Nonequilibrium superfield and lattice Weyl transform transport approach to quantum Hall effect

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February 18, 2020

Abstract

Using Buot’s superfield and lattice Weyl transform nonequilibrium quantum transport formalism, we derive the topological Chern number of the integer quantum Hall effect in electrical conductivity. The method is naturally simple and direct, and employs neither the conventional use of Kubo formula nor the retarded Green’s function in linear response theory. We have identified the topological invariant in \((\vec{p}, \vec{q}, E, t)\)-phase space nonequilibrium quantum transport equation, generally not to first-order in electric field but to first-order in the gradient expansion. We have also derive the Kubo current-current correlation for the Hall current as a by-product of our new approach. The Berry curvature related to orbital magnetic moment is also calculated.
1 Introduction

The quantization of Hall conductance in a two-dimensional periodic potential was first explained by Thouless, Kohmoto, Nightingale, and den Nijs (TKNN) [1] using the Kubo current-current correlation. Similar approach were employed by Streda [2]. Earlier, Laughlin [3], and later Halperin [4], study the effects produced by changes in the vector potential on the states at the edges of a finite system, where quantization of the conductance is made explicit, but it was not obvious that the result is insensitive to boundary conditions. In contrast, the use of Kubo formula by TKNN is for bulk two-dimensional conductors.

These theoretical studies were motivated by the Nobel Prize winning experimental discovery of von Klitzing, Dorda, and Pepper [5] on the quantization of the Hall conductance of a two-dimensional electron gas in a strong magnetic field. The strong magnetic field basically provides the gapped energy structure for the experiments. In the TKNN approach, periodic potential in crystalline solid is being treated. A strong magnetic field is not needed to provide the gapped energy structure in their theory, only peculiar gapped energy-band structures. In principle, in the presence of electric field the discrete Landau levels is replaced by the unstable discrete Stark ladder-energy levels [6, 7].

In this paper, we simply make use of the gapped energy band structure of solids under external electric field. We employ the lattice Weyl transformation technique to go from the bare Hamiltonian to effective or renormalized crystal Hamiltonian, which also provides a rigorous justification of the usual
*ansatz* of substituting the coordinate operator \( \hat{r} \) by \( i \frac{\partial}{\partial p} \) in \( p \)-space (crystal momentum), as well as the crystal group velocity \( v_g = \frac{\partial H}{\partial p} \). We then employ the real-time superfield and lattice Weyl transform nonequilibrium Green’s function (SFLWT-NEGF) \(^8\) quantum transport formalism of Buot \(^9\) \(^10\) in the first-order gradient expansion to derive the topological Chern number of the integer quantum Hall effect (IQHE) for two-dimensional systems.

We find that the quantization of Hall effect occurs strictly not to first-order in the electric field but rather to first-order gradient expansion in the quantum transport equation. The Berry connection and Berry curvature are used to demonstrate the exact quantization of Hall conductance in units of \( e^2/h \), which also happens to coincide with the source and drain contact conductance per spin in mesoscopic quantum transport\(^8\).

The new method employed in this paper employs neither the conventional use of Kubo formula since originally employed by TKNN \(^1\) nor the use of retarded Green’s function in linear response theory. We have identified the topological invariant in \((p,q;E,t)\)-space quantum transport to be given by

\[
\frac{1}{(2\pi\hbar)} \int \int \int d\vec{K}_x d\vec{K}_y dt \left[ \frac{\partial^{(a)} \partial^{(b)}}{\partial K_x \partial K_y} - \frac{\partial^{(a)} \partial^{(b)}}{\partial K_y \partial K_x} \right] H^{(a)}(\vec{K},\mathcal{E}) \left( -iG^<(b) \left( \vec{K},\mathcal{E} \right) \right).
\]

To the author’s knowledge, this is the first time the real-time-dependent quantum superfield nonequilibrium transport in phase space is employed to derive topological invariant in Chern condensed matter system. In the process, we have also derived the Kubo current-current formula strictly from real-time nonequilibrium quantum superfield theory of transport physics adapted to time-dependent electric fields. The orbital magnetic moment and its related Berry curvature is also calculated.

## 2 The Wigner distribution function and density matrix

In the nonequilibrium many-body Green’s function technique, the principal quantities of interest are the “reduced” or single-particle correlation functions defined as

\[
-iG^{<} (1, 2) = Tr \left[ \rho_H \left( \psi_H^\dagger (2) \right) \psi_H (1) \right] = \left\langle \left( \psi_H^\dagger (2) \right) \psi_H (1) \right\rangle,
\]

\[
iG^{>} (1, 2) = Tr \left[ \rho_H \left( \psi_H (1) \psi_H^\dagger (2) \right) \right] = \left\langle \left( \psi_H (1) \psi_H^\dagger (2) \right) \right\rangle,
\]

where \( \psi_H (1) \) and \( \psi_H^\dagger (2) \) are the particle annihilation and creation operators in the Heisenberg representation, respectively. The indices 1 and 2 subsume all space-time indices and other quantum-label indices.
If we write the second quantization operator for the one-particle \((\vec{p}, \vec{q}; E, t)\)-phase space distribution function as

\[
\hat{f}_{\lambda\lambda'}(\vec{p}, \vec{q}; E, t) = \sum_v e^{2i\vec{p} \cdot \vec{v}} \psi^\dagger_{\lambda\sigma} (q + v, t + \frac{T}{2}) \psi_{\lambda'\sigma'} (q - v, t - \frac{T}{2}),
\]  
(2)

where \(\lambda\) label the band index and \(\sigma\) the spin index [here we drop the Heisenberg representation subscripts \(H\) for economy of indices], then upon taking the average

\[
\langle \hat{f}_{\lambda\lambda'}(\vec{p}, \vec{q}; E, t) \rangle = \sum_v e^{2i\vec{p} \cdot \vec{v}} \langle \psi^\dagger_{\lambda\sigma} (\vec{q} + \vec{v}, t + \frac{T}{2}) \psi_{\lambda'\sigma'} (\vec{q} - \vec{v}, t - \frac{T}{2}) \rangle,
\]  
(3)

we obtain particle distribution function \(\rho_{\lambda\lambda'}(p, q)\),

\[
\rho_{\lambda\lambda'}(p, q) = \langle \hat{f}_{\lambda\lambda'}(p, q) \rangle,
\]

where we employ the four-dimensional notation: \(p = (\vec{p}, E)\) and \(q = (\vec{q}, t)\).

Equation (3) is indeed the lattice Weyl transform of the density matrix operator \(\hat{\rho}\) as

\[
\rho_{\lambda\lambda'}(p, q) = \langle \hat{\rho} \hat{f}_{\lambda\lambda'}(p, q) \rangle
\]

where the RHS is the lattice Weyl transform (LWT) of the density matrix operator, which is identical to the LWT of \(-iG^< (1, 2)\).

Thus expectation value of one-particle operator \(\hat{A}\) can be calculated in phase-space similar to the classical averages using a distribution function,

\[
Tr \left( \hat{\rho} \hat{A} \right) := \langle \hat{A} \rangle = \sum_{p, q; \lambda\lambda'} A_{\lambda\lambda'}(p, q) \rho_{\lambda\lambda'}(p, q)
\]

clearly exhibiting the trace of binary operator product as a trace of the product of their respective LWT’s. This general observation is crucial in most of the calculations that follows.

The Wigner distribution function \(f_W(\vec{p}, \vec{q}; t)\) maybe given by

\[
f_W(\vec{p}, \vec{q}; t) = \frac{1}{2\pi} \int dE \left( -iG^< (\vec{p}, \vec{q}; E, t) \right)
\]

\[
= \frac{1}{2\pi} \int dE \left( -iG^< (\vec{p}, \vec{q}; E, t) \right).
\]

We further note that

\[
\rho(t) = e^{-\hat{H}_t} \rho(0) e^{\hat{H}_t}
\]

\[
= U(t) \rho(0) U^\dagger(t),
\]

provides the major time dependence in the transport equation that follows.
3 Renormalized Bloch-electron Hamiltonian

In the following, let us consider the crystal-lattice effective Hamiltonian for energy band \( n \) in the presence of uniform electric field obtained through the use of LWT given by [8, 9]

\[
H_{\text{effective}} = E_{\alpha,n}(\hat{\mathbf{K}}) - e\mathbf{F} \cdot \hat{\mathbf{Q}} = \text{LWT (bare Hamiltonian)},
\]

where

\[
\hat{\mathbf{K}} = \hat{\mathbf{P}} - \frac{e}{c} \hat{\mathbf{A}}(t) = \hat{\mathbf{P}} - \frac{e}{c} \mathbf{F} \cdot \hat{\mathbf{q}},
\]

and \( E_{\alpha,n}(\hat{\mathbf{K}}) \) is the energy band function for the band index \( n \). We denote the Bloch state vector which is an eigenvector of the crystal momentum operator \( \hat{\mathbf{P}} \) by \( |\hat{\mathbf{p}}\rangle \) and the Wannier state vector which is an eigenfunction of the lattice position operator \( \hat{\mathbf{Q}} \) by \( |\hat{\mathbf{q}}\rangle \). Of course the Bloch function is given by \( \langle \hat{\mathbf{x}} | \hat{\mathbf{p}} \rangle \) and the Wannier function is given by \( \langle \hat{\mathbf{x}} | \hat{\mathbf{q}} \rangle \).

