

dc conductivity as a geometric phase

Balázs Hetényi
Department of Physics
Bilkent University

TR-06800 Bilkent, Ankara, Turkey
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The zero frequency conductivity (D_c), the criterion to distinguish between conductors and insulators is expressed in terms of a geometric phase. D_c is also expressed using the formalism of the modern theory of polarization. The tenet of Kohn [*Phys. Rev.* **133** A171 (1964)], namely, that insulation is due to localization in the many-body space, is refined as follows. Wavefunctions which are eigenfunctions of the total current operator give rise to a finite D_c and are therefore metallic. These states are also delocalized. Based on the value of D_c it is also possible to distinguish purely metallic states from states in which the metallic and insulating phases coexist. Several examples which corroborate the results are presented, as well as a numerical implementation. The formalism is also applied to the Hall conductance, and the quantization condition for zero Hall conductance is derived to be $\frac{e\Phi_B}{Nhc} = \frac{Q}{M}$, with Q and M integers.

I. INTRODUCTION

What makes conductors conducting and insulators insulating? In classical physics this question is answered by considering the localization of *individual* charge carriers. Localized, bound charges do not contribute to conduction. Quantum mechanics has rendered the answering of this question more difficult. In band theory, conduction can be attributed to the density of electron states at the Fermi level: if $\rho(\epsilon_F) \neq 0$, the system is conducting, if $\rho(\epsilon_F) = 0$ it is insulating. However, simple band theory is not able to explain insulation of strongly correlated systems. In 1964 Kohn suggested [1] that the criterion that distinguishes metals from insulators is localization of the *total position* of all charge carriers. Kohn also derived [1] the quantum criterion of dc conductivity, the Drude weight (D_c).

For several decades, testing Kohn's hypothesis was difficult, due to the fact that in crystalline systems (systems with periodic boundary conditions) the total position operator is ill-defined. This limitation was overcome by the modern theory of polarization [2–5], in which the expectation value of the total position is cast in terms of a geometric phase [6–8]. The geometric phase arises upon varying the crystal momentum across the Brillouin zone. In numerical applications the polarization is easiest to calculate in terms of the ground state expectation value of the total momentum shift operator [9, 10]. These developments have simplified the calculation of the polarization considerably, and are now in widespread use in electronic structure calculations.

Mouloupoulos and Ashcroft [11] have also suggested a connection between conduction and a Berry phase related to the center of mass. Recently, the author has shown [12] that the total current can be expressed as a phase associated with moving the total position across the periodic cell, and that it can be written as a ground state expectation value of the total position shift operator. We note that topological invariants can also characterize metals [13] as well as insulators.

II. PURPOSE

We demonstrate that D_c can also be expressed in terms of a geometric phase. The formal expression for D_c derived here consists of an expectation value of single-body operators and a geometric phase arising from the variation of the total momentum *and* the total position. Its form is similar to that of the Hall conductance [14]. The second term is also expressed in terms of the total momentum and total position shift operators, in other words, based on a formalism similar to that of the “modern” theory of polarization. The resulting formula establishes the precise connection between localization and conductivity as suggested by Kohn [1]. If the ground state wavefunction of a system is an eigenstate of the total current operator, D_c is finite. Such wavefunctions are also delocalized according to the criterion defined by Resta [9, 10]. The calculation of the Drude weight is also straightforward: for metals the $D_c = \frac{\pi\alpha}{L}$. (Eq. (6), where L denotes the size of the system), for insulators it is zero. For wavefunctions corresponding to coexistence between metallic and insulating phases it holds that $0 < D_c < \frac{\pi\alpha}{L}$. One calculates the spread in total current, and if this spread is zero, then $D_c = \frac{\pi\alpha}{L}$. These results are independent of dimensionality. The formalism is also used to derive the Hall conductance [14], and a quantization condition for that quantity being zero is derived. The condition coincides with the well-known experimental results for the fractional quantum Hall effect [15].

