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Interplay between band crossing and charge density wave instabilities

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Our measurements of the Hall coefficient in rare-earth tritelluride compounds reveal a strong hysteresis between cooling and warming in the low-temperature range where a second unidirectional charge density wave (CDW) occurs. We show that this effect results from the interplay between two instabilities: band crossing of the Te p_x and p_y orbitals at the Fermi level and CDW, which have a close energy gain and compete. Calculation of the electron susceptibility at the CDW wave vector with and without band anticrossing reconstruction of the electron spectrum yields a satisfactory estimation of the temperature range of the hysteresis in Hall effect measurements.

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Crossing of electron energy bands near the Fermi level, resulting in the degeneracy and anticrossing of energy levels, always leads to amazing physical properties. The anticrossing of spin-split energy bands with spin-orbit coupling produces nontrivial topologically protected electron states in Weyl and Dirac semimetals, which has been the subject of extensive research for the last decade [1–4]. Even without spin effects, the band anticrossing near the Fermi level modifies the electron spectrum and the Fermi surface (FS). This affects various electronic instabilities such as superconductivity in high-temperature cuprate superconductors [5–7] and spin or charge density waves [8–10]. In this Rapid Communication we unveil the competition of band anticrossing and the charge density wave (CDW) in the family of rare-earth tritelluride compounds. We show, both theoretically and experimentally, that this interplay leads to a hysteretic electronic phase transition with the change of FS topology and of the Hall coefficient.

Layered compounds of the $R\text{Te}_3$ family (R = rare-earth atom) have a weakly orthorhombic crystal structure (space group $Cmcm$). These systems exhibit an incommensurate CDW through the whole R series [8,11,12], with a wave vector $\mathbf{Q}_{\text{CDW1}} = (0, 0, \sim 2/7c^*)$ and a Peierls transition temperature above 300 K for the light atoms (La, Ce, Nd). For the heavier R (Tb, Dy, Ho, Er, Tm) a second CDW occurs at low temperature with the wave vector $\mathbf{Q}_{\text{CDW2}} = (\sim 2/7a^*, 0, 0)$ perpendicular to \mathbf{Q}_{CDW1} .

For our study we chose three compounds from the $R\text{Te}_3$ family: two compounds, ErTe_3 and HoTe_3 , demonstrating bidirectional CDW ordering at $T_{\text{CDW1}} = 270$ and 283 K and $T_{\text{CDW2}} = 160$ and 110 K correspondingly, and TbTe_3 , revealing a unidirectional CDW at $T_{\text{CDW}} = 336$ K. Single crystals of these compounds were grown by a self-flux technique under purified argon atmosphere as described previously [13]. Thin

samples with a typical thickness 1–3 μm having a rectangular shape were prepared by micromechanical exfoliation of relatively thick crystals glued on a sapphire substrate.

The magnetic field was applied parallel to the b axis. The Hall resistance $R_{xy}(B) = [V_{xy}(+B) - V_{xy}(-B)]/I$ was recorded using the van der Pauw method [14,15], sweeping the field between +6 and –6 T at a fixed temperature with a step $\Delta T = 10$ K first by cooling from $T > T_{\text{CDW1}}$ down to 4.2 K and after that by warming back up.

For all measured compounds R_{xy} is a linear function of B at least for temperatures $T \gtrsim 100$ K [16]. So, the Hall constant, $R_H = R_{xy}d/B$, where d is the crystal thickness, is indeed a field-independent quantity. Its temperature dependencies for ErTe_3 , HoTe_3 , and TbTe_3 are shown in Figs. 1(a)–1(c) correspondingly. One can see that for ErTe_3 and HoTe_3 , R_H demonstrates a strong hysteresis between cooling and warming in the temperature range around the second Peierls transition while $R_H(T)$ is completely reversible for TbTe_3 , revealing only a single transition to the CDW state in the studied range of temperature. When measured under cooling and warming the temperature dependence of the resistance $R(T)$ of all three compounds was reversible [16]. It means that the total number of charge carriers remains nearly the same under cooling and warming. We see only one explanation for this effect: There are two types of carriers, and the hysteresis observed is attributed to the change in electron-hole balance as a result of the second CDW formation. Such a scenario is confirmed by the change of the sign of the Hall constant at a certain temperature in HoTe_3 and TbTe_3 .

