3 The Insulating State of Matter: A Geometrical Theory

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1   Introduction

By definition, a macroscopically homogeneous material is insulating whenever its dc longitudinal conductivity vanishes, i.e., when the real symmetric part of the conductivity tensor $\sigma_{\alpha\beta}^{(+)}(\omega)$ goes to zero for $\omega \to 0$. Here and throughout Greek subscripts are Cartesian indices. For a d-dimensional system of volume L^d the conductance G equals $L^{d-2}\sigma$. When measured in klitzing^{-1} (symbol R_{K}^{-1}) conductivity is dimensionless in $d = 2$, while it has the dimensions of an inverse length in $d = 3$. We remind that $1\,R_{\mathrm{K}} = h/e^2 \simeq 25{,}813$ ohm [1].

Longitudinal conductivity is an intensive material property whose most general form can be written as

$$\sigma_{\alpha\beta}^{(+)}(\omega) = D_{\alpha\beta}\left[\delta(\omega) + \frac{i}{\pi\omega}\right] + \sigma_{\alpha\beta}^{(\text{regular})}(\omega) = \sigma_{\alpha\beta}^{(\text{Drude})}(\omega) + \sigma_{\alpha\beta}^{(\text{regular})}(\omega), \qquad (1)$$

where the constant $D_{\alpha\beta}$ goes under the name of Drude weight. The insulating behavior of a material implies that $D_{\alpha\beta} = 0$ and that the real symmetric part of $\sigma_{\alpha\beta}^{(\text{regular})}(\omega)$ goes to zero for $\omega \to 0$ at zero temperature.

Eqn. (1) will be expressed below using linear-response theory (Kubo formulas); it may include—at least in principle—disorder and correlation, but does not include any dissipative mechanisms. The conductivity obeys the f-sum rule

$$\int_0^\infty d\omega\,\mathrm{Re}\,\sigma_{\alpha\alpha}(\omega) = \frac{D_{\alpha\alpha}}{2} + \int_0^\infty d\omega\,\mathrm{Re}\,\sigma_{\alpha\alpha}^{(\text{regular})}(\omega) = \frac{\omega_{\mathrm{p}}^2}{8} = \frac{\pi e^2 n}{2m}, \qquad (2)$$

where n is the electron density and ω_{p} is the plasma frequency. For free electrons (a gas of noninteracting electrons in a flat potential) $\sigma_{\alpha\beta}^{(\text{regular})}(\omega)$ vanishes, while $D_{\alpha\beta}$ assumes the same value as in classical physics [2], i.e, $D_{\alpha\beta} = \pi e^2 (n/m)\,\delta_{\alpha\beta}$: this explains the extraordinary longevity of Drude theory, developed in the year 1900. Given eqn. (2), switching on the potential (one-body and two-body) has the effect of transferring some spectral weight from the Drude peak into the regular term.

Dissipation can be included phenomenologically in the Drude term by adopting a single-relaxation-time approximation, exactly as in the classical textbook case [2], i.e.,

$$\sigma_{\alpha\beta}^{(\text{Drude})}(\omega) = \frac{i}{\pi}\frac{D_{\alpha\beta}}{\omega + i/\tau}, \qquad (3)$$

whose $\tau \to \infty$ limit coincides with first term in the expression (1).

In the special case of a band metal (i.e., a crystalline system of non interacting electrons) $\sigma_{\alpha\beta}^{(\text{regular})}(\omega)$ is a linear-response property, which accounts for interband transitions, and is non-vanishing only at frequencies higher than a finite threshold. Instead, $D_{\alpha\beta}$ is a ground-state property which accounts for the inertia of the many-electron system in the adiabatic limit, and provides an effective value of n/m, where the free-electron value is modified by the periodic potential. After an integration by parts, $D_{\alpha\beta}$ can be equivalently expressed as a Fermi-surface integral, and acquires then the meaning of an "intraband" term [3]. As said above, the free-electron Drude weight is an upper limit for the actual value of $D_{\alpha\beta}$.

In 1964 Kohn published the milestone paper "Theory of the insulating state" [5], according to which insulators and metals differ in their ground state. Even before the system is excited by any probe, a different organization of the electrons is present in the ground state and this is the key feature discriminating between insulators and metals. Kohn's theory remained little visited for many years until the late 1990s, when a breakthrough occurred in electronic structure theory: the modern theory of polarization (for historical presentations see, e.g., Refs. [6–8]).

The many-body version of polarization theory appeared in 1998 [9]; shortly afterwards—inspired by the fact that electrical polarization discriminates qualitatively between insulators and metals— Resta and Sorella [10] provided a definition of many-electron localization rather different from Kohn's, and derived by the theory of polarization. Their program was completed soon after by Souza et al. [11] (hereafter quoted as SWM), thus providing the foundations of the modern theory of the insulating state, deeply rooted in geometrical concepts. A couple of review papers appeared in 2002 [12] and in 2011 [13]. We are going to revisit the theory here. The present viewpoint differs somewhat from the previous one; some of the results given here are original and published for the first time.

2 Linear response and conductivity

To start with, we fix our conventions about Fourier transforms

$$f(\omega) = \int_{-\infty}^{\infty} dt \; e^{i\omega t} f(t) \qquad f(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \; e^{-i\omega t} f(\omega); \tag{4}$$

different conventions can be found in the literature.