III. DEFINITIONS

Let $|\Psi\rangle$ denote the ground state wavefunction of an N particle system. In coordinate space one can write $\Psi(x_1 + X, \dots, x_N + X)$ where X denotes a shift of all coordinates, or equivalently one can write in momentum space $\Psi(k_1 + K, \dots, k_N + K)$. A wavefunction can be labeled by X or K ($|\Psi(X)\rangle$, $|\Psi(K)\rangle$). One can define

the shift operators in position or momentum space as

$$\begin{aligned} e^{-i\Delta K \hat{X}} |\Psi(K)\rangle &= |\Psi(K + \Delta K)\rangle \\ e^{-i\Delta X \hat{K}} |\Psi(X)\rangle &= |\Psi(X + \Delta X)\rangle, \end{aligned} \quad (1)$$

where $\hat{X} = \sum_{i=1}^N \hat{x}_i$, and $\hat{K} = \sum_{i=1}^N \hat{k}_i$. In lattice models the current operator in momentum space takes the form $\hat{K} = \sum_{i=1}^N \sin(\hat{k}_i)$. The explicit construction of the shift operators is given in Refs. [12, 16].

IV. MAIN RESULTS

A. Conductivity as a geometric phase

The Drude weight [1] is defined as

$$D_c = \frac{\pi}{L} \frac{\partial^2 E(0)}{\partial \Phi^2}, \quad (2)$$

where Φ denotes a perturbing field, and the derivative is the adiabatic derivative. The second derivative with respect to Φ can be expressed as

$$\frac{\partial^2 E(0)}{\partial \Phi^2} = \alpha + \gamma, \quad (3)$$

where

$$\alpha = i \sum_j^N \langle \Psi | [\hat{\partial}_{k_j}, \hat{\partial}_{x_j}] | \Psi \rangle, \quad (4)$$

and where

$$\gamma = -\frac{i}{2\pi} \int_{-\pi/L}^{\pi/L} \int_0^L dK dX \quad (5)$$

$$(\langle \partial_K \Psi(K, X) | \partial_X \Psi(K, X) \rangle - \langle \partial_X \Psi(K, X) | \partial_K \Psi(K, X) \rangle).$$

This expression is derived in Appendix B. γ has the form of an integrated Berry curvature over a surface in the two-dimensional space $K - X$, and can be converted into a geometric phase by application of the Stokes theorem. Note that the Drude weight is the sum of two terms, one proportional to the sum of the commutators of each momentum and position, and a “commutator” of the variables related to the total position and total momentum of the system.

B. Analog of D_c based on the modern theory of polarization

D_c , in particular the term γ , can also be expressed using total momentum and total position shift operators. For charge carriers with mass one, the one-body term is

$$\alpha = \begin{cases} N & \text{for continuous models,} \\ -\frac{\langle \Psi | \hat{T}(0) | \Psi \rangle}{2} & \text{for lattice systems.} \end{cases} \quad (6)$$

the geometric phase term can be written as

$$\gamma = -\lim_{\Delta X, \Delta K \rightarrow 0} \frac{1}{\Delta X \Delta K} \left[\text{Im} \ln \frac{\langle \Psi | e^{i\Delta K \hat{X}} e^{i\Delta X \hat{K}} | \Psi \rangle}{\langle \Psi | e^{i\Delta X \hat{K}} | \Psi \rangle} + \text{Im} \ln \frac{\langle \Psi | e^{i\Delta X \hat{K}} e^{-i\Delta K \hat{X}} | \Psi \rangle}{\langle \Psi | e^{i\Delta X \hat{K}} | \Psi \rangle} \right]. \quad (7)$$

This expression is derived in Appendix C.

V. INTERPRETATION

The first term of D_c , proportional to α , is an extensive quantity, a sum over single-body operators. For any non-

trivial system it is expected to be finite. For an insulator the many-body term (proportional to γ) must cancel the single-body term.

We consider a general wavefunction of the form $\Psi(x_1, \dots, x_N)$ corresponding to an unperturbed ground state. Acting on this function with the shift operators according to the first and second terms of γ (Eq. (7)), respectively, results in

$$\begin{aligned} e^{i\Delta K \hat{X}} e^{i\Delta X \hat{K}} \Psi(x_1, \dots, x_N) &= e^{iN\Delta K \Delta X} e^{i\Delta K \sum_{i=1}^N x_i} \Psi(x_1 + \Delta X, \dots, x_N + \Delta X), \\ e^{i\Delta X \hat{K}} e^{-i\Delta K \hat{X}} \Psi(x_1, \dots, x_N) &= e^{-i\Delta K \sum_{i=1}^N x_i} \Psi(x_1 + \Delta X, \dots, x_N + \Delta X). \end{aligned} \quad (8)$$

Evaluating the scalar products, one can then show that apart from the term $e^{iN\Delta K \Delta X}$ in Eq. (8) the two terms in Eq. (7) are complex conjugates of each other. The term

$e^{iN\Delta K \Delta X}$ gives a contribution of $-N$ to the conductivity cancelling the single-body term. When this derivation is valid the system is insulating. This derivation, of course,

has limits of validity, for example, if discontinuities are present in the momentum distribution [17].