One can naturally attribute the observed effect to the hysteresis of the CDW wave vector \mathbf{Q}_{CDW} due to its pinning by crystal imperfections. However, our preliminary x-ray diffraction studies of ErTe_3 , performed at ID28 ESRF beamline [17], showed a completely reversible evolution of

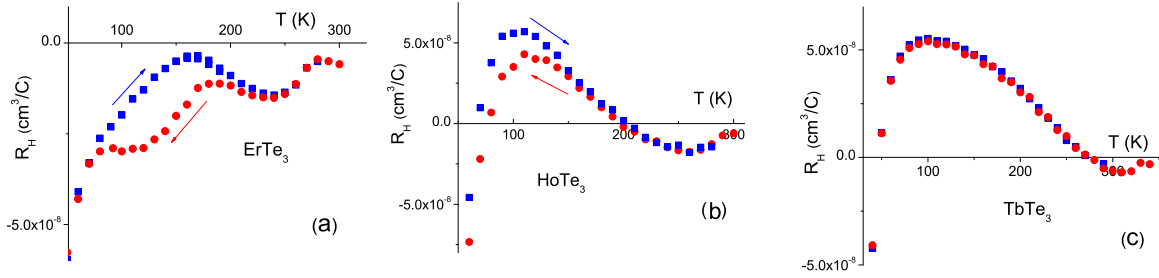


FIG. 1. Hall constant of (a) ErTe_3 , (b) HoTe_3 , and (c) TbTe_3 as a function of temperature. Red circles correspond to cooling, and blue squares correspond to warming.

all structural parameters in the temperature range 100–300 K [16]. Therefore, we consider another possible origin of this hysteresis, based on the interplay of CDW_2 with another type of electronic instability. As a possible candidate for such electronic ordering competing with CDW_2 , we suggest the one due to the electron band crossing at the Fermi level.

Consider two electron bands with electron dispersion $\epsilon_1(\mathbf{k})$ and $\epsilon_2(\mathbf{k})$. Two corresponding Fermi surfaces, given by the equations $\epsilon_1(\mathbf{k}) = E_F$ and $\epsilon_2(\mathbf{k}) = E_F$, intersect along the lines $\{\mathbf{k}_0\}$ in the momentum space. In $R\text{Te}_3$ compounds in the (k_x, k_y) plane below T_{CDW1} there are two such crossing points \mathbf{k}_0 [18], highlighted by solid yellow circles in Fig. 2. At each degeneracy point \mathbf{k}_0 , any small interband coupling $V(\mathbf{Q})$, even at zero momentum transfer $\mathbf{Q} = \mathbf{0}$, leads to the band anticrossing and to the reconstruction of FS (see the upper right inset in Fig. 2). This FS anticrossing has been observed in various $R\text{Te}_3$ compounds by angle-resolved photoemission spectroscopy (ARPES) measurements [12,19]. The interband coupling $V(\mathbf{Q})$ may originate, e.g., from the electron-electron ($e-e$) interaction. Usually, $|V(\mathbf{Q})|$ decreases with an increase of momentum transfer $|\mathbf{Q}|$, and $|V(\mathbf{0})| \equiv V_0$ may considerably exceed $|V(\mathbf{Q} \neq \mathbf{0})|$.

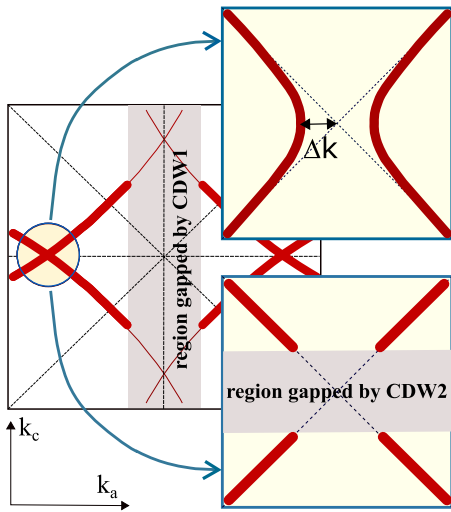


FIG. 2. Schematic representation of the Fermi surface (FS) in $R\text{Te}_3$. Main figure: The full FS with the CDW_1 -gapped region shaded by gray. In the crossing region, highlighted by a solid yellow circle, two FS reconstructions are possible: with band anticrossing shown in the upper right inset, and with an energy gap due to CDW_2 shaded in gray in the lower right inset.