Suppose we have a general input signal $f_{\text{input}}(t)$ and the corresponding output $f_{\text{output}}(t)$, which is due to the response of a time-independent physical system. The most general linear response is given by a convolution

$$f_{\text{output}}(t) = \int_{-\infty}^{\infty} dt' \; \chi(t - t') f_{\text{input}}(t'), \tag{5}$$

where $\chi(t)$ is the generalized susceptibility. It is easily verified that $\chi(t)$ can equivalently be defined as the response an instantaneous δ-like "kick" at $t = 0$; causality implies that $\chi(t) = 0$ for $t < 0$. The convolution theorem yields

$$f_{\text{output}}(\omega) = \chi(\omega) \; f_{\text{input}}(\omega). \tag{6}$$

Within quantum mechanics at zero temperature, we define $\chi(t)$ by means of a perturbation in the Hamiltonian $\Delta \hat{H} = -\delta(t)\hat{A}$ (the "kick"), acting on the system in its ground state. The response is measured as the expectation value of another operator $\hat{B}$. Without loss of generality we simplify our notation by assuming that

$$\langle \Psi_0 | \hat{A} | \Psi_0 \rangle = 0, \quad \langle \Psi_0 | \hat{B} | \Psi_0 \rangle = 0. \tag{7}$$

Time-dependent perturbation theory leads to the Kubo formula for the generalized susceptibility, which we write in the ω domain adopting the compact notation due to Zubarev [14–16]

$$\chi(\omega) = -\langle\!\langle \hat{B}|\hat{A}\rangle\!\rangle_\omega; \tag{8}$$

$$\langle\!\langle \hat{B}|\hat{A}\rangle\!\rangle_\omega = \frac{1}{\hbar} \lim_{\eta\to 0^+} {\sum_{n\neq 0}}' \left(\frac{\langle\Psi_0|\hat{B}|\Psi_n\rangle\langle\Psi_n|\hat{A}|\Psi_0\rangle}{\omega - \omega_{0n} + i\eta} - \frac{\langle\Psi_0|\hat{A}|\Psi_n\rangle\langle\Psi_n|\hat{B}|\Psi_0\rangle}{\omega + \omega_{0n} + i\eta} \right), \tag{9}$$

where $\omega_{0n} = (E_n - E_0)/\hbar$. The positive infinitesimal η ensures causality, and we remind that

$$\lim_{\eta\to 0^+} \frac{1}{\omega \pm i\eta} = \mathcal{P}\frac{1}{\omega} \mp i\pi\delta(\omega), \tag{10}$$

where $\mathcal{P}$ indicates the principal part. We draw attention to the fact that the sign convention adopted in this chapter agrees with Zubarev [14, 15] and Chandler [17], but is opposite the one of McWeeny [16] and other textbooks.

We apply the general linear response theory by addressing an interacting N-electron system, whose most general Hamiltonian we write, in the Schrödinger representation and in Gaussian units, as

$$\hat{H}(\boldsymbol{\kappa}) = \frac{1}{2m} \sum_{i=1}^{N} \left| \mathbf{p}_i + \frac{e}{c}\mathbf{A}(\mathbf{r}_i) + \hbar\boldsymbol{\kappa} \right|^2 + \hat{V}; \tag{11}$$

the potential $\hat{V}$ includes one-body (possibly disordered) and two-body (electron-electron) contributions. Equation (11) is exact in the nonrelativistic, infinite-nuclear-mass limit. The velocity in eqn. (11) is augmented with two terms: $\mathbf{A}(\mathbf{r})$ is a vector potential of electromagnetic origin, and $\boldsymbol{\kappa}$, having the dimensions of an inverse length, is called "flux" or "twist". Setting $\boldsymbol{\kappa} \neq 0$ amounts to a gauge transformation. The electrons are confined in a cubic box of volume L^d and the eigenstates $|\Psi_n(\boldsymbol{\kappa})\rangle$ are normalized to one in the hypercube of volume L^{Nd}; we will adopt the simplifying notation $|\Psi_n(\boldsymbol{\kappa} = 0)\rangle = |\Psi_n\rangle$.

Bulk properties of condensed matter are obtained from the thermodynamic limit: $N \to \infty$, $L \to \infty$, with N/L^d constant. Since the following formulas will comprise $\boldsymbol{\kappa}$-derivatives evaluated at $\boldsymbol{\kappa} = 0$, it is important to stress that the differentiation is performed first, and the thermodynamic limit afterwards.

Two kinds of boundary conditions can be adopted for the given Hamiltonian: either periodic (PBCs) or "open" (OBCs). We briefly address the latter case first: the cubic box confines the electrons in an infinite potential well, the eigenstates $|\Psi_n(\boldsymbol{\kappa})\rangle$ are square-integrable over $\mathbb{R}^{Nd}$, and the position operator $\hat{\mathbf{r}} = \sum_i \mathbf{r}_i$ is the ordinary multiplicative operator. Within OBCs the effect of the gauge is easily "gauged away": the ground-state energy is gauge-independent, while the ground state is $|\Psi_0(\boldsymbol{\kappa})\rangle = e^{-i\boldsymbol{\kappa}\cdot\hat{\mathbf{r}}}|\Psi_0\rangle$.

We will come back below (Sec. 7) to OBCs. For the time being we adopt instead Born-von-Kàrmàn PBCs over each electron coordinate $\mathbf{r}_i$ independently, whose Cartesian components $r_{i,\alpha}$ are then equivalent to the angles $2\pi r_{i,\alpha}/L$. The potential $\hat{V}$ enjoys the same periodicity, which implies that the electric field averages to zero over the sample. As noticed by W. Kohn in 1964 [5], PBCs violate gauge invariance in the conventional sense: for instance, the ground state energy $E_0(\boldsymbol{\kappa})$ actually *depends* on $\boldsymbol{\kappa}$.

In order to address conductivity it is essential to adopt PBCs: there cannot be any steady state current within OBCs. Furthermore, since the multiplicative position $\hat{\mathbf{r}}$ is no longer a legitimate operator within PBCs [9], it is mandatory to adopt the vector-potential gauge for the macroscopic electric field $\boldsymbol{\mathcal{E}}$: the perturbation in the Hamiltonian is therefore an ω-dependent vector potential $\delta\mathbf{A}$, constant in space.