If the function $|\Psi\rangle$ is an eigenfunction of the current operator, then γ is zero, hence the system is metallic. To show this, one considers that the eigenvalue of the current operator for an unperturbed ground state is zero, which means that the total position shift operator will have no effect at all. In this case the two terms of γ are complex conjugates of each other, and their sum will have no imaginary part.

If a wavefunction is an eigenstate of the total current operator, it also follows that the system is delocalized. Indeed the localization criterion defined by Resta [9, 10] is

$$\sigma_X^2 = -\frac{2}{\Delta K^2} \text{Re} \ln \langle \Psi | e^{-i\Delta K \hat{X}} | \Psi \rangle. \quad (9)$$

The function resulting from the total momentum shift operator acting on an eigenfunction of the total current will be orthogonal to the original function, resulting in a divergent σ_X^2 .

To decide whether a particular ground state eigenfunction is an eigenfunction of the current one can calculate the spread in current [12], defined as

$$\sigma_K^2 = -\frac{2}{\Delta X^2} \text{Re} \ln \langle \Psi | e^{-i\Delta X \hat{K}} | \Psi \rangle. \quad (10)$$

If σ_K is zero then the wavefunction is indeed a current eigenstate, the system is metallic, moreover $\gamma = 0$ and the $D_c = \frac{\pi\alpha}{L}$. Otherwise the wavefunction corresponds to an insulating state. To show this one can use the fact that for an eigenfunction of the current with eigenvalue zero the expectation value $\langle \Psi | e^{-i\Delta X \hat{K}} | \Psi \rangle = 1$, must give one, but for any other case $\langle \Psi | e^{-i\Delta X \hat{K}} | \Psi \rangle < 1$. In calculating conductivity, one can also use Eq. (9), but this quantity is expected to diverge when the system becomes metallic, hence calculations based on σ_K can be expected to be more stable.

A wavefunction can also be a linear combination of an eigenstate of the current operator and a localized state corresponding to the coexistence of the insulating and metallic states. In this case the single body term will be partially cancelled by the many-body term and a finite Drude weight will result, but in that case D_c will be smaller than the contribution due to single-particle operators (for continuous models $D_c < N$).

VI. EXAMPLES

A. Fermi sea, BCS

For both the Fermi sea and BCS wavefunctions $D_c = \frac{\pi\alpha}{L}$. The Fermi sea is diagonal in the momentum representation and corresponds to an eigenstate of \hat{K} with eigenvalue zero. A BCS wavefunction consists of a linear combination of wavefunctions with different number of particles, but all have eigenvalue of $\hat{K} = 0$, and the argument for the Fermi sea extends.

B. Gutzwiller metal

The Gutzwiller variational wavefunction was proposed to understand the Hubbard model [18–20], and is of the form

$$|\Psi_G(\tilde{\gamma})\rangle = e^{-\tilde{\gamma} \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}} |FS\rangle. \quad (11)$$

The state $|FS\rangle$ denotes the Fermi sea, out of which doubly occupied sites are projected out via the projector $e^{-\tilde{\gamma} \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}}$. This wavefunction has been shown [21, 22] to be metallic for finite values of the variational parameter $\tilde{\gamma}$, ($D_c = \frac{\alpha\pi}{L}$).

Indeed, the geometric phase term γ vanishes. To see this, consider that the shift operator $e^{i\Delta X \hat{K}}$ commutes with the projector $e^{-\tilde{\gamma} \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}}$, since shifting the position of every particle will not affect the number of doubly occupied sites [12]. Thus $e^{i\Delta X \hat{K}}$ will operate on the Fermi sea, which has eigenvalue $\hat{K}|FS\rangle = 0$, and then the same reasoning applies as in the case of the Fermi sea.

C. Baeriswyl insulating wavefunction for a spinless system

An insulating variational solution for spinless fermions on a lattice with nearest neighbor interaction (t - V model) in one dimension, is the Baeriswyl wavefunction [23], which in this case has the form

$$|\Psi_B(\tilde{\alpha})\rangle = \prod_{\text{RBZ}} [e^{-\tilde{\alpha}\epsilon_k} c_k^\dagger + e^{\tilde{\alpha}\epsilon_k} c_{k+\pi}^\dagger] |0\rangle, \quad (12)$$

where the product is over the reduced Brillouin zone. This wavefunction is easily shown to be insulating [23], hence we expect that it gives $D_c = 0$.

