Theory of quantum anomalous Hall effect and electric-field-induced phase transition in AB-stacked MoTe$_2$/WSe$_2$ moiré heterobilayers

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We propose a new mechanism to explain the unexpected quantum anomalous Hall (QAH) effect and the electric-field-induced Mott-to-QAH phase transition without charge gap closure in AB-stacked MoTe$_2$/WSe$_2$ moiré heterobilayers. We suggest that a hole-occupied band carrying a non-zero Chern number can be generated by an intrinsic band inversion between two topologically distinct Dirac bands and a Coulomb-interaction-induced gap opening in the moiré band structure with broken time-reversal symmetry (TRS). The Dirac-band dispersion is induced by a pseudomagnetic field, which is originated from the Berry phase of Bloch electrons in the presence of a moiré potential. The TRS is broken by valley-polarized interlayer-exciton condensation under an out-of-plane electric field. The valley polarization can be demonstrated by using an excitonic Bose-Hubbard (BH) model and Berezinskii-Kosterlitz-Thouless (BKT) transition to transverse ferromagnetism. In low electric fields, the equilibrium state of the system is a Mott insulator state. At a certain electric field, the exciton condensate combining with the Chern band becomes a more stable state and the Mott-to-QAH transition occurs. Since the band inversion is intrinsic, there is no charge gap closure at the transition.

Introduction.—Quantum anomalous Hall (QAH) insulators and related topological materials have drawn a lot of attention from scientists due to their fundamental importance and potentials to design quantum devices.$^{1-5}$ Moiré material has been found to be a new platform for studying the QAH effect.$^{6-10}$ Recently, a QAH effect in AB-stacked MoTe$_2$/WSe$_2$ moiré heterobilayers and a Mott-to-QAH transition without charge gap closure were observed at $\nu = 1$ hole filling under an out-of-plane electric field.$^{11}$ These observations were unexpected since the moiré band structure of the heterobilayers was thought to be topologically trivial.$^{11,12}$ Several theories have been proposed to explain the observation,$^{12-17}$ but some questions remain.

A suitable theory to explain the QAH effect in the AB-stacked heterobilayers should meet certain theoretical criteria and be able to explain related experimental observations. Theoretically, a QAH insulator must have an occupied band with non-zero Chern number (i.e. a Chern band) and the time-reversal symmetry (TRS) must be broken.$^{12,13}$ Experimentally, in addition to the QAH effect, AB-stacked MoTe$_2$/WSe$_2$ heterobilayers also show the following properties$^{11}$. 1. Quantum spin Hall effect is observed at $\nu = 2$ hole filling. 2. At a small electric field and $\nu = 1$ hole filling, the longitudinal resistance diverges rapidly as temperature decreases, indicating a Mott insulator state. 3. The MoTe$_2$ valence band maximum is about 300 meV above the WSe$_2$ valence band maximum in the absence of electric field. 4. A Mott-to-QAH transition occurs at $\nu = 1$ as the electric field contributes about $-172$ meV shift (with 0.66 V/µm electric-field strength and 2.6 eÅ interlayer dipole moment$^{18}$) to the valence-band energy offset, but no charge gap closure is found. Additionally, a continuous Mott transition is observed in AA-stacked MoTe$_2$/WSe$_2$ heterobilayers at $\nu = 1$ hole filling, but no QAH state is found$^{18}$.

In this letter, we propose that the Chern band in the moiré band structure of AB-stacked heterobilayers is generated by an intrinsic band inversion between two topologically distinct Dirac bands and a Coulomb-interaction-induced gap opening. The Dirac-band dispersion is induced by a pseudo-magnetic field and the TRS is broken due to the formation of a valley-polarized interlayer-exciton condensate. The concepts and formulations of pseudo-magnetic field, Dirac-band dispersion, band inversion mechanism, and TRS breaking are introduced and discussed in the following context. The consistency between the theory and experimental observations is discussed in the end.

Pseudo-magnetic field.—For a charge carrier un-
der a slow-varying external potential \( V(r) \) in a two-dimensional material, the Dirac Hamiltonian \( H(r) = V(r) + \mathbb{I} + m_0^2/2m v_F^2 + v_F \tau (\sigma_3 p_x + \sigma_y p_y) \) can be used to simulate the band structure \[19\], with \( \mathbb{I} \) the two-by-two identity matrix, \( \sigma_x, \sigma_y, \sigma_z \) the Pauli matrices, \( \tau = \pm \) indicating \( \pm K \) valley, \( m \) the mass of the carrier, \( p \) the momentum operator, and \( v_F \) the Fermi velocity. With the Foldy-Wouthuysen (FW) transformation \[20, 24\], the Dirac Hamiltonian can be approximated by

\[
H_{\text{FW}}(r) = \left[ \frac{m_0^2}{2m} + \frac{|p|^2}{2m} + \frac{\tau \Omega}{4} \mathbf{e}_z \cdot \nabla V(r) \times \mathbf{p} \right] \sigma_z + \left[ V(r) + \frac{\Omega}{8} \nabla^2 V(r) \right] \mathbf{I},
\]

with \( \Omega = 1/(m^2 v_F^2) \). The additional terms to the conventional effective mass Hamiltonian correspond to the spin-orbit interaction and the Darwin interaction of a relativistic spin-one-half particle \[20, 22\]. From the band-structure perspective, these additional terms can be interpreted as the Berry-phase effect of Bloch electrons and \( \Omega = |\Omega(k_0)| \) is the norm of Berry curvature \[24, 22\].

Based on the FW-transformed Hamiltonian the effective-mass Hamiltonian for holes in the moiré heterobilayer can be written as \[10\]

\[
H(r) = \begin{pmatrix}
\hbar_+(r) & 0 \\
0 & \hbar_-(r)
\end{pmatrix}, \quad \hbar_{\tau l}(r) = \begin{pmatrix}
\hat{h}_{\tau l}(r) & t_{\tau l}(r) \\
t^*_{\tau l}(r) & \hat{h}_{\tau l}(r)
\end{pmatrix},
\]

where \( \hat{h}_{\tau l}(r) \) is the Hamiltonian for a carrier in the \( l \)-th monolayer and \( t_{\tau l}(r) \) is the interlayer tunneling term, with \( l = 1, 2 \) indicating the up, down layers. The interlayer tunneling term is given by \( t_{\tau l}(r) = w + e^{i\tau \kappa_I} + e^{i\tau \kappa_{II}} \), where \( w \) is the tunneling coupling and \( g_j = k_M |\mathbf{e}_z| \sin(j\pi/3) + e_j \sin(j\pi/3) \) for \( j = 1, 2, \ldots, 6 \) are the reciprocal lattice vectors of the moiré superlattice, with \( k_M = 4\pi/(\sqrt{3}a_M) \) and \( a_M \) the moiré lattice constant. The Hamiltonian for holes in the \( l \)-th monolayer is given by

\[
\hat{h}_{\tau l}(r) = \epsilon_{\tau l} + \frac{|p - \tau \kappa_I|^2}{2m_l} - V_l(r)
\]

\[
+ \frac{\tau}{m_l} \mathbf{A}_l(r) \cdot (p - \tau \kappa_I),
\]

where \( \epsilon_{\tau l} = -\tau M \) and \( \epsilon_{\tau l} = -\tau M \) are band-edge energies with \( D \) the valence-band energy offset and \( M \) a TRS breaking interaction. \( \kappa_1 = (2g_1 - g_2)/3, \kappa_2 = (g_1 - 2g_2)/3 \) are the primitive reciprocal vectors of the moiré superlattice, \( V_l(r) = -(1/2) \sum_{j=1,3,5} \sin(g_j \cdot r) \) is the moiré potential, and \( \mathbf{A}_l(r) = (m_l/4\pi) \mathbf{e}_z \times \nabla V_l(r) \) is the pseudo-vector potential with \( \Omega_l = 1/(m_l^2 v_F^2) \). The pseudo-magnetic field is defined as \( \mathbf{B}_l = \nabla \times \mathbf{A}_l(r) \), with \( \mathbf{b} \) one primitive vector of the moiré superlattice.

The parameters for the MoTe\(_2\) layer are given by \( m_1/m_0 = 0.62, v_F/1 = 2.546 \text{ eVÅ}, \) and the parameters for the WS\(_2\)e layer are given by \( m_2/m_0 = 0.36, v_F/2 = 3.643 \text{ eVÅ} \). The parameters for the AB-stacked heterobilayers are \( D = 300 \text{ meV}, V = 5.0 \text{ meV}, \) and \( w = 1.0 \text{ meV} \). The tunneling coupling is assumed to be small because the interlayer tunneling is spin-forbidden in the leading order approximation for the AB-stacked heterobilayers \[11\]. With these parameters, the effective field strengths of the pseudo-magnetic fields are estimated to be 17 Tesla for the MoTe\(_2\) layer and 13 Tesla for the WS\(_2\)e layer. The moiré band structure can be solved by using plane-wave expansion \[23\]. In Fig.\[1\] the moiré bands in the MoTe\(_2\) layer and WS\(_2\)e layer are shown. In contrast to a previous theoretical work \[12\], the energy shifts induced by the pseudo-magnetic field are small compared with the band dispersion, thus unable to give rise to a band inversion. However, as will be shown by a four band model, the pseudo-magnetic field can introduce a phase term to the Bloch wavefunction that leads to an anisotropic Dirac-band dispersion in the moiré band structure.

**Dirac-band dispersion.**—An anisotropic Dirac-band dispersion is induced in the moiré band structure due to the pseudo-magnetic field. To show that, only the moiré band structure of the MoTe\(_2\) layer is considered since the tunneling coupling is much smaller than the valence-band energy offset and the holes largely reside at the MoTe\(_2\) layer. The layer index \( l \) is set to 1 and kept implicit in the following discussion. The Bloch Hamiltonian in the plane-wave basis reads

\[
\langle \tau \gamma | \mathbf{H}_k | \tau \gamma, G_1 \rangle = \int \phi_{\tau \gamma, k}(r) H_{\tau l}(r) \phi_{\tau, G_1, k}(r) d^2r
\]

with \( \phi_{\tau \gamma, k}(r) = e^{i(k - G) \cdot r} \). The band structure is obtained by solving the eigenvalue problem \( H_k C_{\tau nk} = \varepsilon_{\tau nk} C_{\tau nk} \). By using a four band model with the four main basis states \( |\tau, G \rangle = |+, -\rangle, |+, 0 \rangle, |-, g \rangle, |-, 0 \rangle \) with \( \mathbf{g} = g_1\mathbf{g}_1^2 \), the Hamiltonian matrix can be written as

\[
\mathbf{H}_k = \begin{pmatrix}
\hat{h}_k - \kappa \mathbf{I} & 0 & 0 & 0 \\
0 & \hat{h}^*_k - \kappa \mathbf{I} & 0 & 0 \\
0 & 0 & \hat{h}_k + \kappa \mathbf{I} & 0 \\
0 & 0 & 0 & \hat{h}^*_k + \kappa \mathbf{I}
\end{pmatrix},
\]

where \( \kappa = (\kappa_1 - \kappa_2)/2 \) and

\[
\hat{h}_k = \begin{pmatrix}
|k + g_2^2|/2m & -iV \mathbf{e}_z \times \mathbf{g} \cdot \mathbf{k} \\
-iV \mathbf{e}_z \times \mathbf{g} \cdot \mathbf{k}^* & |k - g_2^2|/2m
\end{pmatrix}.
\]

The Bloch Hamiltonian can be rewritten as \( \hat{h}_k = \hat{h}_{k,0} \mathbf{I} + \hat{h}_k \cdot \sigma, \) with \( \sigma = (\sigma_x, \sigma_y, \sigma_z) \), \( \hat{h}_{k,0} = (\hat{h}_{k,x}, \hat{h}_{k,y}, \hat{h}_{k,z}) \), and \( \hat{h}_{k,0} = k^2_0 + \frac{\Omega_n}{2m} \hat{h}_{k,x} = -\frac{\Omega_n}{2m} \mathbf{e}_z \mathbf{k} \cdot \mathbf{k} = -\nu_k \), \( \hat{h}_{k,y} = V, \hat{h}_{k,z} = k^2_0 - \nu_k \mathbf{k}, \) with \( \nu_k = \sqrt{3} m_k/2m \) and \( V = \sqrt{3} m_k V/2 \). It is found that, apart from \( \hat{h}_{k,0} \), the Bloch band shows an anisotropic Dirac-band dispersion. The Hall conductance of the Bloch band is given by \[1\]

\[
\sigma_H = \frac{e^2}{8\pi^2} \int_{BZ} |\hat{h}_k|^{-2} [\partial_{\xi_x} \hat{h}_k \times \partial_{\xi_y} \hat{h}_k]_{\xi^2}^2 k = \frac{e^2}{2\pi} \frac{\text{sgn}(V)}{2}.
\]

Including the valley index \( \tau \), the Hall conductance is given by \( \sigma_H = \frac{e^2}{2\pi} \frac{\text{sgn}(V)}{2} \). The valley-dependent Hall
conductance might contribute to the quantum spin Hall effect observed [11]. However, since the Hall conductance is half quantized, the QAH effect at ν = 1 filling can not be explained merely by the Dirac-band dispersion.