We have, by suppressing the band indices,

\[
\hat{\mathbf{Q}} |\hat{\mathbf{q}}\rangle = \hat{\mathbf{q}} |\hat{\mathbf{q}}\rangle,
\]

\[
\hat{\mathbf{P}} |\hat{\mathbf{q}}\rangle = i\hbar \nabla_\mathbf{q} |\hat{\mathbf{q}}\rangle,
\]

\[
\hat{\mathbf{P}} |\hat{\mathbf{p}}\rangle = \hat{\mathbf{p}} |\hat{\mathbf{p}}\rangle,
\]

\[
\hat{\mathbf{Q}} |\hat{\mathbf{p}}\rangle = -i\hbar \nabla_\mathbf{p} |\hat{\mathbf{p}}\rangle.
\]

Observe that in the presence of electric field, the effective Hamiltonian depends on both lattice position operator \( \hat{\mathbf{Q}} \) and time \( t \) through the vector potential \( \hat{\mathbf{A}}(t) = \mathbf{F} \cdot \hat{\mathbf{q}} \) and the scalar potential \( V = -e \mathbf{F} \cdot \hat{\mathbf{q}} \). Therefore in general, the LWT is expected to depend on the variables \((\hat{\mathbf{p}}, \hat{\mathbf{q}}, E, t)\).

3.1 Space and time translation operators

Commutation properties of the time and space translation operators, \( \hat{T}(t) \) and \( \hat{T}(\hat{\mathbf{q}}) \), respectively,

\[
\frac{\partial \hat{T}(\hat{\mathbf{q}})}{\partial t} = \frac{i}{\hbar} [\hat{\mathcal{H}}, \hat{T}(\hat{\mathbf{q}})] = \left( \frac{i}{\hbar} e \mathbf{F} \cdot \hat{\mathbf{q}} \right) \hat{T}(\hat{\mathbf{q}}),
\]

\[
\frac{\partial \hat{T}(t)}{\partial \hat{\mathbf{q}}} = \frac{i}{\hbar} [\hat{\mathbf{K}}, \hat{T}(t)] = \left( \frac{i}{\hbar} e \mathbf{F} t \right) \hat{T}(t),
\]

suggest that in the presence of electric field, gauge invariant quantities that are displaced in space and time acquires Peierls phase factors [10]. For example,

\[
\langle \hat{\mathbf{q}}_1, t_1 | \hat{H}^{(1)} | \hat{\mathbf{q}}_2, t_2 \rangle \Rightarrow e^{-i \mathbf{F} \cdot (\hat{\mathbf{q}}_2 - \hat{\mathbf{q}}_1)} e^{-i \mathbf{F} \cdot \hat{\mathbf{q}} (t_1 - t_2)} H^{(1)} (\hat{\mathbf{q}}_1 - \hat{\mathbf{q}}_2, t_1 - t_2),
\]
where
\[
\vec{q} = \frac{1}{2} (\vec{q}_1 + \vec{q}_2), \\
t = \frac{1}{2} (t_1 + t_2).
\]

Using the four dimensional notation: \( p = (\vec{p}, E) \) and \( q = (\vec{q}, t) \), the Weyl transform \( A(p, q) \) of any operator \( \hat{A} \) is defined by

\[
A_{\lambda\lambda'} (p, q) = \sum_{v} e^{i(\vec{p}) \cdot \vec{v}} \langle q - \vec{v}, \lambda | \hat{A} | q + \vec{v}, \lambda' \rangle 
\]

\[
= \sum_{u} e^{i(\vec{q}) \cdot \vec{u}} \langle p + \vec{u}, \lambda | \hat{A} | p - \vec{u}, \lambda' \rangle ,
\]

where \( \lambda \) and \( \lambda' \) stands for other discrete quantum numbers. Viewed as a transformation of a matrix, we see that the Weyl transform of the matrix \( \langle q', \lambda' | \hat{A} | q'', \lambda'' \rangle \) is given by Eq. (11) and the lattice Weyl transform of \( \langle p', \lambda' | \hat{A} | p'', \lambda'' \rangle \) is given by Eq. (12). Denoting the operation of taking the lattice Weyl transform by the symbol \( \mathcal{W} \) then it is easy to see that the lattice Weyl transform of

\[
\mathcal{W} \left( \frac{\partial}{\partial \vec{q}} + \frac{\partial}{\partial \vec{p}} \right) \langle q', \lambda' | \hat{A} | q'', \lambda'' \rangle = \frac{\partial}{\partial \vec{q}} A_{\lambda\lambda'} (p, q).
\]

Similarly

\[
\mathcal{W} \left( \frac{\partial}{\partial \vec{p}} + \frac{\partial}{\partial \vec{q}} \right) \langle p', \lambda' | \hat{A} | p'', \lambda'' \rangle = \frac{\partial}{\partial \vec{p}} A_{\lambda\lambda'} (p, q).
\]

Note that the derivatives on the LHS of Eqs. (13) and (14) operates only on the wavefunction or state vectors.

Writing Eq. (11) explicitly, we have

\[
A_{\lambda\lambda'} (\vec{p}, \vec{q}; E, t) = \sum_{\vec{v}, \tau} e^{(\vec{p}) \cdot \vec{v}} e^{i\vec{E} \cdot \vec{r}} E^\tau \langle \vec{q} - \vec{v}, t - \frac{\tau}{2}, \lambda | q + \vec{v}, t + \frac{\tau}{2}, \lambda' \rangle .
\]

Using the form of matrix elements in Eq. (11), we have

\[
\langle \vec{q} - \vec{v}, t - \frac{\tau}{2}, \lambda | \hat{A} | \vec{q} + \vec{v}, t + \frac{\tau}{2}, \lambda' \rangle = e^{-i\vec{E} \cdot (\vec{q}_1 - \vec{q}_2)} e^{-i\vec{E} \cdot \vec{q} (t_1 - t_2)} A (\vec{q}_1 - \vec{q}_2, t_1 - t_2) = e^{i\vec{E} \cdot (2\vec{r})} e^{i\vec{E} \cdot \vec{q} \tau} A_{\lambda\lambda'} (\vec{q}_1 - \vec{q}_2, t_1 - t_2) .
\]
Thus
\[
A_{\lambda\lambda'}(\vec{p},\vec{q}; E, t) = \sum_{\vec{v}, \tau} e^{i(\vec{r} \cdot \vec{v} + \vec{F} \cdot \vec{q})} e^{i\vec{F} \cdot \vec{q}} A_{\lambda\lambda'}(\vec{q}_1 - \vec{q}_2, t_1 - t_2)
\]
\[
= \sum_{\vec{v}, \tau} e^{i(\vec{r} \cdot \vec{v} + \vec{F} \cdot \vec{q})} e^{i\vec{F} \cdot \vec{q}} A_{\lambda\lambda'}(\vec{q}_1 - \vec{q}_2, t_1 - t_2)
\]
\[
= A_{\lambda\lambda'}(\vec{p} + e\vec{F}t) \cdot (E + e\vec{F} \cdot \vec{q})
\]
\[
= A_{\lambda\lambda'}(\vec{K}; E).
\]
Hence the expected dynamical variables in the phase space including the time variable occurs in particular combinations of \(\vec{K}\) and \(E\). Therefore, besides the crystal momentum varying in time as
\[
\vec{K} = \vec{p} + e\vec{F}t,
\]
the energy variable vary with \(\vec{q}\) as
\[
E = E + e\vec{F} \cdot \vec{q}
\]
\[
= H(\vec{K}) + e\vec{F} \cdot \vec{q}.
\]
(16)
In effect we have unified the use of scalar potential and vector potential for a system under uniform electric fields. Thus,
\[
\frac{\partial \vec{K}}{\partial t} = e\vec{F} \implies \frac{\partial \vec{K}}{\partial t} = \frac{\partial \vec{K}}{\partial \vec{K}} \frac{\partial \vec{K}}{\partial E} = e\vec{F} \frac{\partial E}{\partial \vec{K}},
\]
(17)
\[
\frac{\partial E}{\partial \vec{q}} = e\vec{F} \implies \frac{\partial E}{\partial \vec{q}} = \frac{\partial E}{\partial \vec{K}} \frac{\partial \vec{K}}{\partial E} = e\vec{F} \frac{\partial \vec{K}}{\partial E},
\]
(18)
\[
\frac{\partial}{\partial \vec{K}} = \frac{\partial E}{\partial \vec{K}} \frac{\partial \vec{K}}{\partial \vec{E}} = v_g \frac{\partial}{\partial \vec{E}},
\]
(19)
where \(v_g\) is the group velocity. The LWT of the effective or renormalized lattice Hamiltonian \(\mathcal{H}_{eff} \equiv H(\vec{p}, \vec{q}; E, t)\) can therefore be analyzed on \((\vec{K}, E)\)-space as
\[
H(\vec{p}, \vec{q}; E, t) = H(\vec{K}, E)
\]
\[
= H(\vec{K}) + e\vec{F} \cdot \vec{q}.
\]
The last line is by virtue of Eq. (16). And all gauge invariant quantities are functions of \((\vec{K}, E)\) such as the electric Bloch function[12] or Houston wave-function[13] and electric Wannier function, i.e., the electric-field dependent generalization of Wannier function. In particular, the Weyl transform of a commutator,
\[
\mathcal{W}[H, G^c] = \sin \Lambda,
\]
where \( \Lambda \) is the Poisson bracket operator. We can therefore write the Poisson bracket operator \( \Lambda \), as

