

Theory for the charge-density-wave mechanism of 3D quantum Hall effect

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The charge-density-wave (CDW) mechanism of the 3D quantum Hall effect has been observed recently in ZrTe_5 [Tang *et al.*, *Nature* **569**, 537 (2019)]. Quite different from previous cases, the CDW forms on a 1D band of Landau levels, which strongly depends on the magnetic field. However, its theory is still lacking. We develop a theory for the CDW mechanism of 3D quantum Hall effect. The theory can capture the main features in the experiments. We find a magnetic field induced second-order phase transition to the CDW phase. We find that electron-phonon interactions, rather than electron-electron interactions, dominate the order parameter. We extract the value of electron-phonon coupling constant from the non-Ohmic I - V relation. We point out a commensurate-incommensurate CDW crossover in the experiment. More importantly, our theory explores a rare case, in which a magnetic field can induce an order-parameter phase transition in one direction but a topological phase transition in other two directions, both depend on one magnetic field. It will be useful and inspire further experiments and theories on this emergent phase of matter.

Introduction. – The quantum Hall effect is one of most important discoveries in physics [1–4]. It arises from the Landau levels of 2D electron gas in a strong magnetic field (Fig. 1 Left). When the Fermi energy lies between two Landau levels, the interior of the electron gas is insulating but the deformed Landau levels at the edges can transport electrons dissipationlessly, leading to the quantized Hall resistance and vanishing longitudinal resistance of the quantum Hall effect. The quantum Hall effect is difficult in 3D, where the Landau levels turn to a series of 1D bands of Landau level dispersing with the momentum along the direction of magnetic field (Fig. 1 Center). Because the Fermi energy always crosses some Landau bands, the interior is metallic, which buries the quantization of the edge states, so the quantum Hall effect is usually observed in 2D systems [5]. Nevertheless, searching for a 3D quantum Hall effect has been lasting for more than 30 years [6–23]. One of the famous proposals relies on the formation of charge density wave (CDW), which may gap the 1D Landau band so that the bulk is insulating. In real space, the CDW split the 3D electron gas into layers of decoupled 2D electron gases that each give a quantized Hall effect (Fig. 1 Right) [6]. Quite different from the known cases [24–26], the CDW of Landau bands depends on the magnetic field strongly [27–32]. Nevertheless, lack of experiments prevented further explorations at the quantitative level. Recently, the CDW mechanism of the 3D quantum Hall effect has been observed in 3D crystals of ZrTe_5 [33], providing a platform to study this rare phase of matter where both order

parameter and topological number coexist.

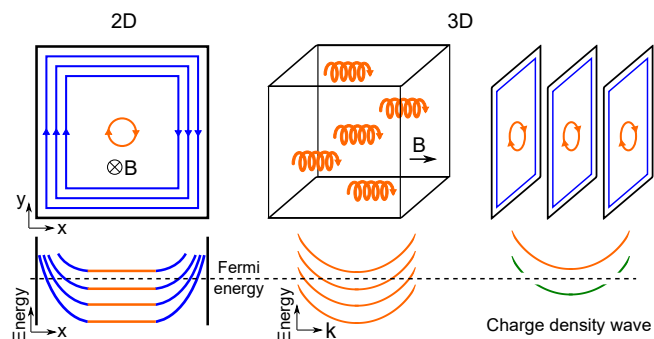


FIG. 1. Left: A strong magnetic field (B) splits a 2D electron gas into the Landau levels (orange). The quantum Hall effect arises when only the edge states (blue) conduct electrons, while more importantly the interior bulk states are insulating as the Fermi energy lies between the Landau levels. Center: In 3D, the Landau levels turn to 1D bands of Landau levels that disperse with the momentum (k) along the direction of magnetic field. The quantum Hall effect is difficult in 3D because the bulk is metallic as the Fermi energy always crosses some Landau bands. Right: The charge density wave may gap the Landau band, so that the bulk is insulating and the quantum Hall effect can be observed.