This can be shown readily by considering again the action of the shift operators on $|\Psi_B(\tilde{\alpha})\rangle$. The scalar products in γ evaluate to

$$\begin{aligned} \langle \Psi_B(\tilde{\alpha}) | e^{i\Delta K \hat{X}} e^{i\Delta X \hat{K}} | \Psi_B(\tilde{\alpha}) \rangle &= \prod_{\text{RBZ}} [e^{i\Delta X \sin(k+\Delta K)} e^{-\tilde{\alpha}(\epsilon_k + \epsilon_{k+\Delta K})} + e^{-i\Delta X \sin(k+\Delta K)} e^{\tilde{\alpha}(\epsilon_k + \epsilon_{k+\Delta K})}], \\ \langle \Psi_B(\tilde{\alpha}) | e^{i\Delta X \hat{K}} e^{-i\Delta K \hat{X}} | \Psi_B(\tilde{\alpha}) \rangle &= \prod_{\text{RBZ}} [e^{i\Delta X \sin(k)} e^{-\tilde{\alpha}(\epsilon_k + \epsilon_{k-\Delta K})} + e^{-i\Delta X \sin(k)} e^{\tilde{\alpha}(\epsilon_k + \epsilon_{k-\Delta K})}]. \end{aligned} \quad (13)$$

U	σ_K	$D_c \times L/\pi$	$-\frac{\langle T \rangle}{2}$	σ_X
0	0	327.95	327.95	—
1	5.8(2)	0.01154(4)	297(7)	38(4)
2	9.8(2)	0.0087(1)	233(3)	17.8(9)
3	12.8(2)	0.0066(2)	175(5)	11.7(5)
4	15.1(2)	0.0051(2)	136(5)	8.4(4)
5	16.7(3)	0.0041(2)	110(5)	6.5(3)

TABLE I. Results from diagonalization of Anderson localization model for a system with 1024 lattice sites and 512 particles. $\Delta K = \Delta X = 0.001$

Substituting into the definition of γ and taking the limits $\Delta K, \Delta X \rightarrow 0$ lead to $D_c = 0$ as expected for an insulating state. The above derivation is also valid for the mean-field spin or charge-density wave solutions of strongly correlated lattice models.

D. Anderson localized system

We have evaluated the above formula for a model which exhibits Anderson localization [24], with Hamiltonian of the form

$$H = -t \sum_i c_i^\dagger c_{i+1} + \text{H. c.} + U \sum_i \xi_i n_i, \quad (14)$$

where ξ_i is a number drawn from a uniform Gaussian distribution. By diagonalizing the Hamiltonian we have calculated the localization parameter [9, 10] for different system sizes, and have found that the larger system sizes are always more localized for finite U (results not

shown). We have also calculated the Drude weight and the quantity σ_K . The results are shown in Table I.

For the metallic state σ_K gives zero as expected, and the Drude weight is equal to minus one-half the kinetic energy. For all insulating cases the Drude weight is very near zero, in particular if one compares its magnitude to that of the kinetic energy. While one can calculate the Drude weight directly, this may be difficult in some applications, since phases have to be evaluated. However evaluating the kinetic energy and the spread in current allows the determination of the Drude weight unambiguously.

VII. HALL CONDUCTANCE

The Hall conductance can also be expressed in terms of a Berry phase [14], similar in form to the conductivity derived above (Eq. (5)). It is possible to express the Hall conductance as a ground state observable. [25, 26] Here we express it via shift operators, and derive a quantization condition for zero Hall conductance in a quantum Hall system. The momentum shift operators in this case take forms which are different from those used in expressing dc conductivity.