\[
\Lambda = \hbar \frac{1}{2} \left[ \frac{\partial (a)}{\partial t} \frac{\partial (b)}{\partial \mathbf{E}} - \frac{\partial (a)}{\partial \mathbf{E}} \frac{\partial (b)}{\partial t} \right]
\]

\[
\Rightarrow \frac{\hbar}{2} \frac{\partial \mathbf{K}}{\partial t} \cdot \left[ \frac{\partial (a)}{\partial \mathbf{K}} \frac{\partial (b)}{\partial \mathbf{E}} - \frac{\partial (a)}{\partial \mathbf{E}} \frac{\partial (b)}{\partial \mathbf{K}} \right]
\]

\[
= \frac{\hbar}{2} e \mathbf{F} \cdot \left[ \frac{\partial (a)}{\partial \mathbf{K}} \frac{\partial (b)}{\partial \mathbf{E}} - \frac{\partial (a)}{\partial \mathbf{E}} \frac{\partial (b)}{\partial \mathbf{K}} \right],
\]

(20)
on \((\mathbf{K}, \mathbf{E})\)-phase space.

4 SFLWT-NEGF transport equation

The nonequilibrium quantum superfield transport equation for interacting Bloch electrons under a uniform electric field has been derived by Buot and Jensen[10]. In the absence of superconducting behavior, the phase-space transport equation reads

\[
\frac{\partial}{\partial t} G^< (\mathbf{p}, \mathbf{q}; \mathbf{E}, t) = 2 \hbar \sin \Lambda \{ H (p, q) G^< (p, q) + \Sigma^< (p, q) \text{Re} G^> (p, q) \}
\]

\[
+ \frac{1}{\hbar} \cos \Lambda \{ \Sigma^< (p, q) A (p, q) - \Gamma (p, q) G^< (p, q) \}.
\]

(21)

If we expand Eq. (21) to first order in the gradient, i.e., \( \sin \Lambda \simeq \Lambda \), we obtain

\[
\frac{\partial}{\partial t} G^< (p, q) = -e \mathbf{F} \cdot \left\{ \frac{\partial}{\partial \mathbf{E}} E_\alpha \left( \mathbf{K} \right) + \frac{\partial \text{Re} \Sigma^> (p, q)}{\partial \mathbf{E}} \right\} \frac{\partial}{\partial \mathbf{K}} G^< (p, q)
\]

\[
+ e \mathbf{F} \cdot \left\{ \frac{\partial}{\partial \mathbf{K}} E_\alpha \left( \mathbf{K} \right) + \frac{\partial \text{Re} \Sigma^> (p, q)}{\partial \mathbf{E}} \right\} \frac{\partial}{\partial \mathbf{E}} G^< (p, q)
\]

\[
- e \mathbf{F} \cdot \left\{ \frac{\partial \Sigma^< (p, q)}{\partial \mathbf{E}} \frac{\partial \text{Re} G^> (p, q)}{\partial \mathbf{K}} \right\} + e \mathbf{F} \cdot \left\{ \frac{\partial \Sigma^< (p, q)}{\partial \mathbf{K}} \frac{\partial \text{Re} G^> (p, q)}{\partial \mathbf{E}} \right\}
\]

\[
+ \frac{1}{\hbar} \{ \Sigma^< (p, q) A (p, q) - \Gamma (p, q) G^< (p, q) \},
\]

(22)

where \( G^> (p, q) \) is the LWT of the retarded Green’s function, \( A (p, q) \) is the spectral function, and \( \Gamma (p, q) \) is the corresponding scattering rate.

4.1 Balistic transport

We will simplify Eq. (22) by neglecting the self-energies, i.e., we limit to non-interacting particles. Then we have the following simplified quantum transport equation,

\[
\frac{\partial}{\partial t} G^< (p, q) = -e \mathbf{F} \cdot \frac{\partial}{\partial \mathbf{E}} E_\alpha \left( \mathbf{K} \right) \frac{\partial}{\partial \mathbf{K}} G^< (p, q)
\]

\[
+ e \mathbf{F} \cdot \frac{\partial}{\partial \mathbf{K}} E_\alpha \left( \mathbf{K} \right) \frac{\partial}{\partial \mathbf{E}} G^< (p, q)
\]

(22)
which can be written in terms of the Poisson bracket of Eq. (20) as
\[
\frac{\partial}{\partial t} G^<(\vec{k}, E) = \frac{2}{\hbar} e \vec{F} \cdot \left( \frac{\partial^{(a)}}{\partial \vec{k}} \frac{\partial^{(b)}}{\partial E} - \frac{\partial^{(a)}}{\partial E} \frac{\partial^{(b)}}{\partial \vec{k}} \right) H^{(a)}(\vec{k}, E) \frac{G^{<(b)}(\vec{k}, E)}{G^{<(b)}(\vec{k}, E)}.
\]
(23)

Therefore
\[
G^<(\vec{k}, E) = e \vec{F} \cdot \int dt \left( \frac{\partial^{(a)}}{\partial \vec{k}} \frac{\partial^{(b)}}{\partial E} - \frac{\partial^{(a)}}{\partial E} \frac{\partial^{(b)}}{\partial \vec{k}} \right) H^{(a)}(\vec{k}, E) \frac{G^{<(b)}(\vec{k}, E)}{G^{<(b)}(\vec{k}, E)}.
\]

Assuming that the electric field is in the x-direction. Then
\[
G^<(\vec{k}, E) = e \left| \vec{F} \right| \int dt \left( \frac{\partial^{(a)}}{\partial k_x} \frac{\partial^{(b)}}{\partial E} - \frac{\partial^{(a)}}{\partial E} \frac{\partial^{(b)}}{\partial k_x} \right) H^{(a)}(\vec{k}, E) \frac{G^{<(b)}(\vec{k}, E)}{G^{<(b)}(\vec{k}, E)}.
\]

The Hall current in the y-direction is thus given by the following equation,
\[
\frac{a^2}{(2\pi \hbar)^2} \int \int d\vec{k}_x d\vec{k}_y \left( \frac{\left| \vec{F} \right|}{a^2 \hbar} \right) \left( \frac{\partial E}{\partial \vec{k}_y} \right)^2 (-iG^<(\vec{k}, E))
\]
\[
= e^2 \left| \vec{F} \right| \frac{1}{(2\pi \hbar)^2} \int \int d\vec{k}_x d\vec{k}_y dt \left( \frac{\partial E}{\partial \vec{k}_y} \right)^2 \left[ \frac{\partial^{(a)}}{\partial k_x} \frac{\partial^{(b)}}{\partial E} - \frac{\partial^{(a)}}{\partial E} \frac{\partial^{(b)}}{\partial k_x} \right] H^{(a)}(\vec{k}, E) \left( -iG^{<(b)}(\vec{k}, E) \right)
\]
\[
= e^2 \left| \vec{F} \right| \frac{1}{(2\pi \hbar)^2} \int \int d\vec{k}_x d\vec{k}_y dt \left[ \frac{\partial^{(a)}}{\partial k_x} \frac{\partial^{(b)}}{\partial \vec{k}_y} \right] H^{(a)}(\vec{k}, E) \left( -iG^{<(b)}(\vec{k}, E) \right).
\]
(24)

If we are only interested in linear response we may consider all the quantities in the integrand to be of zero-order in the electric field, although this is not necessary if we allow very weak electric field leading to time dependence being dominated by the time dependence of the density matrix, as we shall see in what follows.

### 4.2 Quantization of Hall conductance

From Eq. (24), we claim that the quantized Hall conductivity is given by
\[
\sigma_{yz} = \left( \frac{e^2}{\hbar} \right) \left| \vec{F} \right| \frac{1}{(2\pi \hbar)^2} \int \int d\vec{k}_x d\vec{k}_y dt \left[ \frac{\partial^{(a)}}{\partial k_x} \frac{\partial^{(b)}}{\partial \vec{k}_y} - \frac{\partial^{(a)}}{\partial \vec{k}_y} \frac{\partial^{(b)}}{\partial k_x} \right] H^{(a)}(\vec{k}, E) \left( -iG^{<(b)}(\vec{k}, E) \right),
\]
(25)
and is quantized in units of \( \frac{e^2}{\hbar} \), i.e., \( \sigma_{yz} = \frac{e^2}{\hbar} \mathbb{Z} \), where \( \mathbb{Z} \) is in the domain of integers or the first Chern numbers. In doing the integration with respect to time, \( t \), we need to examine the implicit time-dependence of the matrix element of \( G^< \) in the ‘pull back’ representation defined below.