In this Letter, we develop a theory for the CDW mechanism of 3D quantum Hall effect. The theory captures the main features in the experiment of ZrTe_5 at the quantitative level. We find that electron-phonon interactions dominate the formation of the CDW, instead of electron-electron interactions. We extract the value of

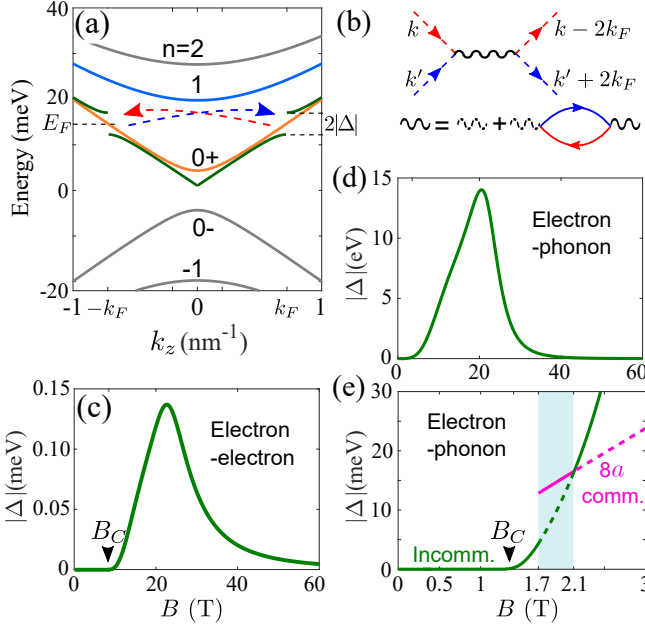


FIG. 2. (a) The 1D energy bands of Landau levels dispersing with the z -direction wave vector k_z in a z -direction magnetic field $B = 1.6$ T. The CDW opens the gap ($2|\Delta|$) at the Fermi energy E_F . n marks the indices of the Landau bands. $n = 0\pm$ are the lowest Landau bands. (b) The g -ology diagrams of CDW. The wavy line stands for interactions under the random phase approximation. [(c)-(e)] The calculated CDW order parameters for electron-electron (c) and electron-phonon [(d)-(e)] interactions, respectively. B_C indicates a threshold magnetic field at which there is a second-order phase transition as Δ overcomes temperature. “Incomm.” and “8a comm.” indicate that incommensurate and commensurate (CDW wavelength/lattice constant = 8) CDWs are assumed, respectively. The parameters are $v_x = 9 \times 10^5$ m/s, $v_y = 1.9 \times 10^5$ m/s, $v_z = 0.3 \times 10^5$ m/s, $M_0 = -4.7$ meV, $M_\perp = 150$ meV·nm², $M_z = 0.01M_\perp$, $a = 7.25$ Å [33, 34], $n_0 = 8.87 \times 10^{16}$ cm⁻³, $\epsilon_r = 25.3$ [35], and the electron-phonon coupling constant $g_0 = 537.3$ eV·nm⁻¹ (determined by comparing with the non-linear I - V data [33] in Fig. 4 (h)), and $T = 0$ K.

electron-phonon coupling constant from the non-Ohmic I - V relation. We point out a **crossover between commensurate and incommensurate CDWs, tunable by the magnetic field**. More importantly, the theory addresses a rare but experiment-accessible scenario, described by an order parameter along one direction but a topological Chern number in other two directions, both tunable by one magnetic field. Our theory will inspire more studies along this promising direction in the future.

1D Landau band in the quantum limit. – We start with a generic Dirac model [36]

$$\hat{\mathcal{H}}(\mathbf{k}) = \hbar(v_x k_x \tau_x \otimes \sigma_z + v_y k_y \tau_y \otimes \sigma_0 + v_z k_z \tau_z \otimes \sigma_x) + [M_0 + M_1(v_x^2 k_x^2 + v_y^2 k_y^2) + M_z k_z^2] \tau_z \otimes \sigma_0, \quad (1)$$

where $\tau_{x,y,z,0}$ and $\sigma_{x,y,z,0}$ are Pauli matrices and unit matrix for orbital and spin degrees of freedom, and $M_{0,1,z}$,

$v_{x,y,z}$ are the model parameters. This model can describe not only ZrTe₅, but also various semimetals and insulators [17, 34, 37–46]. A uniform magnetic field $\mathbf{B} = (0, 0, B)$ along the z direction (crystal b direction) is taken into account by the Landau gauge vector potential $\mathbf{A} = (-By, 0, 0)$, which shifts k_x to $k_x - eBy/\hbar$, where $-e$ is the electron charge and \hbar is the reduced Planck’s constant. The magnetic field splits the energy spectrum into a series of 1D bands of Landau levels, dispersing with k_z , as shown in Fig. 2 (a).