Our starting point is the form derived by Thouless *et al.* [14],

$$\sigma_{xy}^H = \frac{ie^2}{2\pi\hbar} \int dK_x dK_y [\langle \partial_{K_x} \Psi | \partial_{K_y} \Psi \rangle - \text{H.c.}], \quad (15)$$

which, using the formalism above converts to

$$\sigma_{xy}^H = \frac{e^2}{h} \lim_{\Delta K_x \Delta K_y \rightarrow 0} \frac{1}{\Delta K_x \Delta K_y} \left[\text{Im} \ln \frac{\langle \Psi | U_x(\Delta K_x) U_y(\Delta K_y) | \Psi \rangle}{\langle \Psi | U_y(\Delta K_y) | \Psi \rangle} + \text{Im} \ln \frac{\langle \Psi | U_y(\Delta K_y) U_x(-\Delta K_x) | \Psi \rangle}{\langle \Psi | U_y(\Delta K_y) | \Psi \rangle} \right], \quad (16)$$

where $U_x(\Delta K_x)$ and $U_y(\Delta K_y)$ are momentum shift operators in the x and y directions. Using the forms of the total momentum shift operators in Eqs. (1) (applicable when the wavefunctions can be written in the coordinate or momentum representations) we can show that in the limit $\Delta K_x, \Delta K_y \rightarrow 0$ the Hall conductivity takes the form

$$\sigma_{xy}^H = \frac{ie^2}{h} \sum_i \langle \Psi | [\hat{x}_i, \hat{y}_i] | \Psi \rangle. \quad (17)$$

Using Eq. (16) applied to a Landau state one can also derive a quantization condition for the values of the magnetic field at which σ_{xy}^H must be zero. A Landau level has the form

$$\psi(x, y) = e^{ik_x x} \phi_n(y - y_0), \quad (18)$$

where $y_0 = k_x \frac{\hbar c}{eB}$. As far as the x direction is concerned this function is neither in the momentum nor in the position representations. However, the momentum shift operators can be constructed, considering that a momentum

shift in the x -direction is also a position shift in the y direction. It is easy to check that in this case

$$U_x(\Delta K_x) = e^{i\Delta K_x x} e^{i\Delta Y k_y}, \quad (19)$$

with $\Delta Y = \Delta K_x \frac{\hbar c}{eB}$. The momentum shift in the y di-

rection remains

$$U_y(\Delta K_y) = e^{i\Delta K_y y}. \quad (20)$$

Applying the shift operators to the Landau state results in

$$\begin{aligned} U_x(\Delta K_x)U_y(\Delta K_y)\psi(x, y) &= e^{i\Delta K_y(y-y_0)} e^{i\Delta K_x x} \psi(x, y + \Delta y), \\ U_y(\Delta K_y)U_x(-\Delta K_x)\psi(x, y) &= e^{i\Delta K_y \Delta y} e^{i\Delta K_y(y-y_0)} e^{i\Delta K_x x} \psi(x, y - \Delta y), \end{aligned} \quad (21)$$

where $\Delta y = \Delta K_x \frac{\hbar c}{eB}$. If $\Delta K_x \Delta y = \Delta K_x \Delta K_y \frac{\hbar c}{eB} = 2\pi M$, with M integer, then the phase in the second of Eqs. (21) is one, and in this case taking the limits $\Delta K_x, \Delta K_y \rightarrow 0$ results in a Hall conductance of zero. We can take the momentum shifts to be $\Delta K_x = q_x \frac{2\pi}{L_x}$ and $\Delta K_y = q_y \frac{2\pi}{L_y}$, with q_x, q_y integers, which corresponds to equivalent states for the adiabatic case [27, 28] it follows that for a system with N particles the quantization condition is

$$\frac{e\Phi_B}{N\hbar c} = \frac{Q}{M}, \quad (22)$$

where Φ_B denotes the magnetic flux, and Q is an integer. Indeed, the maxima in the Hall resistivity occur [15] precisely at values of the magnetic flux given by Eq. (22).

VIII. CONCLUSION

In this work it was shown that the zero frequency conductivity can be expressed in terms of a Berry phase. Subsequently the conductivity was also expressed in terms of shift operators (total momentum and total position) leading to expressions which provide clear physical insight, as well as a good starting point for numerical work. It was argued that a metallic state is one which is the eigenstate of the total current operator. Such states were also shown to be delocalized. In this case the dc conductivity takes its maximum possible value for a given system (proportional to the number of charge carriers for continuous models). These conclusions were supported by analytic and numerical calculations on a number of examples, both metallic and insulating. If the wavefunction is a linear combination of a total current eigenstate and an insulating wavefunction then a finite dc conductivity results which is smaller than the allowed maximum. Hence, based on the value of the dc conductivity it is possible to distinguish metallic and insulating states from ones in which conducting and insulating states coexist. Subsequently the formalism was used to express the Hall conductance, and to derive the quantization condition at which the Hall conductance is zero. The condition coincides with the well-known experimental results.