### 5 SFLWT-NEGF approach to Hall conductivity

Now to prove the Eq. (25) gives \( \sigma_{yz} = \frac{e^2}{\hbar} n \), where \( n \in \mathbb{Z} \), we need to transform the integral of the equation to the curvature of the Berry connection in a closed
loop. This necessitates a 'pull back' (i.e., undoing) the lattice transformation of Eq. (24).

5.1 'Pull back' of the lattice Weyl transformation

We give the proof that the Hall conductivity \( \sigma_{yx} = \frac{e^2}{2\hbar} \) in Eq. (25) by recasting the Eq. (24) to the expression originally used by TKNN[11], obtained through the Kubo formula in linear response theory, to derive the quantization of integer quantum Hall effect. This means we have to 'pull back' or undo the lattice transformation of SFLWT-NEG transport equation.

Consider the integrand in Eq. (25) given by the partial derivatives of lattice Weyl transformed quantities.

\[
\begin{align*}
\frac{\partial}{\partial K_x} \langle \vec{K}, \mathcal{E} \rangle &= \frac{\partial}{\partial K_x} \left( \frac{e}{\hbar} \left( \kappa, \mathcal{E} \right) \left( \frac{iG^{<}(\vec{K}, \mathcal{E})}{\partial G^{>}(\vec{K}, \mathcal{E})} \right) \right) \\
&= \left[ \frac{\partial}{\partial K_x} \left( \frac{e}{\hbar} \right) \left( \kappa, \mathcal{E} \right) \left( \frac{iG^{<}(\vec{K}, \mathcal{E})}{\partial G^{>}(\vec{K}, \mathcal{E})} \right) \right] \langle \vec{K}, \mathcal{E} \rangle.
\end{align*}
\]

The trick is to 'pull back' (undo) the lattice Weyl transformation to touch base with Berry connection and Berry curvature. Take first the term of Eq. (26)

\[
\frac{\partial}{\partial K_x} \langle \vec{K}, \mathcal{E} \rangle = \frac{\hbar}{\partial \vec{K}_x} \frac{\partial}{\partial \vec{K}_x} \langle \vec{K}, \mathcal{E} \rangle.
\]

From Eq. (14) this can be written as a lattice Weyl transform \( \mathcal{W} \) in the form,

\[
\begin{align*}
\frac{\partial}{\partial K_x} \langle \vec{K}, \mathcal{E} \rangle &= \mathcal{W} \left\{ \left( \frac{\partial}{\partial \vec{K}_x} \right)^2 \left( \mathcal{E} \right) \right\} \\
&= \mathcal{W} \left\{ \left( \frac{\partial}{\partial \vec{K}_x} \right)^2 \left( \mathcal{E} \right) \right\} \\
&= \mathcal{W} \left\{ \left( \frac{\partial}{\partial \vec{K}_x} \right)^2 \left( \mathcal{E} \right) \right\}.
\end{align*}
\]

where \( \left( \frac{\partial}{\partial \vec{K}_x} \right)^2 \left( \mathcal{E} \right) \) symbolically denotes derivative with respect to \( \vec{K}_x \) of the state vector \( \langle \alpha, \vec{K}_x, \mathcal{E} \rangle \) labeled by the three quantum labels. Likewise for \( \beta, \frac{\partial}{\partial \vec{K}_x} \vec{K}_x, \mathcal{E} \).

We also have

\[
\frac{\partial}{\partial K_y} \langle \vec{K}, \mathcal{E} \rangle = \mathcal{W} \left\{ \left( \frac{\partial}{\partial \vec{K}_y} \right)^2 \left( \mathcal{E} \right) \right\}.
\]
where  \( \hat{\rho} \) is the density matrix operator. From Eq. (4), we take the time dependence of \( \langle \beta, \vec{K}, \mathcal{E} \mid (i\hat{\rho}) \mid \alpha, \vec{K}, \mathcal{E} \rangle \) to be given by \( i \langle \beta, \vec{K}, \mathcal{E} \mid \hat{\rho}(0) \mid \alpha, \vec{K}, \mathcal{E} \rangle e^{i\omega_{\alpha\beta}t} \).

We have \(^1\)

\[
\frac{\partial G^{<}(\vec{K}, \mathcal{E})}{\partial K_y} = \mathcal{W} \left\{ \right. \\
\left. \langle \beta, \vec{K}, \mathcal{E} \mid (i\hat{\rho}) \mid \alpha, \vec{K}, \mathcal{E} \rangle \\
+ \langle \beta, \vec{K}, \mathcal{E} \mid \alpha, \frac{\partial}{\partial K_y} \vec{K}, \mathcal{E} \rangle \hat{\rho}_0 \right\} e^{i\omega_{\alpha\beta}t}.
\]

The density matrix operator \( \hat{\rho}_0 \) is of the form,

\[
\hat{\rho}_0 = \sum_m \rho_m |m\rangle \langle m|
\]

\[
\hat{\rho}_0 |m\rangle = \rho_m |m\rangle = f(E_m) |m\rangle
\]

\[
\langle m| \hat{\rho}_0 |n\rangle = \rho_{mn} = f(E_n) \delta_{mn} \text{ or } f(E_m) \delta_{mn}
\]

where the weight function is the Fermi-Dirac function,

\[
\rho^m_0 = f(E_m)
\]

Hence

\[
i \hat{\rho}_0 \mid \alpha, \vec{K}, \mathcal{E} \rangle = i \sum_\gamma |\gamma, \vec{K}, \mathcal{E} \rangle \rho_0^\gamma \langle \gamma, \vec{K}, \mathcal{E} \mid \alpha, \vec{K}, \mathcal{E} \rangle
\]

\[
= i \langle \alpha, \vec{K}, \mathcal{E} | f(E_\alpha) \rangle.
\]

Similarly,

\[
i \langle \beta, \vec{K}, \mathcal{E} | (\hat{\rho}_0) \rangle = i \langle \beta, \vec{K}, \mathcal{E} | \sum_\gamma |\gamma, \vec{K}, \mathcal{E} \rangle \rho_0^\gamma \langle \gamma, \vec{K}, \mathcal{E} \rangle
\]

\[
= if(E_\beta) \langle \beta, \vec{K}, \mathcal{E} \rangle.
\]

Hence

\[
\frac{\partial G^{<}(\vec{K}, \mathcal{E})}{\partial K_y} = \mathcal{W} \left\{ i \langle \beta, \vec{K}, \mathcal{E} \mid \alpha, \frac{\partial}{\partial K_y} \vec{K}, \mathcal{E} \rangle \rho_0^\alpha \right\} e^{i\omega_{\alpha\beta}t}.
\]

Shifting the first derivative to the right, we have

\[
\frac{\partial G^{<}(\vec{K}, \mathcal{E})}{\partial K_y} = \mathcal{W} \left\{ -i \langle \beta, \vec{K}, \mathcal{E} \mid \alpha, \frac{\partial}{\partial K_y} \vec{K}, \mathcal{E} \rangle f(E_\alpha) \right\} e^{i\omega_{\alpha\beta}t}
\]

\[
= \mathcal{W} \left[ \left\{ i (f(E_\beta) - f(E_\alpha)) \langle \beta, \vec{K}, \mathcal{E} \mid \alpha, \frac{\partial}{\partial K_y} \vec{K}, \mathcal{E} \rangle \right\} e^{i\omega_{\alpha\beta}t} \right].
\]

\(^1\)Here we use the definition of Green’s function without the factor \( h \), following traditional treatments, i.e. \( \rho(1,2) = -iG^{<}(1,2) \).
For energy scale it is convenient to chose to use \( f (E_\alpha) \) in the above equation, with the viewpoint that \( \alpha \)-state is far remove from the \( \beta \)-state in gapped states, so that we can set \( f (E_\beta) \approx 0 \). The case \( \alpha = \beta \) is indeterminate so that by setting \( f (E_\beta) \approx 0 \) renders the summation to be well-defined. Therefore

\[
\frac{\partial H (\vec{K}, \vec{E})}{\partial K_x} \frac{\partial G^< (\vec{K}, \vec{E})}{\partial K_y} = \left\{ \mathcal{W} \left[ -\left( E_\beta (\vec{K}, \vec{E}) - E_\alpha (\vec{K}, \vec{E}) \right) \right] \left\{ \left\langle \alpha, \frac{\partial}{\partial K_x} \vec{K}, \vec{E} \right| \left| \beta, \vec{K}, \vec{E} \right\rangle \right\} \right\} \left\{ \mathcal{W} \left[ -i f (E_\alpha) \left\langle \beta, \vec{K}, \vec{E} \right| \alpha, \frac{\partial}{\partial K_y} \vec{K}, \vec{E} \right\rangle e^{i \omega_{\alpha \beta} t} \right\}
\]