One key point is that the vector potential modifies the velocity operator. We stick to the symbol $\hat{\mathbf{v}}$ for the velocity in absence of the perturbation, and at $\kappa = 0$: this may include a *ground-state* vector potential, but not the *perturbing* one, i.e.,

$$\hat{\mathbf{v}} = \frac{1}{m}\sum_{i=1}^{N}\left[\mathbf{p}_i + \frac{e}{c}\mathbf{A}(\mathbf{r}_i)\right]. \tag{12}$$

The current carried by a generic state $|\Psi\rangle$ after the perturbation is switched on is therefore

$$\mathbf{j} = -\frac{e}{L^d}\langle\Psi|\hat{\mathbf{v}}|\Psi\rangle - \frac{e^2 N}{mcL^d}\delta\mathbf{A}. \tag{13}$$

Expansion of the Hamiltonian to first order in the perturbing vector potential $\delta\mathbf{A}$ yields

$$\Delta\hat{H} = \frac{e}{c}\delta\mathbf{A}\cdot\mathbf{v}. \tag{14}$$

If we set $\boldsymbol{\mathcal{E}}$ and $\delta\mathbf{A}$ along the β direction, the linearly induced current in the α direction is

$$j_\alpha = -\frac{e^2 N}{mcL^d}\delta A\,\delta_{\alpha\beta} - \frac{e}{L^d}\langle\langle\,\hat{v}_\alpha\,|\,\frac{e}{c}\,\delta A\,\hat{v}_\beta\rangle\rangle_\omega = -\frac{e^2}{cL^d}\left(\frac{N}{m}\delta_{\alpha\beta} + \langle\langle\hat{v}_\alpha|\hat{v}_\beta\rangle\rangle_\omega\right)\delta A(\omega), \tag{15}$$

where we are restoring the ω dependence. The term in δA^2, being constant in space, has zero matrix elements; it is also second order in $\boldsymbol{\mathcal{E}}$.

In order to arrive at the conductivity we need to express $\delta A(\omega)$ in eqn. (15) in terms of $\mathcal{E}(\omega)$. In the time domain their relationship is $\mathcal{E} = -\frac{1}{c}\partial\delta A/\partial t$; a naive integration would yield $\delta A(\omega) = -ic\mathcal{E}(\omega)/\omega$, but this violates causality. The correct integration yields:

$$\delta A(\omega) = c\mathcal{E}(\omega)\left[\frac{1}{i\omega} - \pi\delta(\omega)\right]. \tag{16}$$

Therefore the current, as expressed directly in terms of the field intensity, is

$$j_\alpha(\omega) = \sigma_{\alpha\beta}(\omega)\,\mathcal{E}_\beta(\omega) = -\frac{e^2}{L^d}\left(\frac{N}{m}\delta_{\alpha\beta} + \langle\langle\hat{v}_\alpha|\hat{v}_\beta\rangle\rangle_\omega\right)\left[\frac{1}{i\omega} - \pi\delta(\omega)\right]\mathcal{E}_\beta(\omega). \tag{17}$$

We then write the Kubo formula as

$$\langle\langle v_\alpha|v_\beta\rangle\rangle_\omega = \frac{1}{\hbar}\lim_{\eta\to 0^+}\sum_{n\neq 0}{}'\left(\frac{\mathcal{R}_{n,\alpha\beta} + i\,\mathcal{I}_{n,\alpha\beta}}{\omega - \omega_{0n} + i\eta} - \frac{\mathcal{R}_{n,\alpha\beta} - i\,\mathcal{I}_{n,\alpha\beta}}{\omega + \omega_{0n} + i\eta}\right), \tag{18}$$

$$\mathcal{R}_{n,\alpha\beta} = \text{Re}\,\langle\Psi_0|v_\alpha|\Psi_n\rangle\langle\Psi_n|v_\beta|\Psi_0\rangle, \quad \mathcal{I}_{n,\alpha\beta} = \text{Im}\,\langle\Psi_0|v_\alpha|\Psi_n\rangle\langle\Psi_n|v_\beta|\Psi_0\rangle, \tag{19}$$

where $\mathcal{R}_{n,\alpha\beta}$ is symmetric and $\mathcal{I}_{n,\alpha\beta}$ antisymmetric. The longitudinal conductivity is the symmetric part $\sigma_{\alpha\beta}^{(+)}(\omega)$ of the tensor. Upon exploiting eqn. (10) we eventually get

$$D_{\alpha\beta} = \frac{\pi e^2}{L^d}\left(\frac{N}{m}\delta_{\alpha\beta} - \frac{2}{\hbar}\sum_{n\neq 0}{}'\frac{\mathcal{R}_{n,\alpha\beta}}{\omega_{0n}}\right), \tag{20}$$

$$\text{Re }\sigma_{\alpha\beta}^{(\text{regular})}(\omega) \;=\; \frac{\pi e^2}{\hbar L^d}{\sum_{n\neq 0}}'\frac{\mathcal{R}_{n,\alpha\beta}}{\omega_{0n}}\big[\,\delta(\omega-\omega_{0n})-\delta(\omega+\omega_{0n})\,\big], \tag{21}$$

$$\text{Im }\sigma_{\alpha\beta}^{(\text{regular})}(\omega) \;=\; \frac{2e^2}{\hbar L^d}{\sum_{n\neq 0}}'\frac{\mathcal{R}_{n,\alpha\beta}}{\omega_{0n}}\frac{\omega}{\omega_{0n}^2-\omega^2}. \tag{22}$$

The two terms $\sigma_{\alpha\beta}^{(\text{Drude})}(\omega)$ and $\sigma_{\alpha\beta}^{(\text{regular})}(\omega)$ obey the Kramers-Kronig relationships *separately*; we also remind that only the longitudinal conductivity $\sigma_{\alpha\beta}^{(+)}(\omega)$ is addressed for the time being. The transverse conductivity $\sigma_{\alpha\beta}^{(-)}$ will be addressed in Secs. 6 and 9.

At any finite-size L the spectrum is discrete and the system is gapped, while in a metal the gap closes in the large-L limit. It is therefore necessary to regularize the singular sums in eqns. (20-22); this can be done in the following way [18]: One starts assuming a finite value of η in the Kubo formula, eqn. (9), with η much larger than the level spacing; then one takes the $L \to \infty$ limit first, and the $\eta \to 0^+$ limit afterwards.