First, consider the toy model with the interband coupling (off-diagonal terms) only at $\mathbf{Q} = \mathbf{0}$. In this model the different momenta are not coupled, and the Hamiltonian writes down as a sum over electron momenta \mathbf{k} , $\hat{H} = \sum_{\mathbf{k}} \hat{H}_{\mathbf{k}}$, where in the basis of two branches $\alpha = 1, 2$ of the electron spectrum each term $\hat{H}_{\mathbf{k}}$ is given by a 2×2 matrix [20],

$$\hat{H}_{\mathbf{k}} = \begin{pmatrix} \epsilon_1(\mathbf{k}) & V_0 \\ V_0 & \epsilon_2(\mathbf{k}) \end{pmatrix}, \quad (1)$$

with two eigenvalues,

$$E_{\pm}(\mathbf{k}) = \frac{\epsilon_1(\mathbf{k}) + \epsilon_2(\mathbf{k})}{2} \pm \sqrt{\left(\frac{\epsilon_1(\mathbf{k}) - \epsilon_2(\mathbf{k})}{2}\right)^2 + V_0^2}, \quad (2)$$

representing two new branches of the electron spectrum. The total electron energy is given by the sum of quasiparticle energies over their quantum numbers,

$$\mathcal{E} = \sum_{\mathbf{k}, \alpha} E_{\alpha}(\mathbf{k}) n_F[E_{\alpha}(\mathbf{k})], \quad (3)$$

where $n_F(\varepsilon) = 1/(1 + \exp[(\varepsilon - E_F)/T])$ is the Fermi-Dirac distribution function. Without band anticrossing the total energy \mathcal{E}_0 is given by the same Eq. (3) with the replacement $E_{\alpha}(\mathbf{k}) \rightarrow \epsilon_{\alpha}(\mathbf{k})$. The difference $\Delta\mathcal{E}_{\text{AC}} = \mathcal{E} - \mathcal{E}_0$ comes mainly from the vicinity of the crossing points \mathbf{k}_0 , where two conditions are satisfied: (i) $|\epsilon_1(\mathbf{k}) - \epsilon_2(\mathbf{k})| \lesssim V_0$, so that the electron spectrum changes considerably, and (ii) $|\epsilon_1(\mathbf{k}) + \epsilon_2(\mathbf{k})| \lesssim 2V_0$, so that the change in the electron spectrum is close to the Fermi level. Near the crossing point \mathbf{k}_0 one may linearize each branch of the electron spectrum,

$$\epsilon_{\alpha}(\mathbf{k}) \approx v_{F\alpha}(\mathbf{k} - \mathbf{k}_0), \quad (4)$$

where $v_{F\alpha}$ is the Fermi velocity v_F of branch α . Then $|\epsilon_1(\mathbf{k}) \pm \epsilon_2(\mathbf{k})| \approx (v_{F1} \pm v_{F2})(\mathbf{k} - \mathbf{k}_0) \sim v_F |\mathbf{k} - \mathbf{k}_0|$, and the contributing momentum area in the vicinity of the crossing point \mathbf{k}_0 is estimated as $(V_0/v_F)^2$. Then the energy difference per unit area per one spin component but including two cross points is

$$\Delta\mathcal{E}_{\text{AC}} \sim -(V_0/\pi\hbar v_F)^2 V_0 \approx -V_0^3 a^2 \rho_F^2, \quad (5)$$

where a is the in-plane lattice constant and $\rho_F = 1/\pi\hbar v_F a$ is the quasi-one-dimensional (1D) density of states (DOS) at the Fermi level per one branch and spin component. Our calculation of $\Delta\mathcal{E}_{\text{AC}}$ by the numerical integration according to Eq. (3) confirms the estimate in Eq. (5), giving a $\Delta\mathcal{E}_{\text{AC}}$ value 20% less than in Eq. (5).