Since it appears as a product of two Weyl transforms, it must be a trace formula in the untransformed or pulled back version, i.e., for the remaining indices \( \alpha \) and \( \beta \) we must be a summation,

\[
\frac{\partial H (\vec{K}, \vec{E})}{\partial K_x} \frac{\partial G^< (\vec{K}, \vec{E})}{\partial K_y} = \mathcal{W} \left\{ \sum_{\alpha, \beta} \left( E_\beta (\vec{K}, \vec{E}) - E_\alpha (\vec{K}, \vec{E}) \right) \right\} \left\{ i f (E_\alpha) \right\}. \]

Similarly, we have

\[
\frac{\partial H (\vec{K}, \vec{E})}{\partial K_y} \frac{\partial G^< (\vec{K}, \vec{E})}{\partial K_x} = \mathcal{W} \left\{ \sum_{\alpha, \beta} \left( E_\beta (\vec{K}, \vec{E}) - E_\alpha (\vec{K}, \vec{E}) \right) \right\} \left\{ i f (E_\alpha) \right\}. \]

Therefore we obtain

\[
\left[ \frac{\partial H (\vec{K}, \vec{E})}{\partial K_x} \frac{\partial G^< (\vec{K}, \vec{E})}{\partial K_y} - \frac{\partial H (\vec{K}, \vec{E})}{\partial K_y} \frac{\partial G^< (\vec{K}, \vec{E})}{\partial K_x} \right] = \mathcal{W} \left\{ \sum_{\alpha, \beta} \left( E_\beta (\vec{K}, \vec{E}) - E_\alpha (\vec{K}, \vec{E}) \right) \right\} \left\{ i e^{i \omega_{\alpha \beta} t} f (E_\alpha) \right\}. \]

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Now the LHS of Eq. (21), namely
\[
\left( \frac{a}{(2\pi\hbar)} \right)^2 \int d\vec{K}_x d\vec{K}_y \frac{e}{a^2} \frac{\partial^2 H}{\partial K_y^2} G^< (\vec{K}, \vec{E}) = \left( \frac{a}{(2\pi\hbar)} \right)^2 \int d\vec{K}_x d\vec{K}_y \frac{e}{a^2} \frac{\partial H}{\partial K_y} G^< (\vec{K}, \vec{E}).
\] (28)

Using the result of Eq. (27), we have
\[
\frac{\partial H (\vec{K}, \vec{E})}{\partial K_y} = \mathcal{W} \left\{ \left[ (E_\alpha (\vec{K}, \vec{E}) - E_\beta (\vec{K}, \vec{E})) \right] \left\langle \alpha, \vec{K}, \vec{E} \right| \beta, \frac{\partial}{\partial K_y} \left\langle \vec{K}, \vec{E} \right) \right\}
\]
\[
= \mathcal{W} \left\{ \left[ (E_\beta (\vec{K}, \vec{E}) - E_\alpha (\vec{K}, \vec{E})) \right] \left\langle \alpha, \frac{\partial}{\partial K_y} \vec{K}, \vec{E} \right| \beta, \vec{K}, \vec{E} \right\}
\]
\[
= \mathcal{W} \left\{ \omega_{\beta\alpha} \left( \alpha, \frac{\partial}{\partial K_y} \vec{K}, \vec{E} \right| \beta, \vec{K}, \vec{E} \right\} = \left( \alpha, \vec{K}, \vec{E} \right| \beta, \vec{K}, \vec{E} \right)
\]

where
\[
\omega_{\beta\alpha} (\alpha, \nabla \vec{p} | \beta, \vec{p}) = \langle \alpha, \vec{p} | \hat{v} | \beta, \vec{p} \rangle
\]

Likewise
\[
G^< (\vec{K}, \vec{E}) = i\mathcal{W} \left( \left\langle \beta, \vec{K}, \vec{E} \right| \hat{\rho} \right) \left\langle \alpha, \vec{K}, \vec{E} \right)
\]

Again since Eq. (28) is a product of lattice Weyl transform, it must be a trace in the untransformed version, i.e.,
\[
\left( \frac{a}{(2\pi\hbar)} \right)^2 \int d\vec{K}_x d\vec{K}_y \frac{e}{a^2} \frac{\partial H}{\partial K_y} G^< (\vec{K}, \vec{E})
\]
\[
= \mathcal{W} \left\{ i \int \left( \frac{1}{2\pi\hbar} \right)^2 d\vec{K}_x d\vec{K}_y \right\} \times \sum_{\alpha, \beta} \left\langle \alpha, \vec{K}, \vec{E} \right| \frac{\partial}{\partial K_y} v_y \left| \beta, \vec{K}, \vec{E} \right\rangle \left\langle \beta, \vec{K}, \vec{E} \right| \hat{\rho} \left| \alpha, \vec{K}, \vec{E} \right\rangle
\]
\[
= \mathcal{W} \left\{ i \mathcal{W} \left( \text{Tr}(\vec{j}_y \hat{\rho}) \right) \right\} = i\mathcal{W} \left( \text{Tr}(\vec{j}_y \hat{\rho}) \right) = i\mathcal{W} \left( \text{Tr}(\vec{j}_y \hat{\rho}) \right)
\]
\[
= i\mathcal{W} \left\{ \{\vec{j}_y(t)\} \right\}
\]

For calculating the conductivity we are interested in the term multiplying the first-order in electric field. We can now convert the quantum transport equation in the transformed space, Eq. (21),
\[
\left( \frac{a}{(2\pi\hbar)} \right)^2 \int d\vec{K}_x d\vec{K}_y \frac{e}{a^2} \frac{\partial H}{\partial K_y} \left[ -ig^< (\vec{K}, \vec{E}) \right]
\]
\[
= e^2 \left| \vec{F} \right| \left\{ \int \int d\vec{K}_x d\vec{K}_y dt \left[ \frac{\partial^{(a)}}{\partial K_x} \frac{\partial^{(b)}}{\partial K_y} - \frac{\partial^{(a)}}{\partial K_y} \frac{\partial^{(b)}}{\partial K_x} \right] H^{(a)} (\vec{K}, \vec{E}) \left( -ig^{(<b)} (\vec{K}, \vec{E}) \right) \right\},
\]
Taking the limit \( \omega \) to the untransformed space by undoing or 'pulling back' the lattice Weyl transformation \( \mathcal{W} \), which amounts to canceling \( \mathcal{W} \) in both side of the equation given by,

\[
\mathcal{W} \{ \langle j_y (t) \rangle \} = \mathcal{W} \left\{ \sum_{\alpha, \beta} \left[ \frac{e^2}{h} \left| \hat{F} \right| \frac{1}{(2\pi \hbar)} \int \int d\vec{k}_x d\vec{k}_y \langle \alpha, \frac{\partial}{\partial k_x} \vec{k}, \vec{E} \rangle \langle \beta, \vec{k}, \vec{E} \rangle \left( \langle \alpha, \frac{\partial}{\partial k_y} \vec{k}, \vec{E} \rangle - \langle \alpha, \frac{\partial}{\partial k_y} \vec{k}, \vec{E} \rangle \right) \right] e^{i \omega_{\alpha \beta} t} \langle f (E_\alpha) \rangle \right\} .
\]

The time integral of the RHS amounts to taking zero-order time dependence [zero electric field] of the rest of the integrand, then we have for the remaining time-dependence, explicitly integrated as,

\[
\int_{-\infty}^{0} dt \exp i \omega_{\alpha \beta} t = \exp \frac{i \omega_{\alpha \beta} \tau}{\omega_{\alpha \beta}} \bigg|_{\tau = -\infty}^{\tau = 0} = \frac{\exp (i (\omega_{\alpha \beta} - i \eta) \tau)}{i \omega_{\alpha \beta}} \bigg|_{\tau = -\infty}^{\tau = 0} = \frac{1}{i \omega_{\alpha \beta}}.
\]

Thus eliminating the time integral we finally obtain.

\[
\langle j_y (t) \rangle = -\frac{e^2}{h} \left| \hat{F} \right| \frac{1}{(2\pi \hbar)} \int \int d\vec{k}_x d\vec{k}_y \sum_{\alpha, \beta} \left[ \left\{ \langle \alpha, \frac{\partial}{\partial k_x} \vec{k}, \vec{E} \rangle \langle \beta, \vec{k}, \vec{E} \rangle \langle \beta, \vec{k}, \vec{E} \rangle \langle \alpha, \frac{\partial}{\partial k_y} \vec{k}, \vec{E} \rangle \right\} \right] \int \int d\vec{k}_x d\vec{k}_y \sum_{\alpha, \beta} f (E_\alpha) \left\{ \langle \alpha, \frac{\partial}{\partial k_x} \vec{k}, \vec{E} \rangle \langle \beta, \vec{k}, \vec{E} \rangle \langle \beta, \vec{k}, \vec{E} \rangle \langle \alpha, \frac{\partial}{\partial k_y} \vec{k}, \vec{E} \rangle \right\} (30)
\]