**Band inversion mechanism.**—The Chern band is generated by an intrinsic band inversion and a Coulomb-interaction-induced gap opening. The Chern number C of the bands can be related to the quantized Hall conductance by σ_H = e^2/2\pi C. For interacting systems, the Chern number can be calculated by [23, 32–35]

\[
C = \sum_{\mu \nu \rho} \frac{\epsilon_{\mu \nu \rho}}{6} \int \text{Tr} \left[ G^{\dagger} \frac{\partial G}{\partial k_\mu} \frac{\partial G^\dagger}{\partial k_\nu} \frac{\partial G}{\partial k_\rho} \right] \frac{d^2 k}{(2\pi)^2},
\]

with \(\mu, \nu, \rho \in \{0, x, y\}\), \(\epsilon_{\mu \nu \rho}\) the Levi-Civita symbol, \(k = (\omega, k_x, k_y)\), and \(\tilde{G}(k) = \tilde{G}_{\mu \nu}(\omega)\) the single-particle Green’s function, which can be solved by \(\tilde{G}_{\mu \nu}(\omega) = \left[ \omega - \tilde{H}_k - \tilde{\Sigma}_k(\omega) \right]^{-1}\) and the self-energy \(\tilde{\Sigma}_k(\omega)\) has included the effect of interactions. To study the effect of Coulomb interaction on band topology, the band structure can be determined by the Hartree-Fock equation \(\hat{F}_k C_{nk} = \varepsilon_{nk} C_{nk}\) and the Chern number can be found by solving Eq. (7) with the self-energy \(\tilde{\Sigma}_k(\omega) = \hat{F}_k - \hat{H}_k\). In this scheme, the Fock matrix can be viewed as an effective single-particle Hamiltonian. The topological properties of the band structure can be studied by identifying band inversions among topological distinct bands and gap opening induced by the Coulomb interaction [23].

For the present problem, we assume that the Coulomb potential for the intralayer hole-hole interaction can be approximated by the contact potential \(U \delta(r_1 - r_2)\) with \(U \approx 70 \text{ meV}\). The Fock matrix is given by [23]

\[
\langle a, G_1 | \hat{F}_k | b, G_2 \rangle = \langle a, G_1 | \hat{H}_k | b, G_2 \rangle - U \langle a, G_1 | P | b, G_2 \rangle + \delta_{ab} U \sum_{c} \langle c, G_1 | P | c, G_2 \rangle, \tag{8}
\]

where \(\langle a, G_1 | P | b, G_2 \rangle = (1/N) \sum_{nk,G} n_{nk} C_{a,G+G_1,nk} \times C_{b,G+G_2,nk}\) is the reduced density matrix with \(n_{nk}\) the occupation number and \(N\) the number of moiré unit cell. For the four-band model, the Fock matrix at \(\nu = 1\) can be written approximately as

\[
\hat{F}_k \approx \frac{U \varrho_0}{2} + \begin{pmatrix}
\hat{h}_{k-\kappa} - M^\dagger & -U \varpi \sigma_x \\
-U \varpi \sigma_x & \hat{h}^*_{k-\kappa} + M^\dagger
\end{pmatrix}, \tag{9}
\]

with \(\varrho_0 = \sum_\tau \langle \tau, 0 | \varpi | \tau, 0 \rangle\) and \(\varpi = (-, |g|P|+, 0)\). The results of Hartree-Fock calculation is shown in Fig. 2 (b), (d). A band inversion and a gap opening between two highest bands are found near the \(\kappa^*\) point in the moiré Brillouin zone with an artificially added TRS-breaking interaction \(M = 10 \text{ meV}\) in Fig. 2 (c) and (d). The magnitude of TRS-breaking interaction is exaggerated to show the effect and the origin of this interaction will be discussed below. It is found that the contact interaction contributes to an exchange field on the moiré band structure and induces an antiferromagnetic order by breaking the lattice translational symmetry. The band inversion mechanism create a topologically nontrivial Skyrmion spin texture described by the spinor Hamiltonian \(\hat{h}_k \cdot \sigma\) and contribute a winding number to the hole-occupied band [2].

However, there are two major problems in the above argument. Firstly, the TRS-breaking interaction \(M\) in the discussion is artificially introduced to the model. If there is no external magnetic field or intrinsic magnetization, the TRS can not be broken and the Chern band can not be generated. Secondly, the bandwidth of the hole-occupied band in the first Brillouin zone is about \(E_W = k^2_{\text{F}}/(2m) \approx 43 \text{ meV}\). Since \(U > E_W\), the equilibrium state should be a Mott insulator and thus the band-structure picture to describe the electronic structure is artificial. To resolve these problems, we suggest that a valley-polarized interlayer-exciton condensate can be formed at \(\nu = 1\) filling under the out-of-plane electric field. A ferromagnetic order is generated and the TRS is broken by the valley polarization. At a certain electric field, the exciton condensate with the Chern band becomes a more stable state as compared with the Mott insulator, such that a Mott-to-QAH transition occurs after the formation of the exciton condensate. Therefore, the band-structure picture can still be applied.

**TRS breaking.**—The TRS is broken by valley-polarized interlayer-exciton condensation. Exciton condensation is Bose-Einstein condensation (BEC) of excitons [36–44], and interlayer-exciton condensation has been observed in layered materials [45, 48]. An interlayer-exciton condensate (with the intralayer Coulomb repulsion being omitted, which will be discussed later) can be studied by the
where $\Delta_{r,k}=0$ and exciton density $n_X$ v.s. electric-field strength $F_z$. While $F_z=0.66\ V/\text{nm}$ and $\hat{D}=108\ \text{meV}$ at the Mott-to-QAH transition \cite{11}, the condition is satisfied.

The equilibrium exciton condensate can be described by the Bardeen-Cooper-Schrieffer (BCS)-like wavefunction $|\Phi_{\text{BCS}}\rangle=\prod_{r,k}(\hat{u}_{r,k}+\hat{v}_{r,k}\hat{d}_{r,k}^\dagger)|\Phi_{\text{He}}\rangle$, where $u_{r,k}$ and $v_{r,k}$ are variational coefficients subject to the normalization condition $u_{r,k}^2+v_{r,k}^2=1$ \cite{36,40}. The variational coefficients can be solved as $u_{r,k}^2=(1+\Xi_{r,k}/E_{\text{He}})/2$, $v_{r,k}^2=(1-\Xi_{r,k}/E_{\text{He}})/2$, where $E_{\text{He}}=\sqrt{E_{\text{He}}^2+|\Delta_{r,k}|^2}$ and $\Xi_{r,k}=(\epsilon_{r,k}^\dagger+\epsilon_{r,k})/2$. The exciton density is given by $n_X=\sum_{r,k}v_{r,k}^2/N$, and the order parameter $\Delta_{r,k}$ can be solved from the gap equation $\Delta_{r,k}=1/(2\Xi)\sum_{k,c}W_{c}^{\text{eh}}\Delta_{r,k}/E_{\text{He}}$. The results of the gap-equation calculation are shown in Fig. 3. The exciton condensate is formed at the electric-field strength about $0.58\ V/\text{nm}$, which is lower than the observed value $0.66\ V/\text{nm}$ at the Mott-to-QAH transition \cite{11}. Note that an additional electric-field strength may be required for the equilibrium exciton condensate to become a more stable state than the Mott-insulator state. The correlation-induced screening effect and Pauli-blocking effect are not considered here because the exciton radius ($a_X$) is shorter than the lattice constant ($a_M$), and the exciton density is low \cite{53}. However, with a denser population of excitons under a higher electric field, these correlation effects may cause the dissociation of excitons and the formation of electron-hole plasma \cite{53}. It could explain the observed insulator-to-metal transition \cite{11,12}.

Note that the moiré periodicity and the intralayer Coulomb repulsion were not considered in the EHL Hamiltonian in Eq. (10). The moiré periodicity and the Coulomb repulsion can lead to the localization of an exciton in each moiré unit cell. Such an effect on the exciton condensate can be described by the moiré Bose-Hubbard (BH) Hamiltonian \cite{54,55},

$$\hat{H}_{\text{BH}}=-t\sum_{\tau,(R',R)}\hat{x}_{\tau,R}\hat{x}_{\tau,R'}+U\sum_{R}\hat{x}_{\tau,R}\hat{x}_{\tau,R}+U'\sum_{\tau,R}\hat{x}_{\tau,R}\hat{x}_{\tau,R}(\hat{x}_{\tau,R}\hat{x}_{\tau,R}-1),$$

where $\hat{x}_{\tau,R} = \frac{1}{\sqrt{N}}\sum_{K} e^{-iK\cdot R} \hat{X}_{\tau,K}$ is the exciton creation operator on the moiré unit cell at $R$ site, with $\hat{X}_{\tau,K} = \sum_{k} \Psi_{\tau,k} \hat{d}_{k-k}^\dagger \Psi_{\tau,k}/S$ variationally \cite{22,53}. It is found to be $E_X=129\ \text{meV}$ and the projected in-plane exciton radius is $a_X=16\ \text{Å}$. It is known that an exciton condensate exists if the exciton binding energy is larger than the band gap \cite{23,38,39,40}, indicating $E_X>D$ with $D=D-\delta D-\Delta_{r,k}F_z$ the reorganized band gap.
becomes one exciton per unit cell. If $|\tilde{u}| \ll \tilde{U}, \tilde{U}'$, the BH Hamiltonian with the filling number being one can be approximated by the anisotropic Heisenberg (XXZ) Hamiltonian \cite{58, 61}

$$\hat{H}_{\text{XXZ}} = \sum_{(\mathbf{r}, \mathbf{r}')}(J_z + J_z') \hat{S}_{\mathbf{r}}^z \hat{S}_{\mathbf{r}'}^z - J_\perp \left( \hat{S}_{\mathbf{r}}^x \hat{S}_{\mathbf{r}'}^x + \hat{S}_{\mathbf{r}}^y \hat{S}_{\mathbf{r}'}^y \right)$$ \hspace{1cm} (14)

with $J_z = 4t^2/\tilde{U} - 4t^2/\tilde{U}'$, $J_\perp = 4t^2/\tilde{U}$ and $\hat{S}_{\mathbf{r}}^{x,y,z}$ being spin-1/2 operators with the basis $|+\rangle, |-\rangle$. The model exhibits a transverse ferromagnetic order if $J_z > J_\perp$ \cite{60, 62}. The ferromagnetic order implies valley polarization and TRS breaking. It is estimated that $U \approx U' \approx e^2/(\epsilon_c a_M) \approx 70$ meV, $t \approx 0.015U \approx 1$ meV \cite{55}, and $n_X \approx 0.10$ at the QAH state. We get $U = Un_X \approx 7$ meV, $J_\perp \approx 0.6$ meV, and $J_z \approx 0$ meV. The Berezinskii-Kosterlitz-Thouless (BKT) temperature \cite{62} in a triangular lattice is estimated to be about $T_{\text{BKT}} \approx (1/0.69)J_\perp/(2k_B)$ \cite{63}, which gives $T_{\text{BKT}} \approx 5$ K. This scale is consistent with the observed Curie temperature for the ferromagnetic transition \cite{11}.

Discussions.— A theory to explain the QAH effect and the Mott-to-QAH transition in AB-stacked MoTe$_2$/WSe$_2$ heterobilayers is provided. Compared with other theories \cite{12, 15}, the present theory shows a better consistency with experimental observations. For the valence-band energy offset about 300 meV and the electric-field-induced shift about $-172$ meV \cite{11}, band inversions between moiré bands in different layers \cite{13, 14, 17} is unlikely to happen. Besides, no charge gap closure was observed \cite{11}. The valley polarization of holes to break the TRS \cite{12, 17} is also unlikely, since the moiré bands are not flat enough for the hole occupation to be fully polarized \cite{64} and the observed Mott-to-QAH transition seem to be continuous \cite{11}. Intrinsic band inversion and valley-polarized interlayer-exciton condensation gives more suitable explanations. The observed insulator-to-metal transition at a higher electric field \cite{11} which was lack of a well-accepted explanation now can also be explained by exciton dissociation. Our theory may provide a new viewpoint to search QAH insulators among correlated materials.

Note: a discussion of the topology of Chern band being unaltered in the presence of the exciton condensate is given in the supplemental material.

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[1] M. König, H. Buhmann, L. W. Molenkamp, T. Hughes, C.-X. Liu, X.-L. Qi, and S.-C. Zhang, The Quantum Spin Hall Effect: Theory and Experiment, J. Phys. Soc. Jpn., **77**, 031007 (2008).
[2] B. A. Bernevig, Topological insulators and topological superconductors, Princeton university press (2013).
[3] M. Hohenadler and F. F. Assaad, Correlation effects in two-dimensional topological insulators, J. Phys.: Condens. Matter, **25**, 143201 (2013).
[4] H. Weng, R. Yue, X. Huc, X. Daia, and Z. Fang, Quantum anomalous Hall effect and related topological electronic states, Advances in Physics, **64**, 227 (2015).
[5] C.-X. Liu, S.-C. Zhang, and X.-L. Qi, The Quantum Anomalous Hall Effect: Theory and Experiment, Annu. Rev. Condens. Matter Phys., **7**, 301 (2016).
[6] G. Chen, A. L. Sharpe, E. J. Fox, Y.-H. Zhang, S. Wang, L. Jiang, B. Lyu, H. Li, K. Watanabe, T. Taniguchi, Z. Shi, T. Senthil, D. Goldhaber-Gordon, Y. Zhang, and F. Wang, Tunable correlated Chern insulator and ferromagnetism in a moiré superlattice, Nature, **579**, 56 (2020).
[7] M. Serlin, C. L. Tschirhart, H. Polshyn, Y. Zhang, J. Zhu, K. Watanabe, T. Taniguchi, L. Balents, A. F. Young, Intrinsic quantized anomalous Hall effect in a moiré heterostructure, Science, **367**, 900 (2020).
[8] C. L. Tschirhart, M. Serlin, H. Polshyn, A. Shragai, Z. Xia, J. Zhu, Y. Zhang, K. Watanabe, T. Taniguchi, M. E. Huber, and A. F. Young, Imaging orbital ferromagnetism in a moiré Chern insulator, Science, **372**, 1323 (2021).
[9] Y.-H. Zhang, D. Mao, Y. Cao, P. Jarillo-Herrero, and T. Senthil, Nearly flat Chern bands in moiré superlattices, Phys. Rev. B, **99**, 075127 (2019).
[10] F. Wu, T. Lovorn, E. Tutuc, I. Martin, and A. H. MacDonald, Topological Insulators in Twisted Transition Metal Dichalcogenide Homobilayers, Phys. Rev. Lett., **122**, 086402 (2019).
[11] T. Li, S. Jiang, B. Shen, Y. Zhang, L. Li, Z. Tao, T. Devakul, K. Watanabe, T. Taniguchi, L. Fu, J. Shan, K. F. Mak, Quantum anomalous Hall effect from intertwined moiré bands, Nature, **600**, 641 (2021).
[12] Y.-M. Xie, C.-P. Zhang, J.-X. Hu, K. F. Mak, K. T. Law, Theory of Valley Polarized Quantum Anomalous Hall State in Moiré MoTe$_2$/WSe$_2$ Heterobilayers, Phys. Rev. Lett., **128**, 026402 (2022).
[13] Y. Zhang, T. Devakul, and Liang Fu, Spin-textured Chern bands in AB-stacked transition metal dichalcogenide bilayers, PNAS, **118**, 36 (2021).
[14] Y. Su, H. Li, C. Zhang, K. Sun, and S.-Z. Lin, Massive Dirac fermions in moiré superlattices: a route toward correlated Chern insulators, arXiv:2110.02537 (2021).
[15] H. Pan, M. Xie, F. Wu, and S. Das Sarma, Topological Phases in AB-stacked MoTe$_2$/WSe$_2$: Z2 Topological Insulators, Chern Insulators, and Topological Charge Density Waves, arXiv:2111.01152 (2021).
[16] T. Devakul and L. Fu, Quantum anomalous Hall effect from inverted charge transfer gap, arXiv:2109.13909 (2021).
[17] L. Rademaker, Spin-Orbit Coupling in Transition Metal Dichalcogenide Heterobilayer Flat Bands, arXiv:2111.06208 (2001).
[18] T. Li, S. Jiang, L. Li, Y. Zhang, K. Kang, J. Zhu, K. Watanabe, T. Taniguchi, D. Chowdhury, L. Fu, J. Shan, and K. F. Mak, Continuous Mott transition in semiconductor moiré superlattices, Nature, **597**, 350 (2021).
[19] D. Xiao, G.-B. Liu, W. Feng, X. Xu, and W. Yao, Coupled spin and valley physics in monolayers of MoS$_2$ and
other group-VI dichalcogenides, Phys. Rev. Lett., 108, 196802 (2012).