The first term in the parenthesis in eqn. (20) yields the free-electron Drude weight, while the second term accounts for the (always negative) correction due to the one-body potential and to the electron-electron interaction. We have given here the Kubo formula for a many-body Hamiltonian; for independent electrons eqn. (18) is easily transformed into a double sum over occupied and unoccupied orbitals [3].

3   Drude weight

We have arrived at eqn. (20) by means of linear-response theory, while we have stressed above that $D_{\alpha\beta}$ must be regarded as a ground-state property, which measures the inertia of the many-electron system in the adiabatic limit. In order to show this, we follow W. Kohn, who in 1964 adopted the "twisted" Hamiltonian, eqn. (11). By expanding $E_0(\boldsymbol{\kappa})$ to second order one gets

$$E_0(\boldsymbol{\kappa}) \simeq \frac{N\hbar^2}{2m}\kappa^2 - \hbar\,\kappa_\alpha\kappa_\beta\,\text{Re}{\sum_{n\neq 0}}'\frac{\langle\Psi_0|\hat{v}_\alpha|\Psi_n\rangle\langle\Psi_n|\hat{v}_\beta|\Psi_0\rangle}{\omega_{0n}}; \tag{23}$$

the expansion is essentially the many-body analogue of the elementary $\mathbf{k}\cdot\mathbf{p}$ expansion for the band energy, leading to the effective mass.

By comparing eqn. (23) to (20) one immediately gets Kohn's result:

$$D_{\alpha\beta} = \frac{\pi e^2}{\hbar^2 L^d}\frac{\partial^2 E_0(\boldsymbol{\kappa})}{\partial\kappa_\alpha\partial\kappa_\beta}\bigg|_{\boldsymbol{\kappa}=0}. \tag{24}$$

We remind that it is crucial to set $\boldsymbol{\kappa} = 0$ in the derivative *before* the thermodynamic limit is taken: this ensures that we are following the ground state adiabatically [19]. In insulators the second derivative is zero: this can be proved in various ways.

In the simple case of a band metal eqn. (24) becomes the Brillouin-zone (BZ) integral [3]:

$$D_{\alpha\beta} = \pi e^2\sum_j\int_{\text{BZ}}[d\,\mathbf{k}]\,\theta(\mu-\varepsilon_{j\mathbf{k}})\,m_{j,\alpha\beta}^{-1}(\mathbf{k}), \tag{25}$$

where $[dk] = d\mathbf{k}/(2\pi)^d$, μ is the Fermi level, $\varepsilon_{j\mathbf{k}}$ are band energies, and the effective inverse mass tensor of band j is

$$m_{j,\alpha\beta}^{-1}(\mathbf{k}) = \frac{1}{\hbar^2}\frac{\partial^2\varepsilon_{j\mathbf{k}}}{\partial k_\alpha \partial k_\beta}. \tag{26}$$

4   The Resta-Sorella approach

We consider a special value $\boldsymbol{\kappa}_0 = \frac{2\pi}{L}\mathrm{e}_\alpha$, where e_α is the unit vector in any Cartesian direction. For this special $\boldsymbol{\kappa}_0$ the effect of the gauge is easily gauged away; in fact the state vector

$$|\tilde{\Psi}_0(\boldsymbol{\kappa}_0)\rangle = \mathrm{e}^{-i\boldsymbol{\kappa}_0\cdot\hat{\mathbf{r}}}|\Psi_0\rangle \tag{27}$$

obeys PBCs, and is an eigenstate of $\hat{H}(\boldsymbol{\kappa}_0)$ with eigenvalue E_0, similarly to the OBCs case. Now the issue is whether $|\tilde{\Psi}_0(\boldsymbol{\kappa}_0)\rangle$ coincides or not with the genuine $|\Psi_0(\boldsymbol{\kappa}_0)\rangle$, obtained, as said above, by following the ground state adiabatically while $\boldsymbol{\kappa}$ is switched on continuously. Eqn. (24) shows that whenever $D \neq 0$ the state $|\Psi_0(\boldsymbol{\kappa}_0)\rangle$ has an energy higher than E_0: it is therefore an excited eigenstate of $\hat{H}(\boldsymbol{\kappa}_0)$, orthogonal to $|\tilde{\Psi}_0(\boldsymbol{\kappa}_0)\rangle$. If instead $D = 0$, then the state $|\Psi_0(\boldsymbol{\kappa}_0)\rangle$ coincides—apart for a phase factor—with $|\tilde{\Psi}_0(\boldsymbol{\kappa}_0)\rangle$ (we are assuming a nondegenerate ground state):

$$\langle\tilde{\Psi}_0(\boldsymbol{\kappa}_0)|\Psi_0(\boldsymbol{\kappa}_0)\rangle = \langle\Psi_0|\mathrm{e}^{i\boldsymbol{\kappa}_0\cdot\hat{\mathbf{r}}}|\Psi_0(\boldsymbol{\kappa}_0)\rangle = 0, \quad D \neq 0, \tag{28}$$

$$\langle\tilde{\Psi}_0(\boldsymbol{\kappa}_0)|\Psi_0(\boldsymbol{\kappa}_0)\rangle = \langle\Psi_0|\mathrm{e}^{i\boldsymbol{\kappa}_0\cdot\hat{\mathbf{r}}}|\Psi_0(\boldsymbol{\kappa}_0)\rangle = \mathrm{e}^{i\gamma}, \quad D = 0. \tag{29}$$

We notice, en passant, that γ is the single-point Berry phase determining the polarization [9]; we are not discussing the issue here.