We will focus on the quantum limit, in which the Fermi energy E_F crosses only the $n = 0+$ Landau band [47]. At the critical magnetic field B_Q when entering the quantum limit, $E_F = E_{k_z=k_F}^{(0+)} = E_{k_z=0}^{(1)}$, where the Fermi wave vector [48]

$$k_F = 2\pi^2 \hbar n_0 / eB, \quad (2)$$

n_0 is carrier density, the energy dispersion of the $n = 0+$ Landau band $E_{k_z}^{(0+)} = \sqrt{(\hbar v_z k_z)^2 + (M_0 + M_\perp/\ell_B^2 + M_z k_z^2)^2}$, $M_\perp = M_1 v_x v_y$, the magnetic length is $\ell_B = \sqrt{\hbar/eB}$, the bottom of the $n = 1$ Landau band $E_{k_z=0}^{(1)} = \sqrt{(M_0 + 3M_\perp/\ell_B^2)^2 + 2v_x v_y \hbar^2/\ell_B^2}$. Using $B_Q = 1.3$ T in the above equations, n_0 is found as 8.87×10^{16} cm⁻³, comparable with the experiment [33], showing that our model and parameters can well capture the non-interacting energy spectrum. At this low carrier density, the electron pocket at the M point does not play a role [49].

Theory of CDW for the Landau band. – We study the CDW of the $0+$ Landau band by using a mean-field approach, which can well capture the physics of 1D CDWs [24, 25]. Exact diagonalization and density matrix renormalization group are advanced tools but are difficult to compare with the tens of thousands layers of CDW with high Landau degeneracy in the experiment. Quite different from previous theories (e.g., [26]), the 1D Landau band here strongly depends on the magnetic field, e.g., the changing k_F in Eq. (2), the nesting momentum k_{cdw} , and CDW wave length λ_{cdw} .

As shown by the g -ology diagram in Fig. 2 (b), the CDW gap (described by the order parameter Δ) can be opened by the coupling between the electrons near k_F and $-k_F$, through either electron-electron or electron-phonon interactions. The electron-electron interaction reads [29, 32, 50, 51]

$$\hat{H}_{ee} = - \sum_{\mathbf{k}} |\Delta| \left(e^{i\phi} \hat{d}_{\mathbf{k}+}^\dagger \hat{d}_{\mathbf{k}-} + h.c. \right) + \frac{2|\Delta|^2 V}{U(2k_F)}, \quad (3)$$

where the order parameter is defined as $\Delta = \Delta_{ee} = [U(2k_F)/2V] \sum_{\mathbf{k}} \langle \hat{d}_{\mathbf{k}-2k_F e_z}^\dagger \hat{d}_{\mathbf{k}} \rangle$ and V is the volume. $\Delta = |\Delta| e^{i\phi}$, where ϕ is the phase. $\hat{d}_{\mathbf{k}\pm}^\dagger$ and $\hat{d}_{\mathbf{k}\pm}$ are the creation and annihilation operators in the vicinity of $\mp k_F$,

respectively, where $\mathbf{k}\pm \equiv k_z \pm k_F$. In solids, the electron-electron potential takes the Yukawa form [52] $U(2k_F) = e^2 / \{\epsilon_r \epsilon_0 [(2k_F)^2 + \kappa^2]\}$, where ϵ_r (ϵ_0) is the relative (vacuum) dielectric constant, $1/\kappa$ is the screening length. Under the random phase approximation [Fig. 2 (b)], we have $\kappa = \sqrt{e^3 B / (4\pi^2 \epsilon \hbar^2 v_F)}$ with $\epsilon = \epsilon_0 \epsilon_r$. The electron-phonon interaction can be written as [24, 51, 53]

$$\hat{H}_{e-ph} = \sum_{\mathbf{k}} |\Delta| (e^{i\phi} \hat{d}_{\mathbf{k}+}^\dagger \hat{d}_{\mathbf{k}-} + h.c.), \quad (4)$$