[20] L. L. Foldy and S. A. Wouthuysen, On the Dirac theory of spin 1/2 particles and its non-relativistic limit, Phys. Rev., 78, 29 (1950).

[21] E. Eriksen, Foldy-Wouthuysen transformation. Exact solution with generalization to the two-particle problem, Phys. Rev., 111, 1011 (1958).

[22] A. J. Silenko, Foldy-Wouthuysen transformation and semilocal limit for relativistic particles in strong external fields, Phys. Rev. A, 77, 012116 (2008).

[23] See supplemental material.

[24] Y.-W. Chang and Y.-C. Chang, Foldy-Wouthuysen transformation for gapped Dirac fermions in two-dimensional semiconducting materials and valley excitons under external fields, arXiv:2107.14474 (2021).

[25] D. Xiao, J. Shi, and Q. Niu, Berry Phase Correction to the ground state of an electron-hole gas-II. Spin states, screening and band structure effects, J. Physique, 43, 1083 (1982).

[26] J. Fernández-Rossier and C. Tejedor, Spin degree of freedom in two dimensional exciton condensates, Phys. Rev. Lett., 78, 4809 (1997).

[27] H. Chu and Y. C. Chang, Theory of optical spectra of exciton condensates, Phys. Rev. B, 54, 5020 (1996).

[28] F.-C. Wu, F. Xue, and A. H. MacDonald, Theory of two-dimensional spatially indirect equilibrium exciton condensates, Phys. Rev. B, 92, 165121 (2015).

[29] J. I. A. Li, T. Taniguchi, K. Watanabe, J. Hone and C. R. Dean, Excitonic superfluid phase in double bilayer graphene, Nat. Phys., 13, 751 (2017).

[30] Z. Wang, D. A. Rhodes, K. Watanabe, T. Taniguchi, J. C. Hone, J. Shan, and K. F. Mak, Evidence of high-temperature exciton condensation in two-dimensional atomic double layers, Nature, 574, 76 (2019).

[31] L. Ma, P. X. Nguyen, Z. Wang, Y. Zeng, K. Watanabe, T. Taniguchi, A. H. MacDonald, K. F. Mak, and J. Shan, Strongly correlated excitonic insulator in atomic double layers, Nature, 598, 585 (2021).

[32] J. Gu, L. Ma, S. Liu, K. Watanabe, T. Taniguchi, J. C. Hone, J. Shan, K. F. Mak, Dipolar excitonic insulator in a moiré lattice, Nat. Phys. (2022).

[33] N. S. Rytova, Vestn. Mosk. Univ. Fiz. Astron., 3, 30 (1967).

[34] L. V. Keldysh, JETP Lett., 29, 658 (1979).

[35] M. Van der Donck and F. M. Peeters, Interlayer excitons in transition metal dichalcogenide heterostructures, Phys. Rev. B, 98, 115104 (2018).

[36] Y.-W. Chang and Y.-C. Chang, Variationally optimized orbital approach to trions in two-dimensional materials, 155, 024110 (2021).

[37] K. Asano and T. Yoshioka, Exciton–Mott physics in two-dimensional electron–hole systems: Phase diagram and single-particle spectra, J. Phys. Soc. Jpn., 83, 084702 (2014).

[38] B. Remez and N. R. Cooper, Dark and leaky exciton condensates in transition metal dichalcogenide moiré bilayers, arXiv:2110.07628 (2021).

[39] N. Götting, F. Lohof, and C. Gies, Moiré-Bose-Hubbard model for interlayer excitons in twisted transition metal dichalcogenide heterostructures, arXiv:2201.10877 (2022).

[40] E. J. Mueller, T.-L. Ho, M. Ueda, and G. Baym, Fragmentation of Bose-Einstein condensates, Phys. Rev. A, 74, 033612 (2006).

[41] M. Ueda, Fundamentals and new frontiers of Bose-Einstein condensation, World Scientific, 2010.

[42] A. B. Kuklov and B.V. Svistunov, Counterflow superfluidity of two-species ultracold atoms in a commensurate optical lattice, Phys. Rev. Lett., 90, 100401 (2003).

[43] E. Altman, W. Hofstetter, E. Demler and M. D Lukin, Phase diagram of two-component bosons on an optical lattice, New J. Phys., 5, 113 (2003).

[44] L.-M. Duan, E. Demler, and M. D. Lukin, Controlling spin exchange interactions of ultracold atoms in optical lattices, Phys. Rev. Lett., 91, 090402 (2003).

[45] L. He, Y. Li, E. Altman, and W. Hofstetter, Quantum phases of Bose-Bose mixtures on a triangular lattice,
Phys. Rev. A, 86, 043620 (2012).

[62] J. M. Kosterlit and D. J. Thouless, Ordering, metastability and phase transitions in two-dimensional systems, J. Phys. C: Solid State Phys., 6, 1181 (1973).

[63] P. Butera and M. Comi, High-temperature study of the Kosterlitz-Thouless phase transition in the XY model on the triangular lattice, Phys. Rev. B, 50, 3052 (1994).

[64] Y. Nagaoka, Ferromagnetism in a narrow, almost half-filled s band, Phys. Rev., 147, 392 (1966).
Supplemental Material: Theory of quantum anomalous Hall effect and electric-field induced phase transition in AB-stacked MoTe$_2$/WSe$_2$ moiré heterobilayers

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In this supplemental material, we introduce the moiré band theory to study the moiré band structure of transition metal dichalcogenide heterobilayers in the beginning. The Foldy-Wouthuysen (FW) transformation for two-dimensional Dirac fermions under a slow-varying potential is introduced and the plane-wave expansion method to solve the band structure is derived. Subsequently, we review the Hall conductance formula for Chern insulators based on field-theoretical formulation and Ward-Takahashi identity. Finally, we review the theory of exciton condensation and the conditions of excitonic instability, and introduce the variational method to solve the exciton binding energy. A discussion of the topology of Chern band being unaltered in the presence of the exciton condensate is given in the end.
I. MOIRÉ BAND THEORY

The moiré band theory for transition metal dichalcogenide heterobilayers is given in this section. In addition to the MoTe$_2$/WSe$_2$ heterobilayers studied here, the theory can also be applied to the study of other heterobilayers. In Sec. I A, the Foldy-Wouthuysen (FW) transformation for two-dimensional Dirac fermions under a spatially slow-varying potential is introduced. In Sec. I B, the geometry informations of moiré superlattices are introduced and the effective mass model for moiré heterobilayers is written based on these informations. In Sec. I C, the Hartree-Fock theory for band structures is reviewed. Finally, in Sec. I D, the plane-wave expansion method to solve the moiré band structures is introduced.

A. FW transformation

The FW transformation has been known to be useful to study relativistic quantum few-particle problems[1–4]. Consider the Dirac Hamiltonian in two dimensions,

$$H(r) = V(r)\mathbb{1} + m v_F^2 \beta + v_F \alpha \cdot p,$$

(1)

where $\alpha = \tau \sigma_z e_z + \sigma_y e_y$, $\beta = \sigma_z$, $V(r)$ is a slow-varying potential, $I$ is a two-by-two identity matrix, $\sigma_z, \sigma_y, \sigma_z$ are the Pauli matrices, $\tau = \pm$ indicates the $\pm K$ valley, $m$ is the mass, $p = -i \nabla_r$ is the momentum operator, and $v_F$ is the Fermi velocity. To derive a generalized form of FW transformed Hamiltonian, Eriksen assume that the initial Hamiltonian can be divided into

$$H = \beta m v_F^2 + E + \mathcal{O},$$

(2)

with $\mathcal{E}$ an even operator and $\mathcal{O}$ an odd operator, which fulfill $\beta \mathcal{E} = \mathcal{E} \beta$, $\beta \mathcal{O} = -\mathcal{O} \beta$. The FW transformation connecting the initial Hamiltonian $\mathcal{H}$ and the transformed Hamiltonian $\mathcal{H}_{FW}$ can be written as

$$\mathcal{H}_{FW} = \mathcal{U}_{FW} \left( \mathcal{H} - \frac{i}{\hbar} \frac{\partial}{\partial t} \right) \mathcal{U}_{FW}^\dagger + \frac{i}{\hbar} \frac{\partial}{\partial t},$$

(3)

where $\mathcal{U}_{FW}$ is a unitary operator named as the FW transformation operator. The FW transformation operator up to the order of $1/m^2$ has the expression $\mathcal{U}_{FW} = \exp \left(i \mathcal{S}' \right) \exp \left(i \mathcal{S}\right)$, where $\mathcal{S} = -\frac{\beta \mathcal{O}}{2 m v_F^2}$, $\mathcal{S}' = -\frac{1}{2} \left[ \mathcal{O}, \mathcal{G} \right] / \left( 4 m^2 v_F^4 \right)$, with the generator $\mathcal{G} = \mathcal{E} - i \partial/\partial t$. The FW Hamiltonian which is corrected up to the order of $1/m^2$ can be written as

$$\mathcal{H}_{FW} = \beta m v_F^2 + \mathcal{E} + \beta \mathcal{O}^2 \frac{1}{2 m v_F^2} - \frac{\left[ \mathcal{O}, \left[ \mathcal{O}, \mathcal{G} \right] \right]}{8 m^2 v_F^4},$$

(4)
In the present case, the correspondence between the Dirac Hamiltonian and the Eriksen’s Hamiltonian are given by
\[ O = v_F \alpha \cdot p, \quad \mathcal{E} = V(r) I. \] (5)
We can find \( O^2 = v_F^2 |p|^2 \) and
\[ [O, [O, \mathcal{G}]] = -v_F^2 [\nabla^2 V(r) + 2 \tau \beta e_z \cdot \nabla V(r) \times p]. \] (6)
The FW Hamiltonian becomes
\[ \mathcal{H}_{FW} = \left[ m v_F^2 + \frac{|p|^2}{2m} + \frac{\tau \Omega}{4} e_z \cdot \nabla V(r) \times p \right] \beta + \left[ V(r) + \frac{\Omega}{8} \nabla^2 V(r) \right] I, \] (7)
with \( \Omega = 1/(m^2 v_F^2) \) the valley-orbit coupling, which can be interpreted as the Berry curvature of Bloch electrons in the presence of moiré potential [4–8].

**B. Effective-mass model for moiré heterobilayers**

For a hexagonal lattice system, the lattice vectors of the moiré superlattice can be defined as \( \mathbf{a}_1 = a_M[(\sqrt{3}/2)e_x + (1/2)e_y], \mathbf{a}_2 = a_M[(-\sqrt{3}/2)e_x + (1/2)e_y] \). The primitive vectors of the moiré superlattice are given by \( \mathbf{b}_1 = -(2\mathbf{a}_1 + \mathbf{a}_2)/3, \mathbf{b}_2 = (\mathbf{a}_1 + 2\mathbf{a}_2)/3, \) and \( \mathbf{b}_3 = (\mathbf{a}_1 - \mathbf{a}_2)/3 \). The lattice constant of the moiré supercell \( a_M \) as a function of twisted angle \( \theta \) and the lattice mismatch \( \delta = |a'_0 - a_0|/a_0 \), with \( a_0 \) the lattice constant for the atomistic lattice, is given by
\[ a_M = \frac{(1 + \delta)a_0}{\sqrt{2(1 + \delta)(1 - \cos \theta)} + \delta^2}. \] (8)
The reciprocal lattice vectors can be solved from \( g_i \cdot \mathbf{a}_j = 2\pi \delta_{ij} \) for \( i, j = 1, 2 \). We get \( g_1 = \sqrt{3}k_M[(1/2)e_x + (\sqrt{3}/2)e_y], \quad g_2 = \sqrt{3}k_M[(-1/2)e_x + (\sqrt{3}/2)e_y], \quad g_3 = 4\pi/(3a_M). \) And other reciprocal lattice vectors are given by
\[ g_j = \sqrt{3}k_M [e_x \cos(j\pi/3) + e_y \sin(j\pi/3)] \] (9)
with \( j = 1, 2, \cdots, 6 \). The reciprocal lattice vectors and the moiré Brillouin zone are shown in Fig. 1 (b). With these geometry informations of moiré superlattices, we can write down the effective-mass Hamiltonian for moiré heterobilayers.