The CDW energy gain per spin component is [21,22]

$$\Delta\mathcal{E}_{\text{CDW}} = -\Delta^2\rho_F, \quad (6)$$

where Δ is the CDW energy gap. The extra small parameter $\eta \equiv V_0\rho_F a^2 = V_0 a/\pi\hbar v_F \ll 1$ in the band crossing energy gain in Eq. (5) as compared to Eq. (6) comes from the small momentum region of contributing electrons, while in a CDW a considerable part of the electrons on the Fermi level participates in the Peierls instability, so that a similar small factor $a^2\rho_F\Delta$ does not appear. Hence, the CDW₂ energy gain may be larger than the energy gain from band anticrossing, although its energy gap $\Delta_2 \ll V_0$.

We estimate the value of V_0 from the FS distortion at the crossing point \mathbf{k}_0 observed in ARPES. This FS distortion Δk along the x axis is about 3% of the Brillouin zone width $2\pi\hbar/a$ [12,19], where the lattice constant $a = 4.28 \text{ \AA}$ in ErTe₃. This Δk corresponds to the condition $|\epsilon_1(\mathbf{k}) + \epsilon_2(\mathbf{k})| = 2V_0$, giving the boundary of electron states with a gap on the Fermi level according to Eq. (2). In RTe₃ compounds the FSs of two bands cross at almost a right angle, as shown in Fig. 2. Substituting the electron dispersion (4) with $v_F \approx 1.3 \times 10^8 \text{ cm/s}$, we obtain in ErTe₃ compounds $V_0 \approx v_F \Delta k/\sqrt{2} \approx 250 \text{ meV}$. For comparison, in ErTe₃ the CDW₁ energy gap $\Delta_1 \approx 175 \text{ meV}$, and the CDW₂ energy gap is $\Delta_2 \approx 55 \text{ meV}$ [23]. The parameter $\eta = V_0 a/\pi\hbar v_F \approx 0.04$ is indeed $\ll 1$, and the ratio of energy gains from the band anticrossing and from CDW₂ is $\Delta\mathcal{E}_{\text{AC}}/\Delta\mathcal{E}_{\text{CDW}_2} \approx \eta V_0^2/\Delta_2^2 \approx 0.8$, i.e., slightly less than unity. This means a strong temperature-dependent interplay of these two electronic instabilities, making CDW₂ slightly more energetically favorable at low T . However, since $V_0/\Delta_2 \approx 5 \gg 1$, the band anticrossing appears at a much higher temperature than T_{CDW_2} , even higher than T_{CDW_1} .

The band anticrossing and CDW₂ hinder each other by changing the electron spectrum. The CDW₂ creates an energy gap on the Fermi level just at the spots of FS intersection (see the lower right inset in Fig. 2), thus suppressing or making irrelevant the band anticrossing. The influence of band anticrossing on CDW₂ is less obvious, because the FS has an approximate nesting property both with and without the band anticrossing. Moreover, our calculation of the DOS with and without band anticrossing gives nearly the same result in both

cases. Hence, to substantiate that band anticrossing hinders the CDW₂ instability, we need to compare the electronic susceptibility $\chi(\mathbf{Q}, T)$ at the CDW₂ wave vector \mathbf{Q} in both cases: with and without band anticrossing reconstruction of the electron spectrum. The CDW₂ transition temperature T_c is given by the equation [21] $|U\chi(\mathbf{Q}_{\text{max}}, T_c)| = 1$, where \mathbf{Q}_{max} is the wave vector where the susceptibility χ takes a maximum value. The larger the susceptibility χ , the higher is the CDW transition temperature, because susceptibility increases with a decrease of temperature.

For calculations we use the well-known formula for the static susceptibility of free-electron gas at a finite wave vector \mathbf{Q} . Electron spin only leads to a factor 4 in susceptibility, but the summation over the band index α must be retained. Then the real part of electron susceptibility is

$$\chi(\mathbf{Q}) = \sum_{\alpha, \alpha'} \int \frac{4d^d \mathbf{k}}{(2\pi)^d} \frac{n_F(E_{\mathbf{k}, \alpha}) - n_F(E_{\mathbf{k}+\mathbf{Q}, \alpha'})}{E_{\mathbf{k}+\mathbf{Q}, \alpha'} - E_{\mathbf{k}, \alpha}}, \quad (7)$$

where d is the dimension of space. In RTe₃ compounds under study there are two bands crossing the Fermi level, $\alpha, \alpha' = 1, 2$, and we may take $d = 2$ because the dispersion in the z direction is weak. Equation (7) differs only by the summation over α and α' from the common expression, e.g., given in Eq. (1.7) of Ref. [21].