Taking the Fourier transform of both sides, we obtain

\[
\langle j_y (\omega) \rangle = \frac{e^2}{h} \left| \hat{F} \right| \frac{\delta (\omega)}{(2\pi)} \int \int d\vec{k}_x d\vec{k}_y \sum_{\alpha, \beta} \left\{ \langle \alpha, \frac{\partial}{\partial k_x} \vec{k}, \vec{E} \rangle \langle \beta, \vec{k}, \vec{E} \rangle \langle \beta, \vec{k}, \vec{E} \rangle \langle \alpha, \frac{\partial}{\partial k_y} \vec{k}, \vec{E} \rangle \right\} \int \int d\vec{k}_x d\vec{k}_y \sum_{\alpha, \beta} f (E_\alpha) \left\{ \langle \alpha, \frac{\partial}{\partial k_x} \vec{k}, \vec{E} \rangle \langle \beta, \vec{k}, \vec{E} \rangle \langle \beta, \vec{k}, \vec{E} \rangle \langle \alpha, \frac{\partial}{\partial k_y} \vec{k}, \vec{E} \rangle \right\} \left(31\right)
\]

Taking the limit \( \omega \rightarrow 0 \) and summing over the states \( \beta \), we readily obtain the conductivity, \( \sigma_{yx} \).

\[
\sigma_{yx} = \frac{e^2}{h} \sum_{\alpha} f (E_\alpha) \frac{i}{(2\pi)} \int \int d\vec{k}_x d\vec{k}_y \left[ \langle \alpha, \frac{\partial}{\partial k_x} \vec{k}, \vec{E} \rangle \langle \alpha, \frac{\partial}{\partial k_y} \vec{k}, \vec{E} \rangle \right] . \quad (32)
\]
where $\vec{K} \rightarrow \vec{P}$ from Eq. (6) in both Eqs. (31) and (32). This is the same expression that can obtained to derive the integer quantum Hall effect from Kubo formula [1].

We now prove that for each statevector, $|\alpha, \vec{k}\rangle$, the expression,

$$ \frac{i}{(2\pi)} \int \int d\vec{k}_x d\vec{k}_y f \left( E_\alpha \left( \vec{k} \right) \right) \left[ \left\langle \frac{\partial}{\partial \vec{k}_x} |\alpha, \vec{k}\rangle |\alpha, \vec{k}\rangle \rightangle - \left\langle \frac{\partial}{\partial \vec{k}_y} |\alpha, \vec{k}\rangle |\alpha, \vec{k}\rangle \right\rangle \right],$$

(33)
is the winding number around the occupied contour in the Brillouin zone. First we can rewrite the terms within the square bracket as

$$ = \left\langle \frac{\partial}{\partial \vec{k}} |\alpha, \vec{k}\rangle \times \frac{\partial}{\partial \vec{k}} |\alpha, \vec{k}\rangle \right\rangle = \nabla_{\vec{k}} \times \left\langle \frac{\partial}{\partial \vec{k}} |\alpha, \vec{k}\rangle |\alpha, \vec{k}\rangle \right\rangle. \quad (34)$$

The last term indicates the operation of the curl of the Berry connection which is related to the quantization of Hall conductivity. This quantization is due to the uniqueness of the parallel-transported wavefunction. To understand this, first we discuss how the phase of the wavefunction relates to the Berry connection and Berry curvature. This is given in the next section.

### 5.2 Change of the phase of the wavefunction under parallel transport

To relate to the phase of the wavefunction, we recall that for parallel transport

$$ \frac{\partial \psi_\alpha \left( \vec{k} \right)}{\partial t} = \left( -\Gamma^j_{\vec{k}, \beta} \frac{d\vec{k}}{dt} \right) \psi_\beta \left( \vec{k} \right) $$

$$ = \left( -\left\langle \alpha, \vec{k} | \frac{\partial}{\partial \vec{k}} | \beta, \vec{k} \right\rangle \frac{d\vec{k}}{dt} \right) \psi_\beta \left( \vec{k} \right). $$

In the adiabatic case, this becomes (assuming energy band $\alpha$ is far remove from the other bands),

$$ \frac{\partial \psi_\alpha \left( \vec{k} \right)}{\partial t} = \left( -\left\langle \alpha, \vec{k} | \frac{\partial}{\partial \vec{k}} | \alpha, \vec{k} \right\rangle \cdot \frac{d\vec{k}}{dt} \right) \psi_\alpha \left( \vec{k} \right). $$

Thus,

$$ \frac{d \ln \psi_\alpha \left( \vec{k} \right)}{dt} = \left( -\left\langle \alpha, \vec{k} | \frac{\partial}{\partial \vec{k}} | \alpha, \vec{k} \right\rangle \cdot \frac{d\vec{k}}{dt} \right), $$

$$ d \ln \psi_\alpha \left( \vec{k} \right) = -\left\langle \alpha, \vec{k} | \frac{\partial}{\partial \vec{k}} | \alpha, \vec{k} \right\rangle \cdot d\vec{k}, $$

and

$$ d\phi = i \left\langle \alpha, \vec{k} | \frac{\partial}{\partial \vec{k}} | \alpha, \vec{k} \right\rangle \cdot d\vec{k}, $$

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where $i\phi$ is the change of phase of the wavefunction along a curve in $\vec{k}$-space (Brillouin zone). Around a closed curve the total change of phase must be a multiple of $2\pi$, i.e., $\Delta\phi = 2\pi n \ (n \in \mathbb{Z})$ for the wavefunction to return to its original state.

We can write

$$\frac{i}{(2\pi)} \int \int dk_x dk_y \ f \left( E_\alpha \left( \vec{k} \right) \right) \left[ \nabla_{\vec{k}} \times \left\langle \alpha, \vec{k} \left| \frac{\partial}{\partial \vec{k}} \right| \alpha, \vec{k} \right\rangle \right]_{\text{plane}}$$

5.3 First Chern number and quantization of QHE

At low temperature, we can just write

$$\sigma_{yx} = \frac{ie^2}{2\pi \hbar (2\pi)} \sum_\alpha \int \int_{\text{occupiedBZ}} dk_x dk_y \left[ \nabla_{\vec{k}} \times \left\langle \alpha, \vec{k} \left| \frac{\partial}{\partial \vec{k}} \right| \alpha, \vec{k} \right\rangle \right]_{\text{plane}}$$

Now

$$i\Delta\phi_{\text{total}} = - \oint_{\text{contour}} dk_c \left[ \left\langle \alpha, \vec{k} \right| \frac{\partial}{\partial \vec{k}_c} \left| \alpha, \vec{k} \right\rangle \right]_{\text{contour}}$$

$$\Delta\phi_{\text{total}} = \frac{i}{2\pi} \oint_{\text{contour}} dk_c \left[ \left\langle \alpha, \vec{k} \right| \frac{\partial}{\partial \vec{k}_c} \left| \alpha, \vec{k} \right\rangle \right]_{\text{contour}}$$

$$\frac{\Delta\phi_{\text{total}}}{2\pi} = \frac{i}{2\pi} \oint_{\text{contour}} dk_c \left[ \left\langle \alpha, \vec{k} \right| \frac{\partial}{\partial \vec{k}_c} \left| \alpha, \vec{k} \right\rangle \right]_{\text{contour}}$$ is the winding number or the Chern number.

Therefore

$$\sigma_{yx} = \frac{ie^2}{2\pi \hbar (2\pi)} \sum_\alpha \int \int_{\text{occupiedBZ}} dk_x dk_y \left[ \nabla_{\vec{k}} \times \left\langle \alpha, \vec{k} \left| \frac{\partial}{\partial \vec{k}} \right| \alpha, \vec{k} \right\rangle \right]_{\text{plane}}$$

$$= \frac{e^2}{2\pi \hbar (2\pi)} \sum_\alpha \oint_{\text{contour or Wilson loop over BZ}} dk_c \left[ \left\langle \alpha, \vec{k} \right| \frac{\partial}{\partial \vec{k}_c} \left| \alpha, \vec{k} \right\rangle \right]$$

over all occupied bands $\alpha$, where $n_\alpha \in \mathbb{Z}$ is the topological first Chern (or winding) number. Thus the the Hall conductivity is quantized in units of $\frac{e^2}{\hbar}$ as derive from Eq. (25) of the new method used here.
6 Kubo current-current correlation formula

To touch base with a time-dependent perturbation of the Kubo current-current correlation we recall that in this particular approach, a time varying electric field is indirectly used. To get to QHE the limiting case of $\omega \rightarrow 0$ is taken after Fourier transformation of a convolution integral. In adapting to our approach, this means that the time integral in the expression of the RHS of Eq. (29) when transformed to current-current correlation is a convolution integral before taking the Fourier transform.