![FIG. 1. (a) The first Brillouin zones of the MoTe$_2$ layer (inside purple hexagonal) and the WSe$_2$ layer (inside red hexagonal). The filled green zone is the first moiré Brillouin zone of moiré heterobilayers. (b) A closer look at the first moiré Brillouin zone of moiré heterobilayers and the high symmetry points.](image-url)
Based on Fig. 1 (a), (b) and Ref. [9], the effective-mass Hamiltonian for moiré heterobilayers can be written as

\[ H(r) = \begin{pmatrix} \hat{h}_+ (r) & 0 \\ 0 & \hat{h}_- (r) \end{pmatrix}, \quad \hat{h}_r (r) = \begin{pmatrix} h_{\tau l} (r) & t_{\tau} (r) \\ t_{\tau}^* (r) & h_{\tau 2} (r) \end{pmatrix}, \]

(10)

where \( h_{\tau l} (r) \) is the effective-mass Hamiltonian for a carrier in the \( l \)-th layer and \( t_{\tau} (r) \) is the interlayer tunneling term. The effective-mass Hamiltonian in the \( l \)-th layer is given by

\[ h_{\tau l} (r) = \epsilon_{\tau l} + \frac{|p - \tau \kappa_l|^2}{2m_l} - \frac{q}{e} V_l (r) + \frac{\tau}{m_l} A_l (r) \cdot (p - \tau \kappa_l), \]

(11)

where \( \kappa_1 = (2g_1 - g_2) / 3 \) and \( \kappa_2 = (g_1 - 2g_2) / 3 \) are reciprocal primitive vectors, \( \epsilon_{\tau l} \) is a constant energy shift, \( q \) is the charge with \( q = -e \) for the electron and \( q = e \) for the hole, \( m_l \) the effective mass,

\[ V_l (r) = 2V \sum_{j=1,3,5} \cos (g_j \cdot r - \chi_l), \]

(12)

is the the moiré potential with \( V \) and \( \chi_l \) being the amplitude and the phase angle of the potential,

\[ A_l (r) = \frac{m_l \Omega_l}{4} e_z \times \nabla V_l (r), \]

(13)

is the pseudo-vector potential with \( \Omega_l = 1/(m_l^2 \varepsilon_{F j}^2) \) the Berry curvature. We choose the phase angle \( \chi_l = (-1)^l \pi / 2 \), such that the moiré potential becomes

\[ V_l (r) = (-1)^l 2V \sum_{j=1,3,5} \sin (g_j \cdot r). \]

(14)

The interlayer tunneling term is given by

\[ t_{\tau} (r) = w (1 + e^{i \pi g_1 \cdot r} + e^{i \pi g_2 \cdot r}), \]

(15)

where \( w \) is the tunneling coupling. Note that \( t_{\tau} (b_1) = t_{\tau} (b_2) = t_{\tau} (b_3) = 0 \) and \( t_{\tau} (0) = t_{\tau} (a_1) = t_{\tau} (a_2) = 3w \), \( V_l (b_1) = V_l (b_2) = V_l (b_3) = -V_l (-b_1) = -V_l (-b_2) = -V_l (-b_3) = (-1)^l 3\sqrt{3} V \) and \( V_l (0) = V_l (a_1) = V_l (a_2) = 0 \). All the symmetry points are the critical points in the moiré potential or the tunneling coupling. If the coordinate is transformed as \( r \rightarrow r + b_2 \), the moiré potential becomes

\[ V'_l (r) = (-1)^l 2V \sum_{j=1,3,5} \sin (g_j \cdot (r + b_2)) = (-1)^l 2V \sum_{j=1,3,5} \sin \left( g_j \cdot r + \frac{2\pi}{3} \right), \]

(16)

and the tunneling coupling becomes

\[ t'_{\tau} (r) = w \left( 1 + e^{i \pi g_1 \cdot (r + b_2)} + e^{i \pi g_2 \cdot (r + b_2)} \right) = w \left[ 1 + e^{i \pi (g_1 \cdot r + \frac{2\pi}{3})} + e^{i \pi (g_2 \cdot r + \frac{2\pi}{3})} \right]. \]

(17)

The later formulation of moiré potential and interlayer tunneling term is seen in literatures more often, but actually the two formulations are equivalent.

C. Hartree-Fock theory for band structures

The many-particle Hamiltonian for multi-component particle fields is given by

\[ \hat{H} = \sum_{ab} \int \Psi_d^\dagger (r) H_{ab} (r) \Psi_b (r) d^2 r + \frac{1}{2} \sum_{ab} \int W_{ab} (r_{12}) : \hat{\rho}_a (r_1) \hat{\rho}_b (r_2) : d^2 r_1 d^2 r_2, \]

(18)

where \( a \) is the component index. For the present case, \( a = \{ \tau, l \} \), where \( \tau = \pm \) indicates the \( \pm K \) valley and \( l = 1, 2 \) denoting the MoTe2 and WSe2 layer, respectively. \( H_{ab} (r) \) is the effective-mass Hamiltonian, \( W_{ab} (r_{12}) \) is the Coulomb potential, \( \Psi_d^\dagger (r) \) and \( \Psi_a (r) \) are charge creation and annihilation operators, \( \hat{\rho}_a (r) = \Psi_d^\dagger (r) \Psi_a (r) \) is the density operator.
The number ordering for the density operators in the Coulomb interaction is assumed. The quasiparticle creation and annihilation operators can be transformed as

$$\hat{\psi}^\dagger_{a}(\mathbf{r}) = \sum_{nk} \psi^*_{a,nk}(\mathbf{r}) c^\dagger_{nk}, \quad \hat{\psi}_{a}(\mathbf{r}) = \sum_{nk} \psi_{a,nk}(\mathbf{r}) c_{nk},$$

with $\psi_{a,nk}(\mathbf{r})$ the quasiparticle wavefunction. By using linear variational method, it is found that the quasiparticle wavefunction can be solved by the Hartree-Fock equation

$$\sum_{b} \int F_{ab}(\mathbf{r}_1, \mathbf{r}_2) \psi_{b,nk}(\mathbf{r}_2) d^2r_2 = \varepsilon_{nk} \psi_{a,nk}(\mathbf{r}_1),$$

where $n$ is the band index, $\varepsilon_{nk}$ is the quasiparticle energy. The Fock operator is defined by

$$F_{ab}(\mathbf{r}_1, \mathbf{r}_2) = \delta(\mathbf{r}_1 - \mathbf{r}_2) [H_{ab}(\mathbf{r}_1) + \delta_{ab} K_{aa}(\mathbf{r}_1)] - J_{ab}(\mathbf{r}_1, \mathbf{r}_2),$$

where $K_{aa}(\mathbf{r}_1) \equiv \sum_{c} \int W_{ac}(\mathbf{r}_1) P_{ac}(\mathbf{r}_3; r_3) d^2r_3$ is the Coulomb operator, $J_{ab}(\mathbf{r}_1, \mathbf{r}_2) \equiv W_{ab}(\mathbf{r}_1) P_{ba}(\mathbf{r}_2, \mathbf{r}_1)$ is the exchange operator, and

$$P_{ab}(\mathbf{r}_1, \mathbf{r}_2) = \sum_{nk} n_{nk} \psi_{a,nk}(\mathbf{r}_1) \psi^*_{b,nk}(\mathbf{r}_2)$$

is the density-matrix operator, where $n_{nk} = \langle \hat{c}^\dagger_{nk} \hat{c}_{nk} \rangle$ is the occupation number of charges in the band $n$ with the momentum $\mathbf{k}$. The Hartree-Fock ground-state energy is given by

$$E_{HF} = \sum_{nk} n_{nk} \varepsilon_{nk} - \frac{1}{2} \sum_{a} \int K_{aa}(\mathbf{r}) P_{aa}(\mathbf{r}, \mathbf{r}) d^2r + \frac{1}{2} \sum_{ab} \int J_{ab}(\mathbf{r}_1, \mathbf{r}_2) P_{ba}(\mathbf{r}_2, \mathbf{r}_1) d^2r_1 d^2r_2.$$

### D. Plane-wave expansion

The quasiparticle wavefunction of a carrier in the moiré superlattice can be expanded in terms of plane-wave basis functions as

$$\psi_{nk}(\mathbf{r}) = \sum_{\alpha} C(\alpha, \mathbf{G}_a, nk) \phi_{\mathbf{G}_a, \mathbf{k}(\mathbf{r})},$$

where $\phi_{\mathbf{G}_a, \mathbf{k}}(\mathbf{r})$ denotes a plane-wave basis function and $C(\alpha, \mathbf{G}_a, nk)$ is the wavefunction coefficient. The plane-wave basis function is written as

$$\phi_{\mathbf{G}_a, \mathbf{k}}(\mathbf{r}) = e^{i \mathbf{k} \cdot \mathbf{r}} / \sqrt{S},$$

with $S = N(\sqrt{3}/2)a_0^2$ the area of the moiré lattice. By using the plane-wave expansion, the Hamiltonian matrix element is given by $\langle a, \mathbf{G}_a | H_k | b, \mathbf{G}_b \rangle = \int \phi_{\mathbf{G}_a, \mathbf{k}}^*(\mathbf{r}) H_{ab}(\mathbf{r}) \phi_{\mathbf{G}_b, \mathbf{k}}(\mathbf{r}) d^2r$ and the diagonal part is given by

$$\langle a, \mathbf{G}_a | \hat{H}_k | a, \mathbf{G}_\beta \rangle = \delta_{\alpha\beta} \frac{|k - \mathbf{G}_a - \tau_a \kappa_{la}|^2}{2m_{la}} \quad \frac{q}{e} \langle a, \mathbf{G}_a | \hat{V}_{la, \mathbf{k}} | a, \mathbf{G}_\beta \rangle + \frac{\tau_a}{m_{la}} \langle a, \mathbf{G}_a | \hat{A}_{la, \mathbf{k}} | a, \mathbf{G}_\beta \rangle \cdot (k - \mathbf{G}_\beta - \tau_a \kappa_{la}),$$

with

$$\langle a, \mathbf{G}_a | \hat{V}_{la, \mathbf{k}} | a, \mathbf{G}_\beta \rangle = -i V \sum_{j} (-1)^l a + j \delta (\mathbf{G}_a - \mathbf{G}_\beta - \mathbf{g}_j)$$

and

$$\langle a, \mathbf{G}_a | \hat{A}_{la, \mathbf{k}} | a, \mathbf{G}_\beta \rangle = -\frac{V}{4} \Omega \sum_{j} (-1)^l a + j \mathbf{e}_z \times \mathbf{g}_j \delta (\mathbf{G}_a - \mathbf{G}_\beta - \mathbf{g}_j).$$

The off-diagonal Hamiltonian matrix element is given by

$$\langle a, \mathbf{G}_a | \hat{H}_k | b, \mathbf{G}_\beta \rangle = \delta_{\tau_a, \tau_b} \delta_{l_a, l_b + 1} \left[ \delta (\mathbf{G}_a - \mathbf{G}_\beta) + \sum_{j=1,2} \delta (\mathbf{G}_a - \mathbf{G}_\beta - \tau \mathbf{g}_j) \right]$$

$$+ \delta_{\tau_a, \tau_b} \delta_{l_a + 1, l_b} \left[ \delta (\mathbf{G}_a - \mathbf{G}_\beta) + \sum_{j=1,2} \delta (\mathbf{G}_a - \mathbf{G}_\beta + \tau \mathbf{g}_j) \right].$$
The wavefunction coefficient can be obtained by the Hartree-Fock equation
\[
\tilde{F}_k C_{nk} = \varepsilon_{nk} C_{nk}.
\] (30)

The Fock matrix is given by
\[
\langle a, \mathbf{G}_\alpha | \tilde{F}_k | b, \mathbf{G}_\beta \rangle = \langle a, \mathbf{G}_\alpha | \tilde{H}_k | b, \mathbf{G}_\beta \rangle + \delta_{ab} \langle a, \mathbf{G}_\alpha | \tilde{K}_k | a, \mathbf{G}_\beta \rangle - \langle a, \mathbf{G}_\alpha | \tilde{J}_k | b, \mathbf{G}_\beta \rangle.
\] (31)

The Coulomb integral is given by
\[
\langle a, \mathbf{G}_\alpha | \tilde{K}_k | a, \mathbf{G}_\beta \rangle = \frac{1}{S} \sum_{q, \mathbf{G}, c} \langle c, \mathbf{G} + \mathbf{G}_\alpha | \tilde{P}_q | c, \mathbf{G} + \mathbf{G}_\beta \rangle \tilde{W}_{ac}(\mathbf{G}_\alpha - \mathbf{G}_\beta),
\] (32)
and the exchange integral is given by
\[
\langle a, \mathbf{G}_\alpha | \tilde{J}_k | b, \mathbf{G}_\beta \rangle = \frac{1}{S} \sum_{q, \mathbf{G}} \langle a, \mathbf{G} + \mathbf{G}_\alpha | \tilde{P}_q | b, \mathbf{G} + \mathbf{G}_\beta \rangle \tilde{W}_{ab}(\mathbf{G} + \mathbf{k} - \mathbf{q}),
\] (33)

where the density matrix is given by
\[
\langle a, \mathbf{G}_\alpha | \tilde{P}_k | b, \mathbf{G}_\beta \rangle = \sum_n n_{nk} C_{(a, \mathbf{G}_\alpha), nk} C_{(b, \mathbf{G}_\beta), nk}.
\] (34)

and \(\tilde{W}_{ab}(\mathbf{k}) = \int \exp(-i \mathbf{k} \cdot \mathbf{r}) W_{ab}(\mathbf{r}) d^2 r\) is the Fourier transform of the Coulomb potential.