where $\Delta = \Delta_{e-ph} = (\alpha_{\mathbf{q}}/V)(\langle \hat{b}_{\mathbf{q}} \rangle + \langle \hat{b}_{-\mathbf{q}}^\dagger \rangle)$, $\hat{b}_{\mathbf{q}}^\dagger$ and $\hat{b}_{\mathbf{q}}$ are the creation and annihilation operators for the phonons with momentum $\mathbf{q} = \pm 2k_F \mathbf{e}_z$, the electron-phonon coupling [51] $\alpha_{\mathbf{q}} = -iqV_{\mathbf{q}}\sqrt{N_{\text{ion}}\hbar}/(2M\omega_{\mathbf{q}})$, $V_{\mathbf{q}} = -Ze^2/[\epsilon(q^2 + \kappa^2)]$ is the Yukawa potential, Ze is the ionic charge, M is the ionic mass, and N_{ion} is the ionic number. The Hamiltonian for the phonons is $\hat{H}_{ph} = \sum_{\mathbf{q}} \hbar\omega_{\mathbf{q}} \hat{b}_{\mathbf{q}}^\dagger \hat{b}_{\mathbf{q}}$, where the phonon dispersion is given by $\omega_{\mathbf{q}} = v_s q$ with the velocity of sound v_s . Near $\pm k_F$, the mean-field Hamiltonian of the 0+ Landau band can be written as

$$\mathcal{H}_{k_z}^{0+} = \begin{pmatrix} \hbar v_F(k_z \pm k_F) & \Delta \\ \Delta^* & -\hbar v_F(k_z \pm k_F) \end{pmatrix}, \quad (5)$$

where $\hbar v_F \equiv |\partial E_{k_z}^{(0+)} / \partial k_z|_{k_z=k_F}$. The eigen energies of $\mathcal{H}_{k_z}^{0+}$ can be found as $E_{k_z} = E_F \pm \text{sgn}(k_z \mp k_F) \sqrt{[v_F \hbar(k_z \mp k_F)]^2 + |\Delta|^2}$ near $\pm k_F$ [green curves in Fig. 2 (a)], respectively, where $\text{sgn}(x)$ is the sign function.

The CDW order parameter is calculated self-consistently from the gap equation defined by $\partial E_g / \partial |\Delta| = 0$, where the ground-state energy $E_g \equiv \langle \hat{H}_m \rangle$ is found as

$$E_g = \sum_{\mathbf{k}} (E_{k_z} - E_F) \Theta(E_F - E_{k_z}) + \frac{|\Delta|^2 V}{g_{2k_F}}, \quad (6)$$

$\Theta(x)$ is the step function, $\hat{H}_m = \sum_{\mathbf{k}} \hat{\Psi}_{\mathbf{k}}^\dagger \mathcal{H}_{k_z}^{0+} \hat{\Psi}_{\mathbf{k}} + |\Delta|^2 V / g_{2k_F}$, $\hat{\Psi}_{\mathbf{k}} \equiv (\hat{d}_{\mathbf{k}+}, \hat{d}_{\mathbf{k}-})^T$, and $\mathcal{H}_{k_z}^{0+}$ has been given in Eq. (5). The coupling $g_{2k_F} = e^2 / \{2\epsilon[(2k_F)^2 + \kappa^2]\}$ for electron-electron interactions and $g_{2k_F} = g_0 / [(2k_F)^2 + \kappa^2]^2$ for electron-phonon interactions with the coupling constant $g_0 = N_{\text{ion}} Z^2 e^4 / (M v_s^2 \epsilon^2)$. Different from non-magnetic-field theories, here the summation $\sum_{k_x, k_y} = S_{xy} / (2\pi \ell_B^2)$ gives the Landau degeneracy, with the area S_{xy} in the $x-y$ plane, $V = S_{xy} L_z$, and the length L_z along the z direction. The gap equation is found as

$$|\Delta| = \left| (v_F \hbar k_F) \text{csch} \left(\frac{4\pi^2 \hbar^2 v_F}{g_{2k_F} e B} \right) \right|, \quad (7)$$

where $\text{csch}(x)$ is the hyperbolic cosecant function.