Taking the tight-binding bare electron dispersion $\epsilon_{1,2}(\mathbf{k})$ commonly used [9,24] for RTe₃ compounds and given by Eqs. (2) of Ref. [24], we calculate the susceptibility in Eq. (7) as a function of the wave vector \mathbf{Q} and temperature T for two cases: without the band crossing effect, i.e., for bare electron dispersion $\epsilon_{1,2}(\mathbf{k})$, and for a reconstructed dispersion given by Eq. (2). The results are shown in Fig. 3. The integration over momentum in Eq. (7) is performed only at $k_x > k_{x0} \approx 0.29 \text{ \AA}^{-1}$, because in the momentum region $|k_x| < k_{x0}$ the electron spectrum at the Fermi level has a large energy gap Δ_1 due to CDW₁.

The summation over α and α' in Eq. (7) gives four terms: two intraband terms χ with $\alpha = \alpha'$ and two interband terms $\Delta\chi$ with $\alpha \neq \alpha'$. The intraband ‘‘diagonal’’ terms, enhanced by a rather good FS nesting, are much larger than the ‘‘off-diagonal’’ interband terms, because the latter correspond to almost perpendicular FS sheets and do not have such a nesting

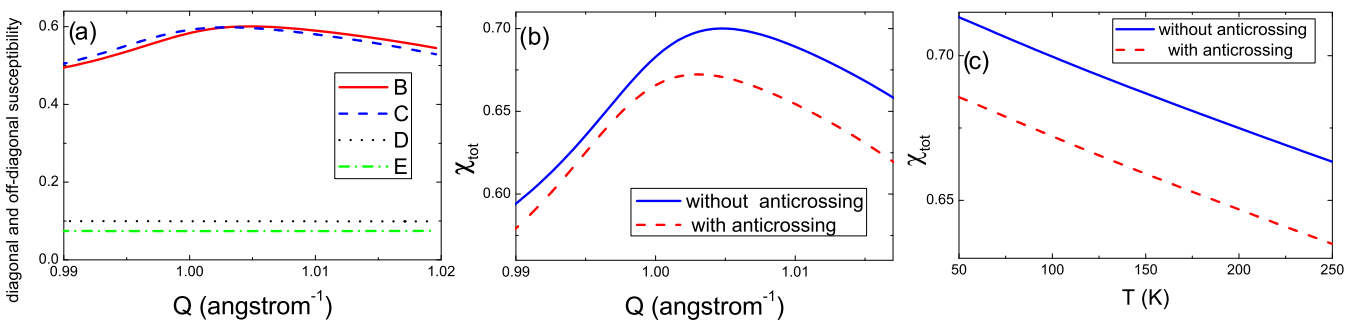


FIG. 3. Calculated electron susceptibility. (a) The electron susceptibility contributions without (solid blue and green lines) and with the band crossing reconstruction (dashed red and black lines). The upper two curves (blue and red) show the calculated ‘‘diagonal’’ intraband contributions χ , while the two lower curves (green and black) show ‘‘off-diagonal’’ interband contributions $\Delta\chi$ to susceptibility. (b) Total susceptibility $\chi_{\text{total}} = \chi + \Delta\chi$ as a function of wave vector Q_x near its maximum without (solid blue line) and with the band crossing reconstruction (dashed red line). (c) The temperature dependence of maximal total susceptibility without (solid blue line) and with the band crossing reconstruction (dashed red line).

enhancement [see Fig. 3(a)]. Hence, the intraband contribution, shown by the upper blue and red curves in Fig. 3(a), have a maximum at the CDW₂ wave vector \mathbf{Q} , resulting in a similar maximum on the total susceptibility in Fig. 3(b), while the interband contribution, shown by the lower green and black curves in Fig. 3(a), depends weakly on \mathbf{Q} . Nevertheless, the interband contribution is considerable, being about 20% of the intraband susceptibility. This again illustrates the well-known fact [25,26] that the Fermi-surface nesting does not determine the CDW properties.