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APPENDICES

APPENDIX A: Perturbed Hamiltonian

The dc conductivity [1] is proportional to the second derivative of the ground state energy with respect to the Peierls phase Φ at $\Phi = 0$. For a continuous system, taking the mass of charge carriers to be unity, the Hamiltonian has the form

$$\hat{H}(\Phi) = \sum_j \frac{(\hat{k}_j + \Phi)^2}{2} + \hat{V}, \quad (23)$$

in the case of discrete models one can write

$$\hat{H}(\Phi) = \hat{T} + \hat{V}, \quad (24)$$

with

$$\hat{T}(\Phi) = - \sum_j t e^{i\Phi} c_{j+1}^\dagger c_j + \text{H. c.} \quad (25)$$

For a detailed discussion see Refs. [1] and [29]) For both continuous and lattice Hamiltonians it holds that

$$H'(0) = i[\hat{H}, \hat{X}] = \hat{K}, \quad (26)$$

and

$$H''(0) = i[\hat{K}, \hat{X}], \quad (27)$$

where $\hat{X}(\hat{K})$ are defined as

$$\hat{X} = \sum_j \hat{x}_j \quad (28)$$

$$\hat{K} = \sum_j \hat{k}_j,$$

for continuous systems and

$$\hat{X} = \sum_j j \hat{n}_j \quad (29)$$

$$\hat{K} = -it \sum_j c_{j+1}^\dagger c_j + \text{H.c.},$$

for lattice models. One can also write $H''(0)$ as a sum of one-body operators as

$$H''(0) = -\sum_j [\hat{k}_j, \hat{\partial}_{k_j}] = -\sum_j [\hat{\partial}_{x_j}, \hat{x}_j]. \quad (30)$$

One can also show that

$$H''(0) = \begin{cases} N & \text{for continuous models,} \\ -\hat{T}(0) & \text{for lattice systems.} \end{cases} \quad (31)$$

One can expand the Hamiltonian and the ground state wavefunction up to second order as

$$\begin{aligned} H(\Phi) &\approx H(0) + \Phi H'(0) + \frac{\Phi^2}{2} H''(0) \\ |\Psi(\Phi)\rangle &\approx |\Psi(0)\rangle + \Phi |\Psi'(0)\rangle + \frac{\Phi^2}{2} |\Psi''(0)\rangle \end{aligned} \quad (32)$$

and express the second derivative of the ground state energy with respect to Φ at $\Phi = 0$ as

$$\begin{aligned} \partial_\Phi^2 E(\Phi)|_{\Phi=0} &= \langle \Phi(0) | H''(0) | \Phi(0) \rangle \\ &+ 2\langle \Phi'(0) | H'(0) | \Phi(0) \rangle + 2\langle \Phi(0) | H'(0) | \Phi'(0) \rangle. \end{aligned} \quad (33)$$

APPENDIX B: dc conductivity as a geometric phase

In this appendix the dc conductivity is derived in terms of a geometric phase. As shown in Ref. [12] the first derivative of the ground state energy with respect to Φ for a continuous Hamiltonian is given by

$$\partial_\Phi E(\Phi) = \alpha \Phi - \frac{i}{L} \int_0^L \langle \Psi(X; \Phi) | \partial_X | \Psi(X; \Phi) \rangle, \quad (34)$$

where

$$\alpha = \begin{cases} N & \text{for continuous models,} \\ -\langle \Psi | \hat{T}(0) | \Psi \rangle & \text{for lattice systems.} \end{cases} \quad (35)$$

We can set the derivative in Φ equal to the derivative in the crystal momentum, and set $\Phi = 0$. For now we will

Taking the derivative with respect to Φ and setting Φ to zero results in

$$\begin{aligned} \partial_\Phi^2 E(\Phi)|_{\Phi=0} &= \alpha - \frac{i}{L} \int_0^L dX \\ &[\langle \partial_\Phi \Psi(X) | \partial_X | \Psi(X) \rangle + \langle \Psi(X) | \partial_X | \partial_\Phi \Psi(X) \rangle]. \end{aligned} \quad (36)$$

Since Φ corresponds to a shift in the crystal momentum K the derivative with respect to Φ can be replaced with a derivative with respect to K . Subsequently an average over K can be taken, resulting in

$$\partial_\Phi^2 E(\Phi)|_{\Phi=0} = \alpha + \gamma, \quad (37)$$

with

$$\gamma = -\frac{i}{2\pi} \int_0^L \int_{-\pi/L}^{\pi/L} dX dK \quad (38)$$

$$[\langle \partial_K \Psi(X, K) | \partial_X \Psi(X, K) \rangle - \langle \partial_X \Psi(X, K) | \partial_K \Psi(X, K) \rangle].$$

The quantity γ in Eq. (37) is a surface integral over a Berry curvature, which can be converted into a line integral around the included surface via Stokes theorem, as for the Hall conductivity [14].

The quantity α can be written with the help of Eq. (30) as

$$\alpha = i \sum_j \langle \Psi | [\partial_{x_j}, \partial_{k_j}] | \Psi \rangle. \quad (39)$$

In other words the conductivity corresponds to the difference between the sum of one body commutators of the position and momenta and the commutator of the total position and total momentum.

APPENDIX C: dc conductivity in terms of shift operators

Our starting point is the current [12] written in terms of shift operators [16],

$$\partial_\Phi E(\Phi) = \alpha \Phi - \frac{1}{\Delta X} \text{Im} \ln \langle \Psi(\Phi) | e^{i\Delta X \hat{K}} | \Psi(\Phi) \rangle. \quad (40)$$

Taking the derivative with respect to Φ results in

$$\partial_\Phi E(\Phi) = \alpha + \gamma, \quad (41)$$

with

$$\gamma = \frac{1}{\Delta X} \text{Im} \left[\frac{\langle \partial_\Phi \Psi(\Phi) | e^{i\Delta X \hat{K}} | \Psi(\Phi) \rangle}{\langle \Psi(\Phi) | e^{i\Delta X \hat{K}} | \Psi(\Phi) \rangle} + \frac{\langle \Psi(\Phi) | e^{i\Delta X \hat{K}} | \partial_\Phi \Psi(\Phi) \rangle}{\langle \Psi(\Phi) | e^{i\Delta X \hat{K}} | \Psi(\Phi) \rangle} \right] \quad (42)$$

consider only the first term in Eq. (42) but the steps for the second term are essentially identical. We can write

this term as

$$\frac{1}{\Delta X \Delta K} \text{Im} \ln \left[\frac{\Delta K \langle \partial_K \Psi(0) | e^{i\Delta X \hat{K}} | \Psi(0) \rangle}{\langle \Psi(0) | e^{i\Delta X \hat{K}} | \Psi(0) \rangle} \right], \quad (43)$$

where we have divided and multiplied by ΔK . For small ΔK we can replace this term with

$$\frac{1}{\Delta X \Delta K} \text{Im} \ln \left[1 + \frac{\Delta K \langle \partial_K \Psi(0) | e^{i\Delta X \hat{K}} | \Psi(0) \rangle}{\langle \Psi(0) | e^{i\Delta X \hat{K}} | \Psi(0) \rangle} \right], \quad (44)$$

which can be converted to

$$\frac{1}{\Delta X \Delta K} \text{Im} \ln \left[\frac{\langle \Psi(\Delta K) | e^{i\Delta X \hat{K}} | \Psi(0) \rangle}{\langle \Psi(0) | e^{i\Delta X \hat{K}} | \Psi(0) \rangle} \right], \quad (45)$$

and using the total momentum shift operator results in

$$\frac{1}{\Delta X \Delta K} \text{Im} \ln \left[\frac{\langle \Psi | e^{i\Delta K \hat{X}} e^{i\Delta X \hat{K}} | \Psi \rangle}{\langle \Psi | e^{i\Delta X \hat{K}} | \Psi \rangle} \right]. \quad (46)$$

Applying exactly the same steps to the second term of Eq. (42) results in

$$\gamma = \frac{1}{\Delta X \Delta K} \left[\text{Im} \ln \left(\frac{\langle \Psi | e^{i\Delta K \hat{X}} e^{i\Delta X \hat{K}} | \Psi \rangle}{\langle \Psi | e^{i\Delta X \hat{K}} | \Psi \rangle} \right) + \text{Im} \ln \left(\frac{\langle \Psi | e^{i\Delta X \hat{K}} e^{-i\Delta K \hat{X}} | \Psi \rangle}{\langle \Psi | e^{i\Delta X \hat{K}} | \Psi \rangle} \right) \right], \quad (47)$$

which is the discretized form for the Drude weight.

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