chemical potential (ϵ_F) is added to include the Re doping effect. We employ first a unitary transformation $R_y(\theta) = e^{i\theta/2\sigma_y}$ with $\theta = 3\pi/2$ on the Hamiltonian to obtain

$$H(\mathbf{k}) = (\omega_1 k_x + \omega_2 k_y - \epsilon_F)I_{2 \times 2} + (ak_x + bk_y)\sigma_y + (ck_x + dk_y)\sigma_x - ek_z\sigma_z. \quad (2)$$

Next we give a rotation of the coordinate space with respect to the k_z -axis by an angle $\phi = \tan^{-1}(\omega_2/\omega_1)$ to yield

$$H(\mathbf{k}) = (\omega_\perp k_y - \epsilon_F)I_{2 \times 2} + d_y\sigma_y + d_x\sigma_x + d_z\sigma_z. \quad (3)$$

where $\omega_\perp = \sqrt{\omega_1^2 + \omega_2^2}$, and $d_y = (a \cos \phi + b \sin \phi)k_x + (b \cos \phi - a \sin \phi)k_y$, and $d_x = (c \cos \phi + d \sin \phi)k_x + (d \cos \phi - c \sin \phi)k_y$, and $d_z = -ek_z$. With a further rescaling of the parameters (a , b , c , d , and ϕ), we obtain our simplified Hamiltonian in the main text to be $d_\mu = v_\mu k_\mu$, where $v_x = (b \cos \phi - a \sin \phi)$, $v_y = (c \cos \phi + d \sin \phi)$, and $v_z = -e$. The four Weyl nodes at (in RLU) $(0.0085, 0.0498, 0.101)$, $(0.0290, 0.1696, 0.1819)$, $(-0.2804, 0.1284, 0.1300)$, $(-0.3071, 0.0279, 0.1300)$ in our rotated frame of reference.

A. Modeling strain induced magnetic field

For a strained material, we define displacement field vector which determines the change in the lattice position (relative to original position): $\mathbf{u} = (\mathbf{r}' - \mathbf{r})$. According to the model shown in Fig. , the lowest order term in the displacement of atoms from its equilibrium position is

$$\mathbf{u} = \left(\frac{zx}{R-d}, 0, 0 \right), \quad (4)$$

where d is the depth of the neutral axis from the tip of the bent (along z axis). The strain is along the x -axis which gives the relation as

$$\alpha = \frac{a_x - a_{x0}}{a_{x0}} = \frac{d}{R-d} = \frac{3}{100}, \quad (5)$$

where α is strain amount. Experimental value of strain is $\sim 3\%$. Under this displacement the hopping parameter changes as $t'_x \sigma_x \rightarrow t'_x (1 - u_{xx}) \sigma_x + \sum_{\mu' \neq x} u_{\mu\mu'} t'_{\mu'} \sigma_{\mu'}$, where $u_{xx} = \frac{\partial u_x}{\partial x}$. Now expanding the Hamiltonian around an Weyl node $\vec{Q} = \left(0.0085(\frac{2\pi}{a_x}), 0.0498(\frac{2\pi}{a_y}), 0.1011(\frac{2\pi}{a_z}) \right)$, we get the vector potential :

$$\mathcal{A} = \frac{1}{e} \left(\frac{z}{a_x(R-d)} \tan(Q_x a_x), 0, \frac{x}{a_z(R-d)} \tan(Q_z a_z) \right), \quad (6)$$

pseudo magnetic field as

$$\mathcal{B} = \frac{1}{e} \left(\frac{\tan(Q_x a_x)}{a_x(R-d)} - \frac{\tan(Q_z a_z)}{a_z(R-d)} \right) \hat{y},$$

where $a_x = 3.45\text{\AA}$, $a_y = 13.86\text{\AA}$, $R = 1418\text{\AA}$, $d = \frac{R}{34}$. For $R = 1418\text{\AA}$, $\mathcal{B} \approx 3T$. It is clear that from the last equation we can find the order of the pseudo-magnetic field by estimating the wavelength of ripples, ($35nm$), depth of the neutral axis (d), and consequently the radius of curvature ($R(1418\text{\AA})$).