We start with the RHS of Eq. (29),

\[
\text{RHS} = \frac{e^2}{h} \frac{1}{(2\pi h)} \int \int dK_x dK_y dt \sum_{\alpha,\beta} \left\{ \begin{array}{l}
\frac{E_\beta \left( K_x, E \right) - E_\alpha \left( K_x, E \right)}{\hbar} \\
\times f(E_\alpha) e^{i(\omega_{\alpha,\beta})t} \end{array} \right\}
\]

\[
\text{RHS} = \frac{e^2}{h} \frac{1}{(2\pi h)} \int \int dK_x dK_y dt \sum_{\alpha,\beta} \left\{ \begin{array}{l}
\frac{h\omega_{\beta\alpha}}{\hbar} \\
\times f(E_\alpha) e^{i(\omega_{\alpha,\beta})t} \end{array} \right\}
\]

\[
\text{RHS} = \frac{e^2}{h} \frac{1}{(2\pi h)\hbar^2} \int \int dK_x dK_y dt \sum_{\alpha,\beta} \left\{ \begin{array}{l}
\frac{\omega_{\beta\alpha}}{\hbar} \\
\times f(E_\alpha) e^{i(\omega_{\alpha,\beta})t} \end{array} \right\}
\]

We make use of the general relations

\[
\langle \alpha, \vec{p} | \vec{v} | \beta, \vec{p} \rangle \equiv \omega_{\beta\alpha} \langle \alpha, \nabla_{K_x} | \beta, \vec{p} \rangle
\]

\[
\langle \alpha, \nabla_{K_x} | \beta, \vec{p} \rangle = \frac{\langle \alpha, \vec{p} | \vec{v} | \beta, \vec{p} \rangle}{\omega_{\beta\alpha}} \tag{36}
\]

Similarly, we have

\[
\langle \beta, \vec{p} | \vec{v} | \alpha, \vec{p} \rangle \equiv \omega_{\beta\alpha} \langle \beta, \vec{p} | \nabla_{K_x} | \alpha, \vec{p} \rangle,
\]

\[
\langle \beta, \vec{p} | \nabla_{K_x} | \alpha, \vec{p} \rangle = \frac{\langle \beta, \vec{p} | \vec{v} | \alpha, \vec{p} \rangle}{\omega_{\beta\alpha}}. \tag{37}
\]
Substituting in Eq. (35), we then have the convolution integral with respect to time,

\[
RHS = \frac{\mu^2}{\hbar} \int \int dK_x dK_y \sum_{\alpha, \beta} \left\{ \frac{1}{2\pi a^2} \left[ \alpha, \beta, \mathcal{E} \right] \left| v_x \right| \left[ \beta, \mathcal{K}, \mathcal{E} \right] \left| v_y \right| (t - t') \left| \alpha, \mathcal{K}, \mathcal{E} \right] \times e^{i(\omega_{\alpha, \beta})t'} f(E_{\alpha}) \right\}
\]

Consider the following Fourier transformation,

\[
\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{i\omega t} F(t) \, dt = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{i\omega t} \int_{-\infty}^{0} f(t - t') g(t') \, dt' \, dt,
\]

\[
t - t' = \alpha \implies dt = d\alpha,
\]

\[
t = (t' + \alpha),
\]

\[
\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{i\omega t} F(t) \, dt = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{i\omega t'} \int_{-\infty}^{0} e^{i\omega \alpha} f(\alpha) \, d\alpha.
\]

We can transform the range of integration as follows,

\[
\int_{-\infty}^{0} e^{i\omega \alpha} f(\alpha) \, d\alpha = \int_{-\infty}^{0} e^{-i\omega \alpha} f(-\alpha) (-d\alpha) = \int_{0}^{\infty} e^{-i\omega \alpha} f(-\alpha) \, d\alpha
\]

\[
= \int_{0}^{\infty} e^{-i\omega \alpha} f^\dagger(\alpha) \, d\alpha = \int_{0}^{\infty} e^{-i\omega \alpha} f(\alpha) \, d\alpha,
\]

since \( f(\alpha) \) is the observable current density and hence self-adjoint. We can apply this result in what follows.

Defining the current density as \( j_x = \frac{e\mu}{a^2} \), we obtain, after Fourier transforming the convolution integral as

\[
RHS = \frac{\mu^2}{\hbar} \int \int \left( \frac{a}{(2\pi \hbar)} \right)^2 dK_x dK_y \sum_{\alpha, \beta} \left\{ \left[ \alpha, \mathcal{K}, \mathcal{E} \right] \left| j_x \right| (0) \left[ \beta, \mathcal{K}, \mathcal{E} \right] \left| j_y \right| (t) \left| \alpha, \mathcal{K}, \mathcal{E} \right] \times e^{-i(\omega_{\alpha, \beta})t} f(E_{\alpha}) \right\}
\]

\[
= \frac{\mu^2}{\hbar} \int_{0}^{\infty} dt \, Tr\rho_0 \left\{ [j_x \left(0\right), j_y \left(t\right)] \right\} e^{-i(\omega_{\alpha, \beta})t},
\]

(38)
where $\eta$ is just a regularization exponent at $\infty$. Therefore the Kubo formula for the conductivity is given by

$$\sigma_{yx}(t) = \frac{\alpha^2}{\hbar \omega} \int_0^\infty dt \text{Tr} \rho_0 \{ [j_x(0), j_y(t)] \} e^{-i(\omega-i\eta)t}. \quad (39)$$

This is the Kubo current-current correlation formula for the Hall conductivity.

6.1 Berry curvature and orbital magnetic moment of 2-D systems

Note that the orbital magnetic moment is given by,

$$\langle \vec{M} \rangle = \text{Tr} \rho \frac{e}{2m} \vec{L} = \text{Tr} \rho \frac{e}{2m} \vec{Q} \times \vec{P}$$

$$= -i \frac{e}{2m} \sum_{\alpha,p;\beta,p} f(E_\alpha(p)) \langle \alpha, \vec{p} | \nabla_E | \beta, \vec{p} \rangle \times \langle \beta, \vec{p} | \vec{P} | \alpha, \vec{p} \rangle$$

$$= -i \frac{e}{2} \sum_{\alpha,p;\beta,p} f(E_\alpha(p)) \langle \alpha, \vec{p} | \nabla_E | \beta, \vec{p} \rangle \times \langle \beta, \vec{p} | \vec{v} | \alpha, \vec{p} \rangle$$

Using Eq. (37), we obtain

$$\langle \vec{M} \rangle = -i \frac{e}{2} \sum_{\alpha,p;\beta,p} f(E_\alpha(p)) \omega_{\alpha\beta} \langle \alpha, \vec{p} | \nabla_E | \beta, \vec{p} \rangle \times \langle \beta, \vec{p} | \nabla_E | \alpha, \vec{p} \rangle,$$

or

$$\langle \vec{M} \rangle = -i \frac{e}{2} \sum_{\alpha,p;\beta,p} f(E_\alpha(p)) \frac{\omega_{\alpha\beta}}{\omega_{\alpha\beta}} \langle \alpha, \vec{p} | \vec{v} | \beta, \vec{p} \rangle \times \langle \beta, \vec{p} | \vec{v} | \alpha, \vec{p} \rangle.$$

So Berry’s curvature implies the presence of orbital magnetic moment. \footnote{Using Eq. (37), we obtain as written in some literature}

In fact we can pull out the Berry curvature by rewriting in the Heisenberg picture,

$$\langle \vec{M} \rangle = \text{Tr} \rho \frac{e}{2m} \vec{L} = \text{Tr} \rho \frac{e}{2m} \vec{Q} \times \vec{P}$$

$$= \frac{e}{2m} \sum_{\alpha,p;\beta,p} f(E_\alpha(p)) \langle \alpha, \vec{p} | \vec{Q} | \beta, \vec{p} \rangle \times \langle \beta, \vec{p} | \vec{P} | \alpha, \vec{p} \rangle$$

$$= \frac{e}{2} \sum_{\alpha,p;\beta,p} f(E_\alpha(p)) \langle \alpha, \vec{p} | e^{i\frac{\pi}{2}Ht} \vec{Q} e^{-i\frac{\pi}{2}Ht} | \beta, \vec{p} \rangle \times \langle \beta, \vec{p} | \vec{v} | \alpha, \vec{p} \rangle$$

$$= \frac{e}{2} \sum_{\alpha,p;\beta,p} f(E_\alpha(p)) e^{i\omega_{\alpha\beta}t} \langle \alpha, \vec{p} | \vec{Q} S | \beta, \vec{p} \rangle \times \langle \beta, \vec{p} | \vec{v} | \alpha, \vec{p} \rangle.$$