Electron-electron or electron-phonon interactions?—As shown in Fig. 2 (c), the order parameter calculated using electron-electron interactions is sizable only beyond a threshold magnetic B_C about 10 T, an order larger than those in the experiments [Fig. 3 (a)]. On the other

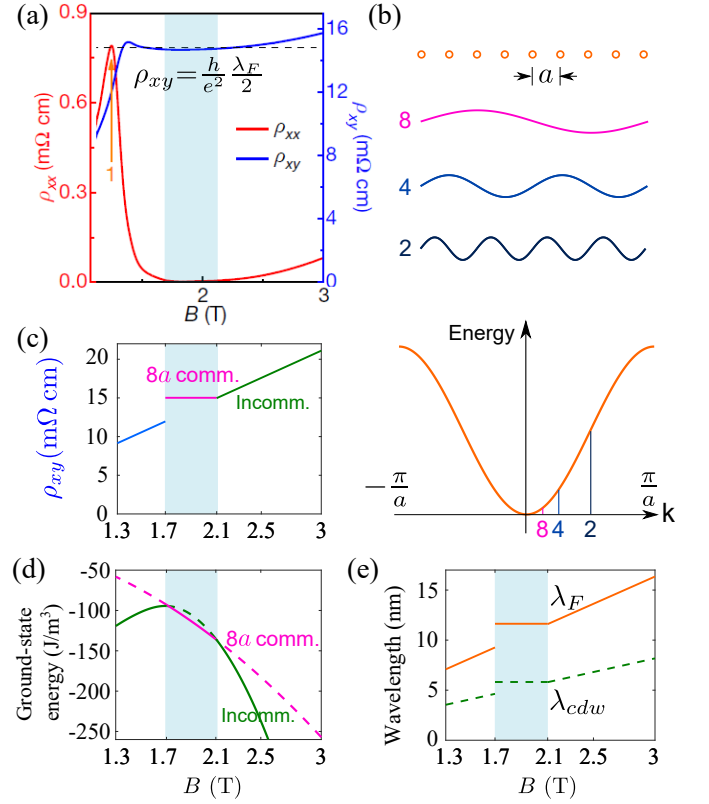


FIG. 3. (a) The Hall (ρ_{xy}) and longitudinal (ρ_{xx}) resistivities adapted from the experiment [33]. (b) Schematic of the commensurate CDWs, whose wave lengths are integer times of the lattice constant a . (c) Our understanding to ρ_{xy} . $B \in [1.3, 1.7]$ T, ρ_{xy} is not quantized due to the broadening of the $n = 1$ Landau band bottom [see also Fig. 4 (e)]; $B \in [1.7, 2.1]$ T, a commensurate CDW pins λ_{cdw} and λ_F , leading to the plateau of ρ_{xy} ; $B \in [2.1, 3]$ T, the incommensurate CDW takes over, so $\rho_{xy} \propto B$. (d) Ground-state energies E_g (per unit volume) of incommensurate and commensurate ($\lambda_{cdw}/a = 8$) CDWs, which shows that the commensurate (incommensurate) CDW has lower energy when $B \in [1.7, 2.1]$ ([2.1, 3] T). (e) The Fermi (λ_F) and CDW (λ_{cdw}) wave lengths.

hand, for electron-phonon interactions with a proper coupling constant ($g_0 = 537.3 \text{ eV}\cdot\text{nm}^{-1}$, determined by the non-Ohmic I-V relation [Fig. 4 (h)]), the threshold B_C could be less than 1.5 T and Δ could be of several to tens of meV [Fig. 2 (e)], both consistent with the experiment. Therefore, electron-phonon interactions may be the mechanism in the ZrTe₅ experiment.

Commensurate-incommensurate crossover. In the experiment, the plateau of the Hall resistivity covers a wide range from 1.7 to 2.1 T, which is surprising for the following reason. According to Fig. 1, the Hall conductivity in units of e^2/h is given by the number of the CDW layers $\sigma_{xy} = \frac{e^2}{h} / \lambda_{cdw}$ per unit length, where λ_{cdw} is the CDW wave length, so the height of plateau should be $\rho_{xy} = 1/\sigma_{xy} = \frac{h}{e^2} \lambda_{cdw}$ when $\sigma_{xx} = 0$. It is known that

the CDW wave length λ_{cdw} is related to the Fermi wave length as [24]

$$\lambda_{cdw} = \lambda_F/2 = \pi/k_F. \quad (8)$$

According to Eq. (2), k_F should decrease with magnetic field, leading to a λ_{cdw} linearly increasing with the magnetic field [e.g., $B > 2.1$ T in Fig. 3 (e)], so ρ_{xy} should increase linearly with B . That is why the plateau in Fig. 3 (a) is surprising.