B. Density of states

If we choose a gauge, which leaves only k_y and to be a good QM numbers ($\mathcal{B}$ is in y direction). The energy spectrum is,

$$E_n^\pm(k) = \omega_\perp k_y - \epsilon_F \pm \sqrt{(v_y k_y)^2 + 2(v_\perp/l_B)^2 n} \quad (7)$$

where $v_{\perp} = \sqrt{|v_x v_z|}$, Green's function:

$$\mathcal{G}(\omega) = \sum_{k_y, n, \pm} \frac{1}{\omega - E_n^{\pm}(k_y) + i\delta} \quad (8)$$

$$DOS = -\frac{Im(\mathcal{G}(\omega))}{\pi} \quad (9)$$

with k_y cutoff= $\pi/20$, and n cutoff=200, we get peaks, which are $\sim 1meV$ apart, in DOS .

C. Lifshitz-Kosevich results and condition for closed Fermi surface

Fitting parameters in $eV \text{ \AA}$ units $\omega_1=-3.39$, $\omega_2=0.58$, $a=0$, $b=0.78$, $c=2.6$, $d=-0.58$, $e=0.0045$. The energy eigenvalues are

$$H(\mathbf{k}) = (\omega_{\perp} k_y - \epsilon_F) I_{2 \times 2} + d_y \sigma_y + d_x \sigma_x + d_z \sigma_z. \quad (10)$$

where $\omega_{\perp} = \sqrt{\omega_1^2 + \omega_2^2}$, and $d_{\mu} = v_{\mu} k_{\mu}$, $v_x = (b \cos \phi - a \sin \phi)$, $v_y = (c \cos \phi + d \sin \phi)$, and $v_z = -e$.

Let us consider a constant energy surface at an energy ϵ , for the $E_{\mathbf{k}}^{-}$ state which gives the condition

$$(\epsilon + \epsilon_F - \omega_{\perp} k_y)^2 = v_x^2 k_x^2 + v_y^2 k_y^2 + v_z^2 k_z^2, \quad (11)$$

This equation can be cast into general equation of quadric surface (by completing square and shifting) as

$$\frac{k_x^2}{A} + \frac{k_y^2}{B} + \frac{k_z^2}{C} = 1. \quad (12)$$

where $A = \frac{G}{v_x^2}$, $B = \frac{G}{v_y^2}$, $C = \frac{G}{v_z^2}$, $G = (\epsilon + \epsilon_F)^2 \left[1 + \frac{\omega_{\perp}^2}{v_y^2 - \omega_{\perp}^2} \right]$

The above equation gives a constant energy surface, which is basically quadric surfaces. The contour we need is the cut of the quadric surface and the plane perpendicular to pseudo-magnetic field. This contour may not be closed depending on the nature of the quadric surface. The nature of quadric surface and therefore the contour can be determined by the signs of the coefficients in (12). For most general case, we consider the closed contour of the electron to be an ellipse. After determining the coefficients, we come to the conclusion that to get an elliptic contour (closed), the orientation of magnetic field is along the y -axis. And the contour equation is,

$$\frac{k_x^2}{\kappa_x^2} + \frac{k_z^2}{\kappa_z^2} = 1, \quad (13)$$

For most general case, we consider the closed contour of the electron to be an ellipse with its semi major, and semi minor axes being κ_x , and κ_z . Now, cyclotron frequency of an closed orbit(semi classical),

$$\omega_c = \frac{2\pi e\mathcal{B}}{\hbar^2} \left(\frac{\partial \mathcal{S}}{\partial \epsilon} \right)^{-1}, \quad (14)$$

where $\mathcal{S}(\epsilon)$ = area of the closed orbit of the constant energy contour ϵ and e =charge of electron, $\mathcal{B}$ = magnetic field. So we have

$$\mathcal{S}(\epsilon) = \pi \kappa_x \kappa_z,$$

Semi-classical quantization is applicable if, $\frac{\hbar\omega_c}{\epsilon_F} \sim 10^{-4}$, and

$$\hbar\omega_c = \frac{2\pi e\mathcal{B}}{\hbar} \left(\frac{\partial \mathcal{S}}{\partial \epsilon} \right)^{-1}_{\epsilon_F}.$$

Now we have

$$\mathcal{B} = \frac{\hbar^2\omega_c}{2\pi e} \left(\frac{\partial \mathcal{S}}{\partial \epsilon} \right)_{\epsilon_F}.$$

We put $\hbar\omega_c = 1.3$ meV, in close agreement with the experimental data and $\epsilon = 0$ and in the above equation.

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