Now we consider that the Coulomb potential is described by the contact potential
\[
W_{ab}(\mathbf{r}) = \delta_{la, lb} \sqrt{3} a_m^2 U \delta(\mathbf{r}),
\] (35)
whose Fourier transform is given by
\[
\tilde{W}_{ab}(\mathbf{k}) = \delta_{la, lb} \sqrt{3} a_m^2 U.
\] (36)

The Coulomb integral is found to be
\[
\langle a, \mathbf{G}_\alpha | \tilde{K}_k | a, \mathbf{G}_\beta \rangle = \frac{U}{N} \sum_{q, \mathbf{G}, c} \langle c, \mathbf{G} + \mathbf{G}_\alpha | \tilde{P}_q | c, \mathbf{G} + \mathbf{G}_\beta \rangle,
\] (37)

and the exchange integral is found to be
\[
\langle a, \mathbf{G}_\alpha | \tilde{J}_k | b, \mathbf{G}_\beta \rangle = \delta_{la, lb} \frac{U}{N} \sum_{q, \mathbf{G}} \langle a, \mathbf{G} + \mathbf{G}_\alpha | \tilde{P}_q | b, \mathbf{G} + \mathbf{G}_\beta \rangle.
\] (38)

By defining a reduced density matrix
\[
\langle a, \mathbf{G}_\alpha | P | b, \mathbf{G}_\beta \rangle = \frac{1}{N} \sum_{q, \mathbf{G}} \langle a, \mathbf{G} + \mathbf{G}_\alpha | \tilde{P}_q | b, \mathbf{G} + \mathbf{G}_\beta \rangle,
\] (39)

the Coulomb and exchange integrals become
\[
\langle a, \mathbf{G}_\alpha | \tilde{K}_k | a, \mathbf{G}_\beta \rangle = U \sum_c \langle c, \mathbf{G}_\alpha | P | c, \mathbf{G}_\beta \rangle,
\] (40)
\[
\langle a, \mathbf{G}_\alpha | \tilde{J}_k | b, \mathbf{G}_\beta \rangle = \delta_{la, lb} U \langle a, \mathbf{G}_\alpha | P | b, \mathbf{G}_\beta \rangle,
\] (41)
and the Fock matrix becomes
\[
\langle a, \mathbf{G}_\alpha | \tilde{F}_k | b, \mathbf{G}_\beta \rangle = \langle a, \mathbf{G}_\alpha | \tilde{H}_k | b, \mathbf{G}_\beta \rangle + \delta_{ab} U \sum_c \langle c, \mathbf{G}_\alpha | P | c, \mathbf{G}_\beta \rangle - \delta_{la, lb} U \langle a, \mathbf{G}_\alpha | P | b, \mathbf{G}_\beta \rangle.
\] (42)

This is the Fock matrix we used in the main text.
II. HALL CONDUCTANCE

In this section, we review the Hall conductance formula for many-particle systems and provide a derivation of the Green’s function formula for calculating Chern numbers

\[
C = \frac{\epsilon_{\mu\nu\rho}}{6} \int \text{Tr} \left[ \hat{G} \frac{\partial \hat{G}^{-1}}{\partial k_\mu} \hat{G} \frac{\partial \hat{G}^{-1}}{\partial k_\nu} \hat{G} \frac{\partial \hat{G}^{-1}}{\partial k_\rho} \right] d^3k (2\pi)^3. \tag{43}
\]

Note that the Einstein summation convention is used in this section for the coordinate index \( \mu, \nu, \rho \). We rewrite the derivation from Ref. \[14\:\[12\] and try to make it more readable. In Sec. II A, the Kubo formula for calculating conductivity tensor is reviewed. In Sec. II B, the extension of the Kubo formula based on field-theoretical formulation is derived. In Sec. II C Eq. (48) is derived by the Green’s function method and the Ward-Takahashi identity.

A. Kubo formula

The dynamical conductivity tensor can be defined by

\[
j^I(t) = \sum_J \int \text{d}t' \sigma_{\text{ret}}^{IJ}(t-t') \mathcal{F}^J(t'), \tag{44}
\]

where \( \mathcal{F} \) is the electric field. By using linear response theory, the dynamical conductivity tensor can be given by

\[
\sigma_{\text{ret}}^{IJ}(t-t') = i\theta(t-t') \langle [\hat{j}^I(t), \hat{\xi}^J(t')] \rangle, \tag{45}
\]

where \( \hat{j} \) is the electric current operator and \( \hat{\xi} \) is the electric dipole operator defined by \( \hat{j} = d\hat{\xi}/dt \). It is also possible to define the current-current response function

\[
\pi_{\text{ret}}^{IJ}(t-t') = i\theta(t-t') \langle [\hat{j}^I(t), \hat{j}^J(t')] \rangle, \tag{46}
\]

such that

\[
\frac{d}{dt} \sigma_{\text{ret}}^{IJ}(t-t') = -i\delta(t-t') \langle [\hat{j}^I(t), \hat{\xi}^J(t')] \rangle + \pi_{\text{ret}}^{IJ}(t-t'). \tag{47}
\]

Using \( e^{i\omega(t-t')} = \frac{1}{\omega} \frac{d}{dt} e^{i\omega(t-t')} \), and assuming \( \sigma^{IJ}(\tau) \rightarrow 0 \) as \( \tau = t - t' \rightarrow \infty \), we get the dynamical conductivity tensor in frequency domain

\[
\hat{\sigma}_{\text{ret}}^{IJ}(\omega + i\eta) = \lim_{\eta \to 0} \int_{-\infty}^{\infty} \frac{d\tau}{\omega + i\eta} \sigma_{\text{ret}}^{IJ}(\tau) d\tau = \lim_{\eta \to 0} \int_{-\infty}^{\infty} \frac{e^{i(\omega+\eta)\tau}}{\omega + i\eta} \frac{d}{dt} \sigma_{\text{ret}}^{IJ}(\tau) d\tau
\]

\[
= -\lim_{\eta \to 0} \left[ \frac{\langle [\hat{j}^I(t), \hat{\xi}^J(t')] \rangle}{\omega + i\eta} + \frac{i\pi_{\text{ret}}^{IJ}(\omega + i\eta)}{\omega + i\eta} \right]. \tag{48}
\]

The current-current correlation function in frequency-domain can be solved by

\[
\hat{\pi}_{\text{ret}}^{IJ}(\omega) = \sum_{NM} \varrho_N \left( \frac{j_{NM}}{\omega_{MN} - \omega} + \frac{j_{NM}}{\omega_{MN} + \omega} \right), \tag{49}
\]

where \( \varrho_N \) is the weight factor, \( \omega_{MN} = E_M - E_N \), and \( j_{NM} = \langle N | \hat{j} | M \rangle \) with \( E_N \) and \( |N\rangle \) being solved from \( \hat{H}|N\rangle = E_N |N\rangle \). It is found that

\[
\hat{\sigma}_{\text{ret}}^{IJ}(0) = -i \lim_{\eta \to 0} \frac{\hat{\pi}_{\text{ret}}^{IJ}(i\eta)}{1\eta} = -i \frac{\partial \hat{\pi}_{\text{ret}}^{IJ}(\omega)}{\partial \omega} |_{\omega=0}. \tag{50}
\]

The response function can be simplified as

\[
\hat{\sigma}_{\text{ret}}^{IJ}(\omega) = \sum_{NM} \varrho_N \left( \frac{j_{NM}}{\omega_{MN} - \omega} + \frac{j_{NM}}{\omega_{MN} + \omega} \right). \tag{51}
\]
Then the Hall conductance can be found as

$$\sigma_H \equiv \tilde{\sigma}_{\text{ret}}^x(0) = 2 \sum_{NM} \frac{\partial \text{Im}(j_{NM}^L j_{MN}^R)}{\omega_{MN}}. \quad (52)$$

Note that the formula can be in general used to study Hall conductance for any many-particle system if the electric current and electric dipole operators are defined. Eq. (50) is known as a Kubo formula and will be used in the following derivation.

### B. Field theoretical formulation

For a multi-component many-particle system, the Hamiltonian can be written as

$$\hat{H} = \sum_{ab} \int \hat{\Psi}_a^\dagger(r) H_{ab}(r) \hat{\Psi}_b(r) d^2r + \frac{1}{2} \sum_{ab} \int W_{ab}(r_{12}) : \hat{\rho}_a(r_1) \hat{\rho}_b(r_2) : d^2r_1 d^2r_2, \quad (53)$$

where $\hat{\Psi}_a^\dagger(r)$, $\hat{\Psi}_a(r)$ are field operators with $a,b$ the component index, $\hat{\rho}_a(r) = \hat{\Psi}_a^\dagger(r) \hat{\Psi}_a(r)$ is the density operator, $H_{ab}(r)$ is the Hamiltonian matrix, $W_{ab}(r_{12})$ is the Coulomb interaction. The continuity equation is given by

$$\frac{\partial \hat{\rho}(r,t)}{\partial t} - \nabla \cdot \hat{\mathbf{J}}(r,t) = 0, \quad (54)$$

where the time-evolving electric density operator and electric current density operator are defined by

$$\hat{\rho}(r,t) = e \sum_a \hat{\Psi}_a^\dagger(r,t) \hat{\Psi}_a(r,t), \quad \hat{\mathbf{J}}^j(r,t) = e \sum_{ab} \hat{\Psi}_a^\dagger(r,t) \gamma^j_{ab} (-\mathbf{i} \nabla) \hat{\Psi}_b(r,t), \quad (55)$$

in Heisenberg picture, with

$$\gamma^j_{ab} (-\mathbf{i} \nabla) = \int \left[ \rho_j^a(p) \hat{H}_{ab}(p) \right] e^{\mathbf{i} \mathbf{p} \cdot \mathbf{r}} \frac{d^3p}{(2\pi)^3} \quad (56)$$

the velocity matrix. The current and dipole operator are given by

$$\hat{\mathbf{J}}^j(t) = \int \hat{\mathbf{j}}^j(r,t) d^2r, \quad \hat{\mathbf{\xi}}^j(t) = -\int r^j \hat{\rho}(r,t) d^2r.$$  

To derive the Hall conductance, we firstly define the following response functions

$$K^j_{\text{ret}}(r-r', t-t') = \mathbf{i} \theta(t-t') \left\langle \left[ \hat{\mathbf{j}}^j(r,t), \hat{\mathbf{\xi}}^j(r',t') \right] \right\rangle, \quad (57)$$

$$\Pi^I_J^J_{\text{ret}}(r-r', t-t') = \mathbf{i} \theta(t-t') \left\langle \left[ \hat{\mathbf{J}}^I(r,t), \hat{\mathbf{J}}^J(r',t') \right] \right\rangle, \quad (58)$$

and the Fourier transformed functions

$$\tilde{K}^I_J^j_{\text{ret}}(\mathbf{k}, \omega) = \int K^j_{\text{ret}}(r,t) e^{\mathbf{i} (\omega t - \mathbf{k} \cdot \mathbf{r})} d^2r dt, \quad \tilde{\Pi}^I_J^J_{\text{ret}}(k, \omega) = \int \Pi^I_J^J_{\text{ret}}(r,t) e^{\mathbf{i} (\omega t - \mathbf{k} \cdot \mathbf{r})} d^2r dt. \quad (59)$$

The dynamical conductivity tensor can be given by

$$\sigma^I_J^j_{\text{ret}}(t-t') = \int r^j K^I_{\text{ret}}(r,t-t') d^2r = \int \left[ \frac{\partial}{\partial k_J} \tilde{K}^I_J^j_{\text{ret}}(\mathbf{k}, \omega) \right]_{\mathbf{k}=0} e^{-\mathbf{i} \omega (t-t')} \frac{d\omega}{2\pi}. \quad (60)$$

The current-current response function can be given by

$$\pi^I_J^j_{\text{ret}}(t-t') = \int \Pi^I_J^J_{\text{ret}}(r,t-t') d^2r = \int \left[ \tilde{\Pi}^I_J^J_{\text{ret}}(0, \omega) \right] e^{-\mathbf{i} \omega (t-t')} \frac{d\omega}{2\pi}. \quad (61)$$

By using Eq. (50), we get

$$\tilde{\sigma}^I_J^j_{\text{ret}}(0) = \mathbf{i} \left. \frac{\partial}{\partial k_J} \tilde{K}^I_J^j_{\text{ret}}(\mathbf{k}, \omega) \right|_{\omega=0, \mathbf{k}=0} = -\mathbf{i} \left. \frac{\partial}{\partial \omega} \tilde{\Pi}^I_J^J_{\text{ret}}(\mathbf{k}, \omega) \right|_{\omega=0, \mathbf{k}=0}. \quad (62)$$
where \( \tilde{\Gamma} \) and the Fourier transform of the correlation function is given by
\[
\partial_k \tilde{\Gamma}^\mu = \partial_t \tilde{\Gamma}^0 - \partial_x \tilde{\Gamma}^x - \partial_y \tilde{\Gamma}^y = \frac{\partial \dot{\rho}(r, t)}{\partial t} - \nabla \cdot \tilde{\mathbf{J}}(r, t) = 0. \tag{63}
\]

The current-density response function is defined as
\[
\Pi^\mu_\text{ret}(r - r') = i \theta(t - t') \left\langle \left[ \tilde{\mathbf{J}}^\mu(r), \tilde{\mathbf{J}}^\nu(r') \right] \right\rangle,
\]
and the Fourier transform of the response function is given by
\[
\tilde{\Pi}^\mu_\text{ret}(k) = \int e^{i k \cdot r} \Pi^\mu_\text{ret}(r) d^3r,
\]
with \( k_\mu = (\omega, -k_x, -k_y) \), \( r^\mu = (t, x, y) \) and \( k \cdot r = \omega t - k_x x - k_y y \). By using Eq. \((50)\) and Eq. \((62)\), the Kubo formula for Hall conductance can be generalized to
\[
\sigma_H = \frac{1}{3!} \epsilon_{\mu\nu\rho} \left. \frac{\partial}{\partial k_\rho} \Pi^\mu_\text{ret}(k) \right|_{k=0},
\]
with \( \partial/\partial k_\rho = (\partial/\partial \omega, \partial/\partial k_x, \partial/\partial k_y) \) and \( \epsilon_{\mu\nu\rho} \) the Levi-Civita tensor.