Replacing now $|\Psi_0(\boldsymbol{\kappa}_0)\rangle$ with $|\Psi_0\rangle$ we are approximating eqns. (28) and (29) to order $1/L$, i.e.,

$$|\mathfrak{z}_N| = |\langle\Psi_0|\mathrm{e}^{i\boldsymbol{\kappa}_0\cdot\hat{\mathbf{r}}}|\Psi_0\rangle| = \mathcal{O}(1/L), \quad D \neq 0, \tag{30}$$

$$|\mathfrak{z}_N| = |\langle\Psi_0|\mathrm{e}^{i\boldsymbol{\kappa}_0\cdot\hat{\mathbf{r}}}|\Psi_0\rangle| = 1 - \mathcal{O}(1/L), \quad D = 0. \tag{31}$$

The Resta-Sorella [10] localization length is defined for an isotropic system in dimension d as

$$\lambda^2 = -\frac{1}{4\pi^2 n^{2/d}}\lim_{N\to\infty} N^{2/d-1}\log|\mathfrak{z}_N|^2 = -\frac{1}{4\pi^2}\lim_{N\to\infty}\frac{L^2}{N}\log|\mathfrak{z}_N|^2, \tag{32}$$

where $n = N/L^d$ is the density. Owing to eqns. (30) and (31) the localization length diverges when $D \neq 0$ and converges to a finite limit otherwise.

A very successful application of this theory concerns the Mott transition in 1-dimensional hydrogen chains within PBCs [20, 21]. We reproduce here Fig. 1 from Ref. [20] by Stella et al. who have performed variational quantum Monte Carlo studies, up to 66 atoms. The crossover between the weakly correlated (band) metallic regime—at small a—and the strongly correlated (Mott) insulating regime—at large a—is clearly visible in both panels of Fig. 1, which indicate the transition at $a \simeq 3.5$ bohr. The bottom panel shows that the modulus of the matrix element in eqns. (30) and (31). Top panel: λ/a. Bottom panel: the modulus of the matrix element
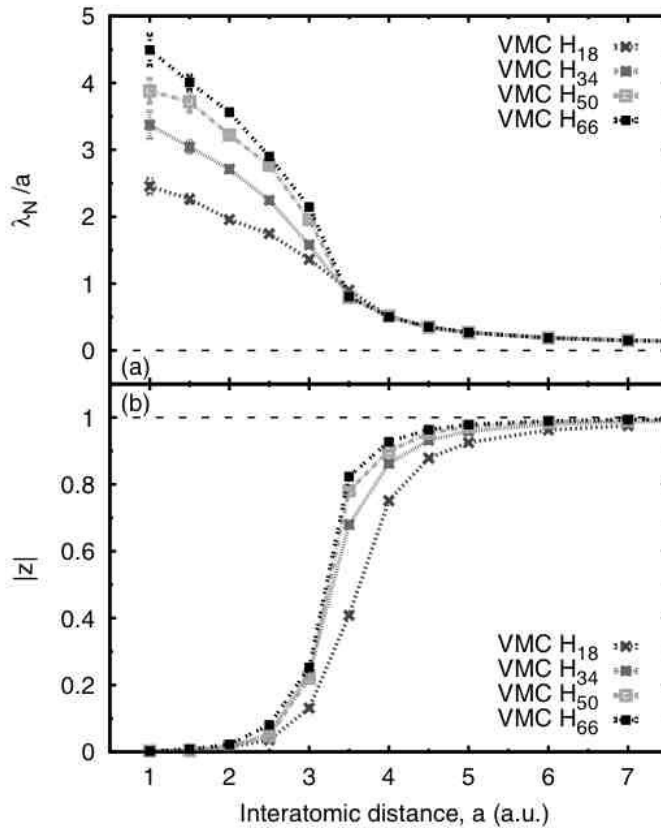
Fig. 1: *Results for chains of H atoms of different lengths as a function of the interatomic distance a, after Ref. [20]. Top panel: λ/a. Bottom panel: the modulus of the matrix element in eqns. (30) and (31).*

switches from zero to one in a narrow a region, the transition becoming sharper with increasing size. The top panel perspicuously shows that in the Mott-insulating regime λ is size-insensitive, while in the metallic regime it diverges with size. Unfortunately, the authors have chosen to plot λ/a instead of λ itself. Therefore the λ value in the large a limit cannot be verified: we expect that it goes to the isolated-atom limit, i.e., $\lambda = 1$ bohr.

5 The Souza-Wilkens-Martin sum rule (periodic boundary conditions)

The modern theory of the insulating state is also rooted in a sum rule, introduced in 2000 by SWM [11]. They define the insulating/metallic character of a homogenous material via the frequency integral

$$I_{\mathrm{SWM}} = \int_0^\infty \frac{d\omega}{\omega} \, \mathrm{Re}\, \sigma_{\alpha\alpha}(\omega); \tag{33}$$

for the sake of simplicity we address isotropic materials only. I_{SWM} converges in all insulators and diverges in all metals. In fact the integral converges at the upper limit—compare to eqn. (2)—but it diverges at the lower one whenever $D_{\alpha\alpha} \neq 0$ and also whenever $\mathrm{Re}\, \sigma_{\alpha\alpha}^{(\mathrm{regular})}(0)$ is finite. The SWM integral has instead a finite value when the system has either a spectral gap or a mobility gap. We evaluate I_{SWM} using the *regular part* only of longitudinal conductivity,

eqn. (22):

$$I_{\mathrm{SWM}} = \frac{\pi e^2}{\hbar L^d} \sideset{}{'}\sum_{n \neq 0} \frac{|\langle \Psi_0 | \hat{v}_\alpha | \Psi_0 \rangle|^2}{\omega_{0n}^2}. \tag{34}$$

The SWM integral is related by a sum rule to the quantum metric, defined according to Provost and Vallee [22], and where the relevant parameter is the twist $\boldsymbol{\kappa}$. The metric-curvature tensor at $\boldsymbol{\kappa} = 0$ is

$$\mathcal{F}_{\alpha\beta} = \frac{1}{N} \big(\langle \partial_{\kappa_\alpha} \Psi_0 | \partial_{\kappa_\beta} \Psi_0 \rangle - \langle \partial_{\kappa_\alpha} \Psi_0 | \Psi_0 \rangle \langle \Psi_0 | \partial_{\kappa_\beta} \Psi_0 \rangle \big), \tag{35}$$

where we have divided by N in order to get an intensive quantity. This tensor is real symmetric in time-reversal invariant system, and may be endowed with an antisymmetric imaginary part if time-reversal invariance is lacking. The latter feature is discussed in the next Section.