The observed ρ_{xy} plateau between 1.7 and 2.1 T implies that there is a commensurate CDW, i.e., the CDW wavelength is pinned at integer times of the lattice constant a [Fig. 3 (b)]. According to the experiment, $\lambda_{cdw}/a = 8.1 \pm 0.8$ [33]. We compare the ground-state energies of commensurate ($\lambda_{cdw}/a = 8$) and incommensurate CDWs near 2.1 T, which can be obtained by minimizing the ground-state energy E_g in Eq. (6). As shown in Fig. 3 (d), the commensurate (incommensurate) CDW has lower energy for $B \in [1.7, 2.1]$ ($[2.1, 3]$) T, so there is a crossover between the commensurate and incommensurate CDWs [$B = 2.1$ T in Fig. 3 (c)].

Non-Ohmic I - V relation.—An evidence of CDW is the non-Ohmic I - V relation, because a bias voltage has to overcome the barriers of CDW [Fig. 4 (a)], which can be used to determine the CDW order parameter and more importantly to fit the electron-phonon interaction coupling constant g_0 by comparing our theory with the experiment. The tunneling current I_{cdw} is found as [24, 54]

$$I_{cdw} = \frac{e}{h} \int_{-\infty}^{\infty} d\epsilon D_{cdw}(\epsilon) D_N(\epsilon + eV_z) [f(\epsilon) - f(\epsilon + eV_z)],$$

with the density of states [Fig. 4 (b)] $D_{cdw}(E_{k_z})/D_N(0) = |E_{k_z} - E_F| \Theta(|E_{k_z} - E_F| - |\Delta|) / \sqrt{(E_{k_z} - E_F)^2 - |\Delta|^2}$, where the normal (N) density of states $D_N(0)$ is assumed energy-independent, and $f(x) = 1/[1 + e^{x/(k_B T)}]$ is the Fermi function. Figure 4 (c) shows the non-Ohmic I_{cdw} - V_z relation at different temperatures. At zero temperature, there is no tunneling current for $|V_z|$ smaller than the threshold voltage $V_{th} \equiv |\Delta|/e$. Finite temperatures can lead to a small tunneling current for $|V_z| < V_{th}$. Figure 4 (d) shows the differential conductance dI_{cdw}/dV_z as a function of bias voltage at different temperatures, in which there is a peak near the threshold V_{th} at $T = 2.5$ K, because of the abrupt increase of I_{cdw} across the threshold. This peak is smeared at higher temperatures.

Figure 4 (h) shows the differential resistance dV_z/dI_z in the experiment [33]. There is a plateau for $|I_z|$ smaller than the threshold current $I_{th} \approx 450 \mu A$, besides the non-Ohmic behavior above I_{th} . This implies that besides the 0+ Landau band, there is another Ohmic channel on the Fermi surface, likely the broadened +1 band bottom which lasts till $B = 1.7$ T [Fig. 4 (e)]. Therefore, we model the z -direction current as $I_z = I_{cdw} + I_N$, where I_{cdw} is the non-Ohmic CDW current from the 0+ band and the normal band is assumed to satisfy the Ohmic law