C. Green’s function formula

The Matsubara Green’s function is defined as
\[
\mathcal{G}_{ab}(r - r') = -\left\langle \tilde{T}_\tau \left[ \hat{\mathbf{\Psi}}_a(r) \hat{\mathbf{\Psi}}_b^\dagger(r') \right] \right\rangle,
\]
with \( r = (\tau, x, y) \), \( \tau = i t \), and \( \tilde{T}_\tau \) the time-ordering operator, and the Fourier transform of the Green’s function is written as
\[
\tilde{\mathcal{G}}(k) = \int e^{i k \cdot r} \mathcal{G}(r) d^3r,
\]
with \( k^\mu = (i \omega, k_x, k_y) \). The current correlation function and its Fourier transform are given as
\[
\Pi_\text{ret}^\mu(\tau = t - t') \left\langle \left[ \tilde{\mathbf{J}}^\mu(r), \tilde{\mathbf{J}}^\nu(r') \right] \right\rangle, \quad \tilde{\Pi}^\mu_\text{ret}(k) = \int e^{i k \cdot r} \Pi^\mu_\text{ret}(r) d^3r.
\]

A three-point correlation function is defined by
\[
\Lambda^\mu(r_1, r, r_2) \equiv -\left\langle \tilde{T}_\tau \left[ \hat{\mathbf{\Psi}}_a(r_1) \tilde{\mathbf{J}}^\mu(r) \hat{\mathbf{\Psi}}_b^\dagger(r_2) \right] \right\rangle,
\]
and the Fourier transform of the correlation function is given by
\[
\int e^{i (q \cdot r + p_1 \cdot r_1 + p_2 \cdot r_2)} \Lambda^\mu(r_1, r, r_2) d^3r_1 d^3r_2 d^3r_2 = -i (2\pi)^3 \delta(p_1 - p_2 + q) \tilde{\mathcal{G}}(p_1) \tilde{\Gamma}^\mu(p_1, p_2) \tilde{\mathcal{G}}(p_2),
\]
where \( \tilde{\Gamma}^\mu(p, q) \) is the vertex function. The vertex function can be related to the Green’s function by the Ward-Takahashi identity
\[
\sum_\mu q_\mu \tilde{\Gamma}^\mu(k + q, k) = \tilde{\mathcal{G}}^{-1}(k + q) - \tilde{\mathcal{G}}^{-1}(k),
\]
and an extension of the identity
\[
\tilde{\Gamma}^\mu(k, k) = \frac{\partial \tilde{\mathcal{G}}^{-1}(k)}{\partial k_\mu}.
\]

The current autocorrelation function can be solved as
\[
\tilde{\Pi}^\mu(q) = -e^2 \int \text{Tr} \left[ \tilde{\Gamma}^\mu(p, p + q) \tilde{\mathcal{G}}(p + q) \tilde{\Gamma}^\nu(p + q, p) \tilde{\mathcal{G}}(p) \right] \frac{d^3p}{(2\pi)^3}. \tag{74}
\]
The current-current response function can be derived from the current autocorrelation function by using the rotation \( \Pi_{\nu\mu}^{\nu\nu}(q) = \Pi_{\nu\mu}(q)|_{\omega \rightarrow -\omega + i\nu} \). We can find

\[
\sigma_H = \frac{1}{3} \epsilon_{\mu\nu\rho} \frac{\partial}{\partial k_\rho} \bar{\Pi}^{\mu\nu}(k) \bigg|_{k=0} = \frac{1}{3} \epsilon_{\mu\nu\rho} \frac{\partial}{\partial k_\rho} \left\{ e^2 \int \text{Tr} \left[ \bar{\Gamma}^{\nu}(p,p + k) \bar{G}(p + k) \bar{\Gamma}^{\nu}(p + k,p) \bar{G}(p) \right] \frac{d^3p}{(2\pi)^3} \right\} \bigg|_{k=0}
\]

\[
= \frac{1}{6} \int \text{Tr} \left[ \bar{G} \frac{\partial \bar{G}^{-1}}{\partial k_\mu} \frac{\partial \bar{G}^{-1}}{\partial k_\nu} \bar{G} \frac{\partial \bar{G}^{-1}}{\partial k_\rho} \right] \frac{d^3k}{(2\pi)^3}.
\]

Note that we have used

\[
\bar{G}^{-1}(k) \bar{G}(k) = 1 \Rightarrow \frac{\partial \bar{G}^{-1}(k)}{\partial k_\mu} \bar{G}(k) + \bar{G}^{-1}(k) \frac{\partial \bar{G}(k)}{\partial k_\mu} = 0
\]

\[
\Rightarrow \frac{\partial \bar{G}(k)}{\partial k_\mu} = -\bar{G}(k) \frac{\partial \bar{G}^{-1}(k)}{\partial k_\mu} \bar{G}(k),
\]

and

\[
\frac{\partial}{\partial k_\rho} \bar{\Gamma}^{\nu}(p + k,p) \bigg|_{k=0} = -\frac{\partial}{\partial k_\rho} \bar{\Gamma}^{\nu}(p,p + k) \bigg|_{k=0} = \frac{\partial^2 \bar{G}^{-1}(p)}{\partial p_\rho \partial p_\mu}.
\]

such that

\[
\int \epsilon_{\mu\nu\rho} \text{Tr} \left[ \frac{\partial \bar{\Gamma}^{\nu}(p,p + k)}{\partial k_\rho} \bar{G}(p) \bar{\Gamma}^{\nu}(p + k,p) \bar{G}(p) + \bar{\Gamma}^{\nu}(p,p + k) \bar{G}(p) \frac{\partial \bar{\Gamma}^{\nu}(p + k,p)}{\partial k_\rho} \bar{G}(p) \right] \frac{d^3p}{(2\pi)^3}
\]

\[
= 2 \int \epsilon_{\mu\nu\rho} \text{Tr} \left[ \frac{\partial^2 \bar{G}^{-1}(p)}{\partial p_\rho \partial p_\mu} \bar{G}(p) \right] \frac{d^3p}{(2\pi)^3} = 0.
\]

By replacing \( k_0 = i\omega \) by \( k_0 = \omega \) for the \( k \)-vector \( k = (k_0, k_x, k_y) \) in Eq. (75) and by referring to the definition of the Chern number by \( \sigma_H = \frac{2}{e^2} C \), it is shown that the Chern number can be given by Eq. (43). Since the derivation is quite general, this formula can be used to study any many-particle Hamiltonian as long as the Ward-Takahashi identity is satisfied.

### III. EXCITON CONDENSATION

In this section, the theory of exciton condensation is presented and reviewed based on references [13–21]. In Sec. III A the variational wavefunction and formalism for exciton condensation are introduced. In Sec. III B the variational method to calculate the exciton binding energy is introduced. In Sec. III C the conditions for exciton instability is discussed. In Sec. III D we argue that the topology of the Chern band will not be altered in the presence of the exciton condensate if there is no band inversion in the single-particle band structure.

#### A. Variational wavefunction for the exciton condensate

The interlayer-exciton condensate can be described by the electron-hole-liquid (EHL) Hamiltonian

\[
\hat{H}_{EHL} = \sum_k \varepsilon^e_k \hat{c}^\dagger_k \hat{c}_k + \sum_{\tau,k} \varepsilon^h_{\tau,k} \hat{d}^\dagger_{\tau,k} \hat{d}_{\tau,k} - \sum_{\tau,qkq'k} \frac{W_{eh}}{S} \varepsilon^e_{\tau,k} \varepsilon^h_{k-q} \hat{d}^\dagger_{\tau,k-q} \hat{d}_{\tau,k+q} \hat{d}_{\tau,k+q} \hat{d}_{\tau,k-q} \hat{c}_k,
\]

where \( \hat{c}^\dagger_k / \hat{c}_k \) is the electron creation/annihilation operator on the unfilled valence (hole-occupied) band in the MoTe₂ layer, \( \hat{d}^\dagger_{\tau,k} / \hat{d}_{\tau,k} \) is the hole creation/annihilation operator on the two-component valence band in the WSe₂ layer with \( \tau = \pm \). The variational state for the exciton condensate is assumed to be the following BCS state

\[
|\Phi_{BCS}\rangle = \prod_{\tau,k} \left( u_{\tau,k} + v_{\tau,k} \hat{d}^\dagger_{\tau,k} \hat{c}_k \right) |\Phi_{HF}\rangle,
\]
where \( u_{\tau,k} \) and \( v_{\tau,k} \) are variational coefficients subject to the normalization condition \( u_{\tau,k}^2 + v_{\tau,k}^2 = 1 \). Note that
\[
\frac{\delta u_{\tau,k}}{\delta v_{\tau',k'}} = -\delta_{\tau,\tau'} \frac{v_{\tau,k}}{u_{\tau,k}}.
\]

The expectation of the Hamiltonian is given by
\[
\langle \hat{H}_{\text{EHL}} \rangle = \sum_{\tau,k} \left( \varepsilon_{\tau,k}^e + \varepsilon_{\tau,k}^h \right) u_{\tau,k}^2 - \sum_{\tau,k \neq k'} \frac{W_{\text{ch}}}{S} v_{\tau,k,u_{\tau,k}u_{\tau,k'}}.
\]

The variation of the energy expectation value is given by
\[
\frac{\delta \langle \hat{H}_{\text{EHL}} \rangle}{\delta v_{\tau,k}} = 2 \left( \varepsilon_{\tau,k}^e + \varepsilon_{\tau,k}^h \right) v_{\tau,k} - 2 \sum_{k'} \frac{W_{\text{ch}}}{S} v_{\tau,k,u_{\tau,k'}} \left( u_{\tau,k} - \frac{v_{\tau,k}^2}{u_{\tau,k}} \right).
\]

Assume \( \delta \langle \hat{H}_{\text{EHL}} \rangle/\delta v_{\tau,k} = 0 \), and
\[
\Delta_{\tau,k} = \sum_{k'} \frac{W_{\text{ch}}}{S} v_{\tau,k,u_{\tau,k'}} \quad \Xi_{\tau,k} = \left( \varepsilon_{\tau,k}^e + \varepsilon_{\tau,k}^h \right)/2, \quad n_X = \sum_{\tau,k} \frac{u_{\tau,k}^2}{N},
\]
we get \( (2v_{\tau,k}u_{\tau,k})\Xi_{\tau,k} - \left( u_{\tau,k}^2 - v_{\tau,k}^2 \right) \Delta_{\tau,k} = 0 \). By replacing \( u_{\tau,k} = \cos \theta_{\tau,k} \) and \( v_{\tau,k} = \sin \theta_{\tau,k} \), we find
\[
\sin(2\theta_{\tau,k})\Xi_{\tau,k} = \cos(2\theta_{\tau,k})\Delta_{\tau,k} \quad \text{and} \quad \cos(2\theta_{\tau,k}) = \Xi_{\tau,k}/\varepsilon_{\tau,k}, \quad \text{with}
\]
\[
\varepsilon_{\tau,k} = \sqrt{|\Xi_{\tau,k}|^2 + |\Delta_{\tau,k}|^2}.
\]

Therefore, we get
\[
\frac{u_{\tau,k}^2}{2} = \frac{1}{2} \left( 1 + \frac{\Xi_{\tau,k}}{\varepsilon_{\tau,k}} \right), \quad \frac{v_{\tau,k}^2}{2} = \frac{1}{2} \left( 1 - \frac{\Xi_{\tau,k}}{\varepsilon_{\tau,k}} \right),
\]
and \( 2v_{\tau,k}u_{\tau,k} = \sin(2\theta_{\tau,k}) = \Delta_{\tau,k}/\varepsilon_{\tau,k} \). The gap equation can be found as
\[
\Delta_{\tau,k} = \sum_{k'} \frac{W_{\text{ch}}}{S} \frac{\Delta_{\tau,k'}}{2\varepsilon_{\tau,k'}}.
\]

The variational ground-state energy is given by
\[
\langle \hat{H}_{\text{EHL}} \rangle = \frac{1}{2} \sum_{\tau,k} \left( \varepsilon_{\tau,k}^e + \varepsilon_{\tau,k}^h \right) \left( 1 + \frac{\Xi_{\tau,k}}{\varepsilon_{\tau,k}} \right) - \sum_{\tau,k \neq k'} \frac{W_{\text{ch}}}{4S} \frac{\Delta_{\tau,k}\Delta_{\tau,k'}}{\varepsilon_{\tau,k}\varepsilon_{\tau,k'}}.
\]

### B. Exciton binding energy

The variational method to solve the exciton binding energy is introduced in this section. Two-dimensional Slater-type orbitals (STOs) are used to expanded the variational exciton wavefunction. A more detailed discussion of this method can be found in Ref. [22]. The kinetic energies of electrons and holes are assumed to be
\[
\varepsilon_{\tau,k}^e + \varepsilon_{\tau,k}^h = \tilde{D} + \frac{k^2}{2\mu_X},
\]
where \( \mu_X = m_em_h/(m_e + m_h) \) is the exciton reduced mass. The interlayer exciton wavefunction \( \Psi_I(r) \) can be solved by the Schrödinger equation
\[
\left[ \tilde{D} - \frac{\nabla^2}{2\mu_X} - W(r) \right] \Psi_I(r) = E_I \Psi_I(r).
\]