The metric tensor at $\boldsymbol{\kappa} = 0$ is the real symmetric part of $\mathcal{F}_{\alpha\beta}$:

$$g_{\alpha\beta} = \frac{1}{N} \big(\operatorname{Re} \langle \partial_{\kappa_\alpha} \Psi_0 | \partial_{\kappa_\beta} \Psi_0 \rangle - \langle \partial_{\kappa_\alpha} \Psi_0 | \Psi_0 \rangle \langle \Psi_0 | \partial_{\kappa_\beta} \Psi_0 \rangle \big); \tag{36}$$

since $g_{\alpha\beta}$ is gauge-invariant, we are going to evaluate it in the parallel-transport gauge, where

$$|\partial_{\kappa_\alpha} \Psi_0 \rangle = \hbar \sideset{}{'}\sum_{n \neq 0} |\Psi_n \rangle \frac{\langle \Psi_n | \hat{v}_\alpha | \Psi_0 \rangle}{E_0 - E_n} = -\sideset{}{'}\sum_{n \neq 0} |\Psi_n \rangle \frac{\langle \Psi_n | \hat{v}_\alpha | \Psi_0 \rangle}{\omega_{0n}}, \tag{37}$$

$$\mathcal{F}_{\alpha\beta} = \frac{1}{N} \sideset{}{'}\sum_{n \neq 0} \frac{\langle \Psi_0 | \hat{v}_\alpha | \Psi_n \rangle \langle \Psi_n | \hat{v}_\beta | \Psi_0 \rangle}{\omega_{0n}^2} = \frac{1}{N} \sideset{}{'}\sum_{n \neq 0} \frac{\mathcal{R}_{n,\alpha\beta} + i\mathcal{I}_{n,\alpha\beta}}{\omega_{0n}^2}. \tag{38}$$

From eqns. (34) and (38) we thus get

$$g_{\alpha\alpha} = \frac{\hbar}{\pi e^2 n} \int_0^\infty \frac{d\omega}{\omega} \operatorname{Re} \sigma_{\alpha\alpha}^{(\mathrm{regular})}(\omega), \tag{39}$$

where $n = N/L^d$. We observe that in eqn. (39) the l.h.s. is a ground-state property, while the r.h.s. concerns the excitations of the system.

In the insulating case $\sigma^{(\mathrm{regular})}$ coincides with the full conductivity; if ε_{g} is either the spectral gap or the mobility gap, the SWM sum rule reads

$$g_{\alpha\alpha} = \frac{\hbar}{\pi e^2 n} \int_{\varepsilon_{\mathrm{g}}/\hbar}^\infty \frac{d\omega}{\omega} \operatorname{Re} \sigma_{\alpha\alpha}(\omega). \tag{40}$$

The f-sum rule leads to the inequality:

$$g_{\alpha\alpha} < \frac{\hbar^2}{\pi e^2 n \, \varepsilon_{\mathrm{g}}} \int_{\varepsilon_{\mathrm{g}}/\hbar}^\infty d\omega \operatorname{Re} \sigma_{\alpha\alpha}(\omega) = \frac{\hbar^2}{2m\varepsilon_{\mathrm{g}}}. \tag{41}$$

From the above it becomes clear that the PBCs metric, when defined via eqn. (36), does *not* discriminate between insulators and metals: in the latter case it misses the (diverging) Drude contribution to eqn. (33). For instance, eqn. (39) vanishes for the paradigmatic metal: the free electron gas.

The author has recently shown how to remove this drawback of the PBCs metric, upon defining it in a somewhat more general way [23]. The novel metric coincides with the established one in the insulating case, but diverges in metals. The theory is incomplete, in that it only addresses independent electrons (in both the crystalline and noncrystalline cases). This recent development is reviewed in Sec. 8.

6 Many-body Chern number

The celebrated TKNN paper (Thouless, Kohmoto, Nightingale, and den Nijs) [24] explains the integer quantum Hall effect as the manifestation of a topological invariant of the electronic ground state in $2d$, the integer $C_1 \in \mathbb{Z}$, called Chern number of the first class. The choice of the sign of C_1 is not uniform across the literature: the one adopted in this Chapter is consistent with most of the recent papers.

Later Niu, Thouless, and Wu [25] addressed the fractional quantum Hall effect, where the many-body wavefunction is known to be strongly correlated. They provided a many-body definition of C_1 which, in the notations of the present work, reads:

$$C_1 = \frac{i}{2\pi} \int_0^{2\pi/L} d\kappa_x \int_0^{2\pi/L} d\kappa_y \left(\langle \partial_{\kappa_x} \Psi_0(\boldsymbol{\kappa}) | \partial_{\kappa_y} \Psi_0(\boldsymbol{\kappa}) \rangle - \langle \partial_{\kappa_y} \Psi_0(\boldsymbol{\kappa}) | \partial_{\kappa_x} \Psi_0(\boldsymbol{\kappa}) \rangle \right). \tag{42}$$

Since the $L \to \infty$ is implicit in the definition, we observed in Ref. [26] that the mean-value theorem yields

$$C_1 = \frac{i}{2\pi} \left(\frac{2\pi}{L} \right)^2 \left(\langle \partial_{\kappa_x} \Psi_0 | \partial_{\kappa_y} \Psi_0 \rangle - \langle \partial_{\kappa_y} \Psi_0 | \partial_{\kappa_x} \Psi_0 \rangle \right). \tag{43}$$

This is clearly proportional to the imaginary part of the metric-curvature tensor, as defined in eqn. (35):

$$C_1 = -4\pi n \operatorname{Im} \mathcal{F}_{xy}, \tag{44}$$

where $n = N/L^2$ is the $2d$ density. A minor detail is worth mentioning: the ground-state wavefunction is a singlet state in the previous Section, while it is instead spin-polarized in the quantum-Hall regime.