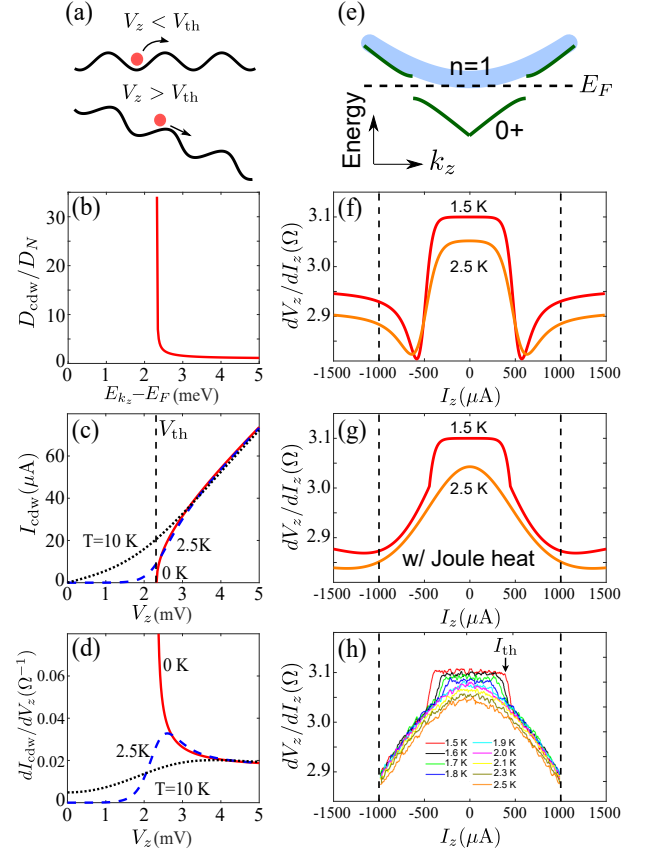


FIG. 4. (a) A bias voltage V_z has to overcome the threshold voltage V_{th} of CDW to yield a current, leading to the non-Ohmic I - V relation. [(b)-(d)] At $B = 1.6$ T, CDW density of states (b), non-Ohmic relation between the tunneling current I_{cdw} and V_z (c), differential conductance dI_{cdw}/dV_z (d). (e) At $B = 1.55$ T, the Fermi energy E_F is assumed to cross both the CDW-gapped $n = 0+$ and broadened $n = 1$ Landau bands. [(f) and (g)] Differential resistance dV_z/dI_z as a function of the z -direction current at $B = 1.55$ T and different temperatures, without (f) and assuming the Joule heat (g). The parameters $\alpha_1 = 7$, $G_{cdw}^{(1)} = 322.58 \text{ m}\Omega^{-1}$, $G_N^{(1)} = 16.64 \text{ m}\Omega^{-1}$, $G_{cdw}^{(2)} = 293.25 \text{ m}\Omega^{-1}$, and $G_N^{(2)} = 49.75 \text{ m}\Omega^{-1}$ at $T = 1.5$ K; $\alpha_2 = 5$, $G_{cdw}^{(3)} = 294.12 \text{ m}\Omega^{-1}$, and $G_N^{(3)} = 53.76 \text{ m}\Omega^{-1}$ at $T = 2.5$ K. (h) Experimental data of dV_z/dI_z [33].

$I_N = G_N V_z$. Then we numerically reproduce the Ohmic plateau and non-Ohmic I_z - V_z relation at different temperatures [Fig. 4 (g)]. Using I_{th} in the experiment, we fit that $g_0 = 537.3 \text{ eV}\cdot\text{nm}^{-1}$. For $T=1.5$ K, we assume that $I_z = I_{cdw}^{(1)}(T) + I_N^{(1)}$ for $I_z < I_{th}$ and $I_z = I_{cdw}^{(2)}(\alpha_1 T) + I_N^{(2)}$ for $I_z > I_{th}$; for $T = 2.5$ K, $I_z = I_{cdw}^{(3)}(\alpha_2 T) + I_N^{(3)}$, where $\alpha_{1,2}$ describe the Joule heat from the abrupt current increase. Without the Joule heat, dV_z/dI_z shows a dip near I_{th} [Fig. 4 (f)], due to the dI_{cdw}/dV_z peak in Fig. 4 (d).

Discussions and perspectives. At higher magnetic fields, signatures of fractional quantum Hall effect have been reported [33, 55]. It could be another commensurate CDW plateau [see Fig. 3 (b)], because the 1D

Landau bands in 3D are naturally “partially-filled”. At lower magnetic fields ($B \in [0.6, 1]$ T), the experiment also shows some plateau-like behaviors in the Hall resistivity [33], implying a simultaneous CDW phase of multiple bands, which could be understood similarly based on our theory. We expect that the CDW mechanism of 3D quantum Hall effect could be realized also in high-quality samples of layered structures HfTe_5 , TaS_2 , NbSe_3 , etc. In Type-II Weyl semimetals [30], the overtilted electron and hole pockets may facilitate nesting, leading to a cascade of CDW even and multiple 3D Hall plateaus for weak interactions.

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