The Fourier transform of the exciton wavefunction can be found by \( \tilde{\Psi}_I(k) = \int e^{-ik\cdot r} \Psi_I(r) d^2r \). The exciton wavefunction can be expanded as
\[
\tilde{\Psi}_I(k) = \sum_\alpha \mathcal{U}_{\alpha,I} \tilde{\Phi}_\alpha(k),
\]
where $\mathcal{U}_{\alpha,l}$ is the wavefunction coefficient and $\tilde{\Phi}_{\alpha}(k)$ is the basis function. The exciton wavefunction coefficient can be solved by the eigenvalue equation

$$
\sum_{\beta} (T_{\alpha\beta} - W_{\alpha\beta}) \mathcal{U}_{\beta,l} = E_l \sum_{\beta} O_{\alpha\beta} \mathcal{U}_{\beta,l}, \tag{92}
$$

where

$$
T_{\alpha\beta} = -\frac{1}{2\mu_x} \int \Phi_\alpha^*(r) \nabla^2 \Phi_\beta(r) d^2 r, \quad W_{\alpha\beta} = \int \Phi_\alpha^*(r) W(r) \Phi_\beta(r) d^2 r, \quad O_{\alpha\beta} = \int \Phi_\alpha^*(r) \Phi_\beta(r) d^2 r \tag{93}
$$

are the kinetic integral, the potential integral, and the overlap integral. By defining

$$
\mathcal{U}_{\alpha,l} = \sum_{\beta} O_{\alpha\beta}^{1/2} \mathcal{U}_{\beta,l}, \tag{94}
$$

the eigenvalue equation becomes

$$
\sum_{\beta} \Omega_{\alpha\beta} \mathcal{U}_{\beta,l} = E_l \mathcal{U}_{\beta,l}, \tag{95}
$$

where

$$
\Omega_{\alpha\beta} = \sum_{\alpha'\beta'} O_{\alpha\beta'}^{-1/2} (T_{\alpha'\beta'} - W_{\alpha'\beta'}) O_{\alpha'\beta'}^{-1/2}. \tag{96}
$$

To solve the exciton eigenvalue equation in Eq. (92), the basis function can be given by a two-dimensional STO, which is written as

$$
\Phi_{\alpha}(r) = \frac{e^{iL_{\alpha} \varphi}}{\sqrt{2\pi}} r N_{\alpha - 1} e^{-z_{\alpha} r}, \tag{97}
$$

where $N_{\alpha}$, $L_{\alpha}$ are the principal quantum number and angular-momentum quantum number of the orbital $\Phi_{\alpha}$, $z_{\alpha}$ is the shielding constant, and $\varphi$ is the azimuth angle. A number of different values of $z_{\alpha}$ can be used to find the optimum shape of the radial part of the wavefunction. The Fourier transform of the two-dimensional STO can be written as

$$
\tilde{\Phi}_{\alpha}(k) = \int \Phi_{\alpha}(r) e^{-ik \cdot r} d^2 r = \frac{e^{iL_{\alpha} \varphi}}{\sqrt{2\pi}} \tilde{R}_{N_{\alpha},L_{\alpha}}(z_{\alpha}, k), \tag{98}
$$

where the radial function in momentum space can be obtained by the generating formula

$$
\tilde{R}_{N,L}(z, k) = \frac{2\pi (-1)^N}{k^{N+1}} \frac{d^N}{dz^N} \left( z - i \eta \sqrt{1 - z^2} \right)^{|L|} \left| z = i z/k \right., \tag{99}
$$

with $\eta = L/|L|$. The kinetic integral is given by

$$
T_{\alpha\beta} = -\frac{\delta_{L_{\alpha},L_{\beta}}}{2\mu_x} \frac{(N_{\alpha} + N_{\beta} - 1)!}{(z_{\alpha} + z_{\beta})^{N_{\alpha} + N_{\beta}}} \left\{ (1 - \delta_{N_{\beta},1}) \frac{[(N_{\beta} - 1)^2 - L_{\beta}^2] (z_{\alpha} + z_{\beta})^2}{(N_{\alpha} + N_{\beta} - 1)(N_{\alpha} + N_{\beta} - 2)} - \frac{[2N_{\beta} - 1] z_{\beta}}{(N_{\alpha} + N_{\beta} - 1)} + z_{\beta}^2 \right\}. \tag{100}
$$

The overlap integral is given by

$$
O_{\alpha\beta} = \delta_{L_{\alpha},L_{\beta}} \frac{(N_{\alpha} + N_{\beta} - 1)!}{(z_{\alpha} + z_{\beta})^{N_{\alpha} + N_{\beta}}}. \tag{101}
$$

The potential integral is given by

$$
W_{\alpha\beta} = \frac{\delta_{L_{\alpha},L_{\beta}}}{(2\pi)^2} \int_0^\infty \tilde{R}_{N_{\alpha} + N_{\beta} - 1,0}(z_{\alpha} + z_{\beta}, k) \tilde{W}(k) dk. \tag{102}
$$

The Coulomb potential can be given by $\tilde{W}(k) = W_{\text{eh}}^{\text{eh}}$. An exciton $I = (N, L)$ can be indicated by a principal quantum number $N$ and an angular momentum $L$, with $L$ being a constant for every orbital in the exciton wavefunction. In the present study, only $L = 0$ is considered.
C. Excitonic instability

If the number of excitons is restricted to be one, by variation

$$\delta \left[ \langle \Phi | \hat{H}_{EHL} | \Phi \rangle - \lambda (Nn_X - 1) \right] / \delta \nu_{\tau, \mathbf{k}} = 0,$$  

with $\lambda$ the Lagrange multiplier, the variational coefficient can be solved by

$$[k^2/(2\mu_X) + E_X] \nu_{\tau, \mathbf{k}} = \sum_{\mathbf{k}' \mathbf{k}'} W_{\mathbf{k}', \mathbf{k}'}^{\text{eh}} \nu_{\tau, \mathbf{k}'} / S,$$  

where $E_X = \hat{D} - \lambda$ is the exciton binding energy. We define the excitonic instability by the condition

$$\Delta_{\tau, \mathbf{k}} \neq 0$$  

for at least one $(\tau, \mathbf{k})$ state. In this section, we intend to show that the necessary condition for the excitonic instability at zero temperature is $\hat{D} \leq E_X$ and the sufficient condition is $\hat{D} < E_X$, with $\hat{D}$ being the effective band gap.

To prove the necessary condition, we rewritten the gap equation by defining

$$\gamma_{\tau, \mathbf{k}} \equiv \nu_{\tau, \mathbf{k}} v_{\tau, \mathbf{k}} = \frac{\Delta_{\tau, \mathbf{k}}}{2 \varepsilon_{\tau, \mathbf{k}}}.$$  

The gap equation can be written as

$$\gamma_{\tau, \mathbf{k}} = \frac{1}{2 \varepsilon_{\tau, \mathbf{k}}} \sum_{\mathbf{k}'} \frac{W_{\mathbf{k}', \mathbf{k}'}^{\text{eh}}}{S} \gamma_{\tau, \mathbf{k}'} \Rightarrow 2 \varepsilon_{\tau, \mathbf{k}} \gamma_{\tau, \mathbf{k}} - \sum_{\mathbf{k}'} \frac{W_{\mathbf{k}', \mathbf{k}'}^{\text{eh}}}{S} \gamma_{\tau, \mathbf{k}'} = 0.$$  

By using

$$\varepsilon_{\tau, \mathbf{k}} = \sqrt{|| \Xi_{\tau, \mathbf{k}} ||^2 + |\Delta_{\tau, \mathbf{k}}|^2} = || \Xi_{\tau, \mathbf{k}} || \sqrt{1 + |\Delta_{\tau, \mathbf{k}}|^2/|| \Xi_{\tau, \mathbf{k}} ||^2} = || \Xi_{\tau, \mathbf{k}} || + g_{\tau, \mathbf{k}},$$

with $g_{\tau, \mathbf{k}} = || \Xi_{\tau, \mathbf{k}} || \left( \sqrt{1 + |\Delta_{\tau, \mathbf{k}}|^2/|| \Xi_{\tau, \mathbf{k}} ||^2} - 1 \right) \geq 0$, and assuming $\Xi_{\tau, \mathbf{k}} > 0$, the gap equation becomes

$$2(\Xi_{\tau, \mathbf{k}} + g_{\tau, \mathbf{k}}) \gamma_{\tau, \mathbf{k}} - \sum_{\mathbf{k}'} \frac{W_{\mathbf{k}', \mathbf{k}'}^{\text{eh}}}{S} \gamma_{\tau, \mathbf{k}'} = 0.$$  

By using Eq. (89), the gap equation can be written as

$$\sum_{\mathbf{k}'} (A_{\mathbf{k}, \mathbf{k}'} + B_{\mathbf{k}, \mathbf{k}'}) \gamma_{\tau, \mathbf{k}'} = 0,$$  

with

$$A_{\mathbf{k}, \mathbf{k}'} = \delta_{\mathbf{k}, \mathbf{k}'} \left[ \hat{D} + k^2/(2\mu_X) - W_{\mathbf{k}', \mathbf{k}'}^{\text{eh}} / S \right] \quad \text{and} \quad B_{\mathbf{k}, \mathbf{k}'} = \delta_{\mathbf{k}, \mathbf{k}'} 2g_{\tau, \mathbf{k}}.$$  

Note that $g_{\tau, \mathbf{k}}$ and $\gamma_{\tau, \mathbf{k}}$ become independent of $\tau$ because Eq. (89) is used. A trivial solution ($\gamma_{\tau, \mathbf{k}} = 0$) of the equation leads to $\Delta_{\tau, \mathbf{k}} = 0$ for every $(\tau, \mathbf{k})$ state. The equation has nontrivial solutions of $\gamma_{\tau, \mathbf{k}}$ only if $\text{Det}(A_{\mathbf{k}, \mathbf{k}'} + B_{\mathbf{k}, \mathbf{k}'}) = 0$, which implies the existence of at least a zero eigenvalue for matrix $\mathbf{A} + \mathbf{B}$. Since $g_{\tau, \mathbf{k}} \geq 0$ for each $\tau$ and $\mathbf{k}$, matrix $\mathbf{B}$ is positive semi-definite. If matrix $\mathbf{A}$ is positive definite, matrix $\mathbf{A} + \mathbf{B}$ will be positive definite, which contradicts to that matrix $\mathbf{A} + \mathbf{B}$ has at least a zero eigenvalue. Therefore, matrix $\mathbf{A}$ is not positive definite. It indicates the lowest eigenvalue of matrix $\mathbf{A}$ is not a positive number. By using the exciton equation in Eq. (104), the lowest eigenvalue of matrix $\mathbf{A}$ is solved by

$$\sum_{\mathbf{k}'} A_{\mathbf{k}, \mathbf{k}'} \Psi_{I, \mathbf{k}'} = E_I \Psi_{I, \mathbf{k}},$$  

with $\Psi_{X, \mathbf{k}}$ being the eigenfunction corresponding to the lowest eigenvalue. The lowest eigenvalue of the equation is given by $E_{I=0} = \hat{D} - E_X$. Therefore, the condition for matrix $\mathbf{A}$ being not positive is given by

$$E_0 = \hat{D} - E_X \leq 0,$$  

which gives the necessary condition $\hat{D} \leq E_X$ for excitonic instability.
To prove the sufficient condition, we assume that the eigenvalue equation of matrix $\mathcal{A}$ can be solved by

$$\sum_{k'} \mathcal{A}_{k',k} \Psi_{I,k'} = E_I \Psi_{I,k},$$  \hspace{1cm} (114)

with $E_I$ the eigenvalue and $\Psi_{I,k}$ the eigenfunction, and the parameter $\gamma_{r,k}$ can be expanded by

$$\gamma_{r,k} = \sum_I C_I \Psi_{I,k},$$  \hspace{1cm} (115)

with $C_I$ being variational coefficient. We get

$$\Delta_{r,k} = \sum_k W_{k-k'}^2 \gamma_{r,k'}/S = - \sum_k (A_{k,k'} - \delta_{k,k'} 2\Xi_{r,k}) \sum_I C_I \Psi_{I,k'} = \sum_I C_I (2\Xi_{r,k} - E_I) \Psi_{I,k}.$$  \hspace{1cm} (116)

The gap equation becomes

$$\sum_I C_I \Psi_{I,k} = \frac{\sum_I C_I (2\Xi_{r,k} - E_I) \Psi_{I,k}}{2 \sqrt{\Xi_{r,k}^2 + |\sum_I C_I (2\Xi_{r,k} - E_I) \Psi_{I,k}|^2}}.$$  \hspace{1cm} (117)

By assigning $k = 0$, the gap equation becomes

$$\sum_I C_I \Psi_{I,0} = \frac{\sum_I C_I (2\Xi_{r,0} - E_I) \Psi_{I,0}}{2 \sqrt{\Xi_{r,0}^2 + |\sum_I C_I (2\Xi_{r,0} - E_I) \Psi_{I,0}|^2}}.$$  \hspace{1cm} (118)

A good approximation for the exciton wavefunctions $\Psi_{I,k}$ is to use the wavefunctions solved from two-dimensional hydrogen-atom problem. The wavefunctions of two-dimensional hydrogen atoms have the properties $\Psi_{I,k} = 0$ for $I > 0$ and $k = 0$. By assuming $\Psi_{I,0} \simeq 0$ for $I > 0$, the gap equation can be reduced to

$$1 \simeq \frac{2\Xi_{r,0} - E_0}{2 \sqrt{\Xi_{r,0}^2 + |C_0 (2\Xi_{r,0} - E_0) \Psi_{0,0}|^2}} \Rightarrow 4\Xi_{r,0}^2 + (2\Xi_{r,0} - E_0)^2 (2C_0 \Psi_{0,0})^2 \simeq (2\Xi_{r,0} - E_0)^2,$$  \hspace{1cm} (119)

such that

$$(2C_0 \Psi_{0,0})^2 \simeq 1 - \frac{4\Xi_{r,0}^2}{(2\Xi_{r,0} - E_0)^2}.$$  \hspace{1cm} (120)