The main result by Niu, Thouless, and Wu is the expression of the quantized Hall conductivity in terms of the many-body Chern number C_1. From eqns. (17) and (18) one gets

$$\operatorname{Re} \sigma_{xy}^{(-)}(\omega) = -\frac{e^2}{\omega L^2} \operatorname{Im} \langle\!\langle v_x | v_y \rangle\!\rangle_\omega = -\frac{2e^2}{\hbar L^2} \sum_{n \neq 0}{}' \frac{\mathcal{I}_{n,xy}}{\omega^2 - \omega_{0n}^2}, \tag{45}$$

and from eqns. (38) and (44) the final result is

$$\operatorname{Re} \sigma_{xy}^{(-)}(0) = \frac{2e^2 n}{\hbar} \operatorname{Im} \mathcal{F}_{xy} = -\frac{e^2}{h} C_1. \tag{46}$$

7 Bounded samples within open boundary conditions

At variance with the PBCs results presented in Sec. 5, the OBCs metric *does* carry the information to discriminate between insulators and metals. As said above, within OBCs the twist is easily gauged away and one has $|\Psi_0(\boldsymbol{\kappa})\rangle = \mathrm{e}^{-i\boldsymbol{\kappa}\cdot\hat{\mathbf{r}}}|\Psi_0\rangle$, where $\hat{\mathbf{r}} = \sum_i \mathbf{r}_i$ is the ordinary position operator, well defined within OBCs.

It is expedient to adopt a $\boldsymbol{\kappa}$-dependent phase factor and write instead:

$$|\Psi_0(\boldsymbol{\kappa})\rangle = \mathrm{e}^{-i\boldsymbol{\kappa}\cdot(\hat{\mathbf{r}}-\mathbf{d})}|\Psi_0\rangle, \quad \mathbf{d} = \langle \Psi_0 | \hat{r} | \Psi_0 \rangle. \tag{47}$$

The gauge-invariant metric, eqn. (36), takes then the form

$$\tilde{g}_{\alpha\beta} = \frac{1}{N} \left(\langle \Psi_0 | \hat{r}_\alpha \hat{r}_\beta | \Psi_0 \rangle - \langle \Psi_0 | \hat{r}_\alpha | \Psi_0 \rangle \langle \Psi_0 | \hat{r}_\beta \Psi_0 \rangle \right), \tag{48}$$

where the different symbol emphasizes the different boundary conditions adopted for $|\Psi_0\rangle$. eqn. (48) clearly shows that $\tilde{g}_{\alpha\beta}$ is the second cumulant moment of the position, or equivalently the ground-state quantum fluctuation of polarization. The basic tenet of the modern theory of the insulating state is that the OBCs metric, eqn. (48), in the large-N limit diverges in all metals and converges in all insulators.

We are going to recast $\tilde{g}_{\alpha\beta}$ in terms of one-body and two body densities, defined as

$$n(\mathbf{r}_1) = N \sum_{\sigma_1} \int d\mathbf{x}_2 d\mathbf{x}_3 \ldots d\mathbf{x}_N |\Psi(\mathbf{x}_1, \mathbf{x}_2, \ldots \mathbf{x}_N)|^2, \tag{49}$$

$$n^{(2)}(\mathbf{r}_1, \mathbf{r}_2) = N(N-1) \sum_{\sigma_1 \sigma_2} \int d\mathbf{x}_3 \ldots d\mathbf{x}_N |\Psi(\mathbf{x}_1, \mathbf{x}_2, \ldots \mathbf{x}_N)|^2, \tag{50}$$

where $\mathbf{x}_i \equiv (\mathbf{r}_i, \sigma_i)$ are the space and spin coordinates of the i-the electron, and a singlet ground state is assumed. Straightforward manipulations lead to the equivalent form:

$$\tilde{g}_{\alpha\beta} = \frac{1}{2N} \int d\mathbf{r} d\mathbf{r}' \, (\mathbf{r} - \mathbf{r}')_\alpha (\mathbf{r} - \mathbf{r}')_\beta [\, n(\mathbf{r}) n(\mathbf{r}') - n^{(2)}(\mathbf{r}, \mathbf{r}') \,], \tag{51}$$

showing that $\tilde{g}_{\alpha\beta}$ is the second moment of the exchange-correlation hole, averaged over the sample.

We have not justified yet why the OBCs metric discriminates between insulators and metals. In a bounded sample there cannot be a steady-state current, nonetheless an oscillating field induces charge sloshing and an oscillating macroscopic current. Therefore at $\omega \neq 0$ a linear relationship of the kind $j_\alpha(\omega) = \tilde{\sigma}_{\alpha\beta}(\omega) E_\beta(\omega)$ holds. The *definition* of the insulating state, making reference to large bounded samples, is that even $\tilde{\sigma}_{\alpha\beta}(\omega)$ vanishes in the $\omega \to 0$ limit. The order of limits is crucial: first $N \to \infty$, and then $\omega \to 0$. The SWM integral bypasses this problem of limits: the insulating state requires that

$$\tilde{I}_{\text{SWM}} = \int_0^\infty \frac{d\omega}{\omega} \, \text{Re} \, \tilde{\sigma}_{\alpha\alpha}(\omega), \tag{52}$$

stays finite in the large-N limit. We stress that $\tilde{\sigma}_{\alpha\beta}(\omega)$ differs from the genuine longitudinal conductivity $\sigma_{\alpha\beta}^{(+)}(\omega)$ in two respects: it lacks the Drude peak, and it includes contributions from the sample boundary. The latter feature enters the Kubo formula by means of the matrix elements.