While the maximum values of the diagonal intraband susceptibility terms are weakly affected by the band anticrossing, the off-diagonal interband terms are suppressed by the band anticrossing reconstruction by more than 20% [see Fig. 3(a)]. This can be easily understood by looking at the FS with and without band anticrossing, shown in Fig. 2. The DOS and the nesting property are not violated by the band anticrossing, hence, the intraband terms remain almost the same (only the optimal CDW₂ wave vector slightly shifts). On the contrary, after the band anticrossing reconstruction, the FSs of different bands become separated by $\Delta k \sim 3\%$ of the Brillouin zone. Two FS sheets even do not intersect, as was without the band anticrossing. Hence, the interband susceptibility decreases considerably.

We have shown that the band anticrossing and CDW₂ interfere, suppressing each other. With a temperature decrease the band anticrossing appears first (at a higher temperature) and reduces the CDW₂ transition temperature to its observed value T_{CDW_2} . At a lower temperature, when CDW₂ develops and the Δ_2 increases, since $|\Delta\mathcal{E}_{\text{CDW}_2}| > |\Delta E_{\text{AC}}|$, the band anticrossing shrinks in favor of CDW₂. This may happen as a first-order phase transition, accompanied by a hysteresis. When the temperature increases again, the CDW₂ disappears at temperature $T_{\text{CDW}_2}^* > T_{\text{CDW}_2}$, because of the changed band crossing energy spectrum. This results in a hysteresis seen by the Hall coefficient sensitive to the FS reconstruction due to CDW₂. We can estimate how strong this hysteresis is by looking at the calculated temperature dependence of susceptibility $\chi(T)$, shown in Fig. 3(c). The calculated optimal wave vector \mathbf{Q} of the CDW₂ instability, i.e., of the susceptibility maximum shown in Fig. 3(b), very slightly increases with temperature from $Q_x \approx 1.004 \text{ \AA}^{-1}$ at $T = 50 \text{ K}$ to $Q_x \approx 1.006 \text{ \AA}^{-1}$ at $T = 200 \text{ K}$. Therefore, this change was not observed in the

x-ray experiment [see the Supplemental Material (SM) [16]]. In Fig. 3(c) we plot the maximum value of $\chi(\mathbf{Q})$ as a function of temperature T without (solid blue line) and with (dashed red line) band crossing reconstruction. They differ by 4.5% only, but since the temperature dependence of susceptibility is also quite weak, the susceptibility value $\chi_c = 0.68$, which the red curve reaches only at $T_c \approx 50 \text{ K}$, the blue curve has already at $T_c^* \approx 175 \text{ K}$. Thus, the expected temperature hysteresis is rather large: $\Delta T = T_c^* - T_c \approx 125 \text{ K}$ [27].

The proposed interplay between band crossing and CDW is rather general and is expected in many other compounds with a FS intersection at the nested parts. For example, a similar effect is expected in the RTe₄ family of compounds, where a large temperature hysteresis of resistance $\Delta T > 100 \text{ K}$ has also been observed recently [10].

The bilayer splitting of the electron spectrum smears the nesting condition [23]. The exact bare electron dispersions $\epsilon_{1,2}(\mathbf{k})$ are unknown. The coupling between two CDWs in the above analysis is taken into account only by neglecting the contribution from the states gapped by CDW₁. These and other factors make the interplay of CDW₂ with other instabilities more complicated, but we expect that the main features of the proposed model remain valid.

To summarize, we observed a strong hysteresis of the Hall coefficient in the rare-earth tritelluride compounds ErTe₃ and HoTe₃, having two CDW phase transitions. We explain this effect by a strong interplay of the low-temperature CDW and the band anticrossing change of the electron spectrum. We estimate the temperature range of this hysteresis by calculating the electron susceptibility at the CDW₂ wave vector with and without band anticrossing. The interplay between these two instabilities is proposed and investigated and may be relevant to other compounds where two electron bands cross at the Fermi level.

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