Therefore, if $E_0 < 0$, there is a nontrivial solution for $|C_0|$, which is given by

$$|C_0| \simeq \frac{1}{2\Psi_{0,0}} \sqrt{1 - \left(\frac{2\Xi_{r,0}}{2\Xi_{r,0} - E_0}\right)^2}.$$  \hspace{1cm} (121)

The gap order parameter can be given approximately by

$$\Delta_{r,k} \simeq C_0 (2\Xi_{r,k} - E_0) \Psi_{0,k} = \pm \frac{2\Xi_{r,k} - E_0}{2} \sqrt{1 - \frac{(2\Xi_{r,0})^2}{(2\Xi_{r,0} - E_0)^2} \Psi_{0,k}}.$$  \hspace{1cm} (122)

By using $2\Xi_{r,k} = \tilde{D} + k^2/(2\mu_X)$, $E_0 = \tilde{D} - E_X$, and by assuming the ground-state exciton wavefunction being given by the ground-state wavefunction of two-dimensional hydrogen atoms,

$$\Psi_{0,k} \simeq \frac{\sqrt{2\pi} 2^{2}}{(k^2 + 2\Xi_{r,0})^{3/2}},$$  \hspace{1cm} (123)

the gap order parameter can be given approximately by

$$\Delta_{r,k} \simeq \pm \theta(E_X - \tilde{D}) \frac{2^3 [E_X + k^2/(2\mu_X)]}{2 (k^2 + 2\Xi_{r,0})^{3/2}} \sqrt{1 - \frac{D^2}{E_X^2}},$$  \hspace{1cm} (124)

with $\theta(x)$ being a step function. The variational coefficient $C_I$ for $I > 0$ and the higher-order corrections of the gap order parameter can be calculated by using the Newton iterative method, and it can be shown that the iteration is converged. Since a nontrivial solution of the gap equation exists, the sufficient condition of exciton instability $\tilde{D} < E_X$ is shown.
The quasiparticle Green’s function is given by

\[ G_{\tau,k}(\tilde{t}) \equiv -\left( \frac{\langle \hat{T} \hat{c}_{-k}(0) \hat{c}_{-k}^\dagger(\tilde{t}) \rangle}{\langle \hat{T} \hat{d}_{\tau,k}(0) \hat{c}_{-k}(0) \rangle} \right), \]  

where \( \hat{T} \) is time-ordering operator and \( \tilde{t} = it \) is the imaginary time variable. By a Fourier transformation \( G_{\tau,k}(i\omega) = \frac{1}{\beta} \int_0^\beta e^{i\omega\tilde{t}} G_{\tau,k}(\tilde{t}) d\tilde{t} \), with \( \beta \) the inverse temperature and \( \omega = (2\nu + 1)\pi/\beta \), the quasiparticle Green’s function can be solved as

\[ \tilde{G}_{\tau,k}^{-1}(i\omega) = \left( \begin{array}{cc} i\omega + \varepsilon_{-k} & -\Delta_{\tau,k} \\ -\Delta_{\tau,k} & i\omega - \varepsilon_{\tau,k}^h \end{array} \right). \]  

The electron creation and annihilation operators can be replaced by the hole creation and annihilation operators by \( \hat{c}_{-k}^\dagger = \hat{d}_k^\dagger, \hat{c}_{-k} = \hat{d}_k \). With including the hole bands in the MoTe$_2$ layer discussed above, the quasiparticle Green’s function can be generalized by the formulation \( G_{nm,k}(\tilde{t}) \equiv -\langle \hat{T} \hat{d}_{nk}(\tilde{t}) \hat{d}_{mk}(0) \rangle \), with \( n, m \) indexing different bands. This hole Green’s function satisfies a Ward-Takahashi identity and thus the Chern number of the hole bands can also be calculated by Eq. (13). Therefore, based on the Green’s function given in Eq. (126), the effect of exciton condensation on the band structure can be realized as the hybridization between the unfilled valence band (hole-occupied band) and the filled conduction band. The topological of Chern band will be preserved with the exciton condensate. Since \( 2\Xi_{\tau,k} > 0 \) is ensured by \( \tilde{D} > 0 \), the topology of Chern band is preserved with the exciton condensate.

In the following context, we illustrate the equivalence between the variational method and the Green’s function formalism. The quasiparticle Green’s function for the exciton condensate is defined as

\[ G_{\tau,k}(i\omega) \equiv -\left( \frac{\langle \hat{T} \hat{c}_{-k}(0) \hat{c}_{-k}^\dagger(i\omega) \rangle}{\langle \hat{T} \hat{d}_{\tau,k}(i\omega) \hat{c}_{-k}(0) \rangle} \right). \]  

where \( \hat{T} \) is time-ordering operator. By a Fourier transformation \( G_{\tau,k}(i\omega) = \frac{1}{\beta} \int_0^\beta e^{i\omega\tilde{t}} G_{\tau,k}(i\omega) d\tilde{t} \), with \( \beta \) the inverse temperature and \( \omega = (2\nu + 1)\pi/\beta \), the quasiparticle Green’s function can be solved as

\[ \tilde{G}_{\tau,k}^{-1}(i\omega) = \left( \begin{array}{cc} i\omega + \varepsilon_{-k} & \Delta_{\tau,k} \\ -\Delta_{\tau,k} & i\omega - \varepsilon_{\tau,k}^h \end{array} \right) = \tilde{G}(i\omega_{\nu}) - \delta\varepsilon_{\tau,k} - \sigma_{\tau}\Xi_{\tau,k} + \sigma_{\tau}\Delta_{\tau,k}, \]  

where

\[ \delta\varepsilon_{\tau,k} = (-\varepsilon_{-k}^h + \varepsilon_{\tau,k}^h)/2. \]

The quasiparticle Green’s function is given by

\[ \tilde{G}_{\tau,k}(i\omega) = \left( \begin{array}{cc} i\omega_{\nu} - \delta\varepsilon_{\tau,k} + \sigma_{\tau}\Xi_{\tau,k} - \sigma_{\tau}\Delta_{\tau,k} & \sigma_{\tau}\Xi_{\tau,k} - \sigma_{\tau}\Delta_{\tau,k} \\ \sigma_{\tau}\Delta_{\tau,k} & (i\omega_{\nu} - \delta\varepsilon_{\tau,k})^2 - \varepsilon_{\tau,k}^h \end{array} \right). \]  

The self-energy is defined as

\[ \tilde{\Sigma}_{\tau,k}(i\omega_{\nu}) = \left( \begin{array}{cc} i\omega_{\nu} + \varepsilon_{-k} & 0 \\ 0 & i\omega_{\nu} - \varepsilon_{\tau,k}^h \end{array} \right) - \tilde{G}_{\tau,k}(i\omega_{\nu}). \]  

By using mean-field approximation, the self-energy can be solved by

\[ \tilde{\Sigma}_{\tau,k}(i\omega_{\nu}) = -\sum_{k'} \frac{W_{k'k}}{S} \int G_{\tau,k'}(i\omega') d\omega'/2\pi, \]  

By comparing the self-energy and the Green’s function, the gap equation at zero-temperature limit can be derived

\[ \Delta_{\tau,k} = \sum_{k'} \frac{W_{k'k}}{S} \frac{\Delta_{\tau,k'}}{2\varepsilon_{\tau,k'}}, \]
and the exciton density is given by

\[ n_X = \sum_{\tau,k} \frac{1}{2N} \left( 1 - \frac{\tilde{\varepsilon}_{\tau,k}}{\varepsilon_{\tau,k}} \right). \quad (134) \]

It is shown that the variational method and the Green’s function method are equivalent at the zero-temperature limit. On the other hand, by replacing the electron creation/annihilation operator by the hole creation/annihilation operator

\[ \hat{c}_{-k}^\dagger = \hat{d}_k, \quad \hat{c}_{-k} = \hat{d}_k^\dagger, \quad (135) \]

the EHL Hamiltonian can be rewritten by the hole representation as

\[ \hat{H}_{EHL} = - \sum_k \varepsilon_{e,k} \hat{d}_{0,k}^\dagger \hat{d}_{0,k} + \sum_{\tau,k} \varepsilon_{h,k} \hat{d}_{\tau,k}^\dagger \hat{d}_{\tau,k} + \sum_{\tau,q,k,k'} \frac{W_{eh}}{S} \hat{d}_{0,k+q}^\dagger \hat{d}_{\tau,k}^\dagger \hat{d}_{\tau,k'} \hat{d}_{0,k}, \quad (136) \]

where \( \hat{d}_{0,k}^\dagger = \hat{c}_{-k} \) and \( \hat{d}_{0,k} = \hat{c}_{-k}^\dagger \) are the hole creation and annihilation operators on the unfilled valence (hole-occupied) band in the MoTe2 layer. \( \hat{\rho}_{\tau,q} = \sum_k \hat{d}_{\tau,k+q}^\dagger \hat{d}_{\tau,k} \) is the hole density operator with \( \tau = \{0, +, -\} \). The hole Green’s function for the many-hole Hamiltonian is defined by

\[ \hat{G}_{\tau,k}(it) = -\frac{\langle \hat{\tau} \hat{d}_{\tau,k}(it) \hat{d}_{\tau,k}^\dagger(0) \rangle}{\langle \hat{\tau} \hat{d}_{\tau,k}(it) \hat{d}_{\tau,k}^\dagger(0) \rangle}, \quad (137) \]

and it is solved by

\[ \tilde{\hat{G}}_{\tau,k}(i\omega) = \begin{pmatrix} i\omega - \varepsilon_{e,k} & 0 \\ 0 & i\omega - \varepsilon_{h,k} \end{pmatrix} - \tilde{\Sigma}_{\tau,k}(i\omega), \quad (138) \]

with the Hartree-Fock self-energy

\[ \tilde{\Sigma}_{\tau,k}(i\omega) = -\sum_{k'} \frac{W_{e-h}}{S} \int \tilde{\hat{G}}_{\tau,k'}(i\omega') \frac{d\omega'}{2\pi}. \quad (139) \]

It is found that the hole Green’s function is the same with the quasiparticle Green’s function. The hole Green’s function can be generalized to the definition \( g_{nm,k}(i\ell) \equiv -\langle \hat{T} \hat{d}_{n,k}(i\ell) \hat{d}_{m,k}^\dagger(0) \rangle \), with \( n, m = \{0, +, -\} \).

[1] L. L. Foldy and S. A. Wouthuysen, On the Dirac theory of spin 1/2 particles and its non-relativistic limit, Phy. Rev., 78, 29 (1950).
[2] E. Eriksen, Foldy-Wouthuysen transformation. Exact solution with generalization to the two-particle problem, Phys. Rev., 111, 1011 (1958).
[3] A. J. Silenko, Foldy-Wouthuysen transformation and semiclassical limit for relativistic particles in strong external fields, Phys. Rev. A, 77, 012116 (2008).
[4] Y.-W. Chang and Y.-C. Chang, Foldy-Wouthuysen transformation for gapped Dirac fermions in two-dimensional semiconducting materials and valley excitons under external fields, arXiv:2107.14474 (2021).
[5] D. Xiao, J. Shi, and Q. Niu, Berry Phase Correction to Electron Density of States in Solids, Phys. Rev. Lett., 95, 137204 (2005).
[6] W. Yao and Q. Niu, Berry Phase Effect on the Exciton Transport and on the Exciton Bose-Einstein Condensate, Phys. Rev. Lett., 101, 106401 (2008).
[7] M.-C. Chang and Q. Niu, Berry curvature, orbital moment, and effective quantum theory of electrons in electromagnetic fields, J. Phys.: Condens. Matter, 20, 193202 (2008).
[8] D. Xiao, and M.-C. Chang, and Q. Niu, Berry phase effects on electronic properties, Rev. Mod. Phys., 82, 1959 (2010).
[9] F. Wu, T. Lovorn, E. Tutuc, I. Martin, and A. H. MacDonald, Topological Insulators in Twisted Transition Metal Dichalcogenide Homobilayers, Phys. Rev. Lett., 122, 086402 (2019).
[10] H. So, Induced Chern-Simons class with lattice fermions, Prog. Theor. Phys., 73, 528 (1985).
[11] K. Ishikawa and T. Matsuyama, A microscopic theory of the quantum Hall effect, Nuclear Physics B, 280, 523 (1987).
[12] T. Matsuyama, Quantization of conductivity induced by topological structure of energy-momentum space in generalized QED3, Prog. Theor. Phys., 77, 711 (1987).
[13] D. Jérôme, T. M. Rice, and W. Kohn, Excitonic Insulator, Phys. Rev., 158, 462 (1967).
[14] J. Zittartz, Theory of the excitonic insulator in the presence of normal impurities, Phys. Rev., 164, 575 (1967).
[15] B. I. Halperin and T. M. Rice, The excitonic state at the semiconductor-semimetal transition, Solid State Physics, 21, 115 (1968).
[16] L. V. Keldysh and A. N. Kozlov, Collective properties of excitons in semiconductors, Sov. Phys. JETP, 27, 521 (1968).
[17] C. Comte and P. Nozières, Exciton Bose condensation: the ground state of an electron-hole gas-I. Mean field description of a simplified model, J. Physique, 43, 1069 (1982).
[18] P. Nozières and C. Comte, Exciton Bose condensation: the ground state of an electron-hole gas-II. Spin states, screening and band structure effects, J. Physique, 43, 1083 (1982).
[19] J. Fernández-Rossier and C. Tejedor, Spin degree of freedom in two dimensional exciton condensates, Phys. Rev. Lett., 78, 4809 (1997).
[20] H. Chu and Y. C. Chang, Theory of optical spectra of exciton condensates, Phys. Rev. B, 54, 5020 (1996).
[21] F.-C. Wu, F. Xue, and A. H. MacDonald, Theory of two-dimensional spatially indirect equilibrium exciton condensates, Phys. Rev. B, 92, 165121 (2015).
[22] Y.-W. Chang and Y.-C. Chang, Variationally optimized orbital approach to trions in two-dimensional materials, 155, 024110 (2021).