\footnote{Using Eq. (37), we obtain as written in some literature}

$$\langle M \rangle = -\frac{e}{2} \sum_{\alpha,p;\beta,p} f(E_\alpha(p)) \frac{(E_\alpha(p) - E_\beta(p))}{E_\alpha(p) - E_\beta(p)} \frac{\langle \alpha, \vec{p} | m \vec{v} | \beta, \vec{p} \rangle}{\langle \beta, \vec{p} | m \vec{v} | \alpha, \vec{p} \rangle}.$$
Moreover, the conventional linearity in the electrical field strength may not be

From Eq. (20), we obtain

\[ \langle M \rangle = -i \frac{e}{2} \sum_{\alpha, p, \beta, p} f(E_{\alpha}(\vec{p})) e^{i \omega_{\alpha, \beta} t} \langle \alpha, \vec{p} | \nabla_{\vec{k}} | \beta, \vec{p} \rangle \times \langle \beta, \vec{p} | \vec{v} | \alpha, \vec{p} \rangle \]

\[ = -i \frac{e}{2} \sum_{\alpha, p, \beta, p} f(E_{\alpha}(\vec{p})) e^{i \omega_{\alpha, \beta} t} \langle \alpha, \vec{p} | \nabla_{\vec{k}} | \beta, \vec{p} \rangle \times \langle \beta, \vec{p} | \nabla_{\vec{k}} | \alpha, \vec{p} \rangle \omega_{\beta \alpha} \]

Integrating the RHS with respect to time, the result is in units of orbital magnetic moment multiplied by time denoted by \( \langle \vec{M} \rangle \),

\[ \langle \vec{M} \rangle = -i \frac{e}{2} \sum_{\alpha, p, \beta, p} f(E_{\alpha}(\vec{p})) \int_{-\infty}^{0} e^{i \omega_{\alpha, \beta} t} dt \omega_{\beta \alpha} \langle \alpha, \vec{p} | \nabla_{\vec{k}} | \beta, \vec{p} \rangle \times \langle \beta, \vec{p} | \nabla_{\vec{k}} | \alpha, \vec{p} \rangle \]

\[ = -i \frac{e}{2} \sum_{\alpha, p, \beta, p} f(E_{\alpha}(\vec{p})) \frac{\omega_{\beta \alpha}}{i \omega_{\alpha \beta}} \int_{\alpha}^{\beta} \langle \alpha, \vec{p} | \nabla_{\vec{k}} | \beta, \vec{p} \rangle \times \langle \beta, \vec{p} | \nabla_{\vec{k}} | \alpha, \vec{p} \rangle \]

\[ = \frac{e}{2} \sum_{\alpha, p, \beta, p} f(E_{\alpha}(\vec{p})) \langle \alpha, \vec{p} | \nabla_{\vec{k}} | \beta, \vec{p} \rangle \times \langle \beta, \vec{p} | \nabla_{\vec{k}} | \alpha, \vec{p} \rangle \]

\[ = \frac{e}{2} \sum_{\alpha, p} f(E_{\alpha}(\vec{p})) \langle \alpha, \nabla_{\vec{k}} \vec{p} | \beta, \vec{p} \rangle \times \langle \beta, \vec{p} | \nabla_{\vec{k}} | \alpha, \vec{p} \rangle \]

The last line is just

\[ \langle \vec{M} \rangle = \frac{e}{2} \frac{a^2}{(2\pi)^2} \sum_{\alpha} \int \int d_k d_y f(E_{\alpha}(\vec{k})) \left[ \frac{\partial}{\partial k_x} \alpha, \vec{k} \right] \frac{\partial}{\partial k_y} \alpha, \vec{k} \]

\[ - \left[ \frac{\partial}{\partial k_y} \alpha, \vec{k} \right] \frac{\partial}{\partial k_x} \alpha, \vec{k} \]

\[ = \frac{e}{2} \frac{a^2}{(2\pi)^2} \sum_{\alpha} \int \int d_k d_y f(E_{\alpha}(\vec{k})) \left[ \frac{\partial}{\partial k_x} \alpha, \vec{k} \right] \frac{\partial}{\partial k_y} \alpha, \vec{k} \]

\[ - \left[ \frac{\partial}{\partial k_y} \alpha, \vec{k} \right] \frac{\partial}{\partial k_x} \alpha, \vec{k} \]

\[ = \frac{e}{2} \frac{a^2}{(2\pi)^2} \sum_{\alpha} f(E_{\alpha}(\vec{k})) \int \int d_k d_y \left[ \nabla_{\vec{k}} \times \langle \alpha, \vec{k} | \partial | \alpha, \vec{k} \rangle \right] \]

explicitly revealing the Berry curvature derived from the expression for the orbital magnetic moment.

### 7 Concluding Remarks

In summary, we have identified topological invariant in \( (\vec{p}, \vec{q}, E, t) \) – phase space quantum transport given by

\[ \frac{1}{(2\pi \hbar)} \int \int dk_xdk_ydt \left[ \frac{\partial^{(a)}(a)}{\partial k_x} \frac{\partial^{(b)}(b)}{\partial k_y} - \frac{\partial^{(a)}(b)}{\partial k_x} \frac{\partial^{(b)}(a)}{\partial k_y} \right] H^{(a)}(\vec{k}, E) G^{<}(b) \left( \vec{k}, E \right) \]

an integral which give results in \( \mathbb{Z} \) manifold, the so-called first Chern numbers. Moreover, the conventional linearity in the electrical field strength may not be
a necessary and sufficient condition to prove the integer QHE, but rather it is the first-order gradient expansion in the real-time SFLWT-NEGF quantum transport equation. In general, nonlinearity in the electric field is still present in the variable \((K, E)\) in the integrand of Eq. (26) based on the assumption of weak electric field and hence weak time dependence. There seems to be experimental evidence on this nonlinearity [11]. It also appears that electron-electron interaction which does not break the symmetry of Eqs. (5)-(9) can be treated in similar manner.

The method employed is based on Buot’s SFLWT-NEGF formalism [8]. It seems more direct and natural for calculating the IQHE. It bypasses the use of linear response theory and Kubo formula for the current-current correlation which is based on time-dependent perturbation, thus the need to take the \(\omega \rightarrow 0\) limit. We believe that this is the first time that real-time SFLWT-NEGF quantum transport formalism is demonstrated to yield the topological invariants of condensed matter systems. In another publication [12], the real-time SFLWT-NEGF multi-spinor quantum transport equations are able to predict various entanglements leading to different topological phases of low-dimensional and nanostructured gapped condensed matter systems.

Acknowledgement 1 The author is grateful for the support of the Balik Scientist Program of the Philippine Council for Industry, Energy and Emerging Technology Research and Development (PCIEERD), Department of Science and Technology (DOST) and for the hospitality of the USC Department of Physics as a Visiting Professor.

References

[1] D. J. Thouless, M. Kohmoto, M. P. Nightingale, and M. den Nijs, Quantized Hall Conductance in a Two-Dimensional Periodic Potential, Phys. Rev. Lett. 49, (6), 405 (1982).
[2] P. Streda, Quantised Hall effect in a two-dimensional periodic potential, J. Phys. C: Solid State Phys. 15 L1299 (1982).
[3] R. B. Laughlin, Quantized Hall conductivity in two dimension, Phys. Rev. B 23, 5632 (1981)
[4] B. I. Halperin, Quantized Hall conductance, current-carrying edge states, and the existence of extended states in a two-dimensional disordered potential, Phys. Rev. B 25, 2185 (1982).
[5] K. von Klitzing, G. Dorda, and M. Pepper, A New Method for High-Accuracy Determination of the Fine–Structure Constant Based on Quantized Hall Resistance, Phys. Rev. Lett, 45, 494 (1980).
[6] F.A. Buot, "Zener Effect", in Encyclopedia of Electrical and Electronics Engineering, Ed. John Webster, Vol. 23, pp. 669-688 (John Wiley, NY 1999). Wiley Online Library 2000 John Wiley & Sons, Inc.
[7] G. H. Wannier, "Dynamics of Band Electrons in Electric and Magnetic Fields", Rev. Mod. Phys. 34, 645 (1962).

[8] Felix A. Buot, "Nonequilibrium Quantum Transport Physics in Nanosystems" (World Scientific, 2009) and references therein.

[9] F. A. Buot, Method for Calculating $\text{Tr}H^n$ in Solid-State Theory, Phys. Rev. B10, 3700 (1974).

[10] F. A. Buot and K. L. Jensen, "Lattice Weyl-Wigner Formulation of Exact Many-Body Quantum Transport Theory and Applications to Novel Quantum-Based Devices", Phys. Rev. B42, 9429-9456 (1990).

[11] N. B. Schade, D. I. Schuster, and S. R. Nagel, A nonlinear, geometric Hall effect without magnetic field, PNAS December 3, 2019 116 (49) 24475-24479; first published November 18, 2019.

[12] F. A. Buot, K. B. Rivero, R. E. S. Otadoy, Generalized nonequilibrium quantum transport of spin and pseudospins: Entanglements and topological phases, Physica B: Condensed Matter 559 42–61 (2019)