We are going to relate $\tilde{I}_{\text{SWM}}$ to the OBCs metric $\tilde{g}_{\alpha\beta}$. To this aim we start converting $\tilde{g}_{\alpha\beta}$ into a sum-over-states form. Using again eqn. (37), we get an expression identical in form to eqn. (38), i.e.,

$$\tilde{g}_{\alpha\beta} = \frac{1}{N} {\sum_{n \neq 0}}' \frac{\langle \Psi_0 | \hat{v}_\alpha | \Psi_n \rangle \langle \Psi_n | \hat{v}_\beta | \Psi_0 \rangle}{\omega_{0n}^2}; \tag{53}$$

the key point is that the velocity matrix elements therein are *very different*, owing to the different boundary conditions. Addressing once more the extreme case of the free electron gas, all matrix elements in eqn. (38) vanish (by an obvious selection rule); they don't vanish for a bounded sample within OBCs, as in eqn. (53).

Within OBCs we may safely adopt the scalar potential gauge, where $\tilde{\sigma}$ has the compact expression

$$\tilde{\sigma}_{\alpha\beta}(\omega) = -\frac{e^2}{L^3} \langle\!\langle \hat{v}_\alpha | \hat{r}_\beta \rangle\!\rangle_\omega \tag{54}$$

in Zubarev's notations. The matrix elements of $\hat{\mathbf{r}}$ are converted into the matrix elements of $\hat{v}$ by means of the commutator $[\hat{H}, \hat{\mathbf{r}}]$, i.e., $\langle\Psi_0|\hat{\mathbf{r}}|\Psi_n\rangle = i\langle\Psi_0|\hat{\mathbf{v}}|\Psi_n\rangle/\omega_{0n}$, to obtain

$$\text{Re}\,\tilde{\sigma}_{\alpha\alpha}(\omega) = \frac{e^2\pi}{\hbar L^3} \sideset{}{'}\sum_{n\neq 0} \frac{|\langle\Psi_0|\hat{v}_\alpha|\Psi_n\rangle|^2}{\omega_{0n}} [\,\delta(\omega - \omega_{0n}) + \delta(\omega - \omega_{0n})\,], \tag{55}$$

leading to the OBCs version of the SWM sum rule

$$\tilde{g}_{\alpha\alpha} = \frac{\hbar}{\pi e^2 n} \int_0^\infty \frac{d\omega}{\omega}\,\text{Re}\,\tilde{\sigma}_{\alpha\alpha}(\omega). \tag{56}$$

Once more, eqns. (55) and (56) are identical in form to their PBCs counterpart, eqns. (21) and (39), but their physical content—as well as their defining quantities—are very different in the metallic case. For instance, $\tilde{\sigma}_{\alpha\beta}(\omega)$ by itself obeys the f-sum rule, while $\sigma^{(\text{regular})}_{\alpha\beta}(\omega)$ does not: see eqn. (2).

In the insulating case, instead, the PBCs conductivity $\sigma(\omega)$ coincides with the OBCs one $\tilde{\sigma}(\omega)$. It follows that the (finite) metric $\tilde{g}_{\alpha\alpha}$ coincides with $g_{\alpha\alpha}$ and obeys the SWM sum rule in the form of eqn. (40). This can be proved in various ways; the basic feature is that the macroscopic polarization $P_\alpha(\omega)$ linearly induced by an oscillating field stays finite for $\omega \to 0$ in insulating materials, and can therefore be evaluated using either OBCs or PBCs, in any gauge.

Finally, we observe that the l.h.s. of eqn. (56) is a ground-state quantum fluctuation, while the r.h.s. is a property of the system *excitations*. Eqn. (56) belongs then to the general class of fluctuation-dissipation theorems.

8   Independent electrons

Owing to eqn. (51), in the noninteracting case the OBCs metric $\tilde{g}_{\alpha\beta}$ is expressed in terms of the one-body density matrix as $\rho(\mathbf{r}, \mathbf{r}') = 2\langle\mathbf{r}|\mathcal{P}|\mathbf{r}'\rangle$ as

$$\tilde{g}_{\alpha\beta} = \frac{1}{N} \int d\mathbf{r} d\mathbf{r}'\, (\mathbf{r} - \mathbf{r}')_\alpha (\mathbf{r} - \mathbf{r}')_\beta\,|\langle\mathbf{r}|\mathcal{P}|\mathbf{r}'\rangle|^2. \tag{57}$$

As said above, the convergence/divergence of $\tilde{g}_{\alpha\beta}$ in the large-N limit discriminates between electrons and metals. For instance, the well known $\mathcal{P}$ expression for the free-electron gas [27], when inserted in eqn. (57), yields a diverging $\tilde{g}_{\alpha\beta}$ in $d = 1$, 2, and 3. This is what is expected in a metal, and is in sharp contrast with the OBCs metric $g_{\alpha\beta}$ which—if defined as in eqn. (36)—vanishes. The difference is to be ascribed to the different order of limits. In this Section we are going to provide a more general definition of the OBCs metric $g_{\alpha\beta}$, which coincides with eqn. (36) in the insulating case, but has the virtue of diverging in the metallic case.

Crystalline systems

Besides the electron-gas case, where $\mathcal{P}$ is known analytically, simulations for model noninteracting systems within OBCs have indeed demonstrated the large-N divergence of the OBCs metric $\tilde{g}$, eqn. (58), in the metallic case [28, 29]. Simulations and heuristic arguments altogether suggest that the metallic divergence of $\tilde{g}$ is of order of the linear dimension L of the system in $d = 1, 2$, or 3.

The PBCs metric $g_{\alpha\beta}$, as defined so far, *does not* diverge in the metallic case and requires therefore a somewhat different definition in order to acquire the same desirable feature. The novel definition provided here follows Ref. [23].

In the crystalline case the PBCs ground-state projector $\mathcal{P}$ is

$$\mathcal{P} = V_{\text{cell}} \sum_j \int_{\text{BZ}} [d\,\mathrm{k}]\, \theta(\mu - \varepsilon_{j\mathbf{k}}) |\psi_{j\mathbf{k}}\rangle\langle\psi_{j\mathbf{k}}|, \tag{58}$$

where BZ is the Brillouin-zone, $|\psi_{j\mathbf{k}}\rangle = \mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}}|u_{j\mathbf{k}}\rangle$ are the Bloch states (normalized to one over the unit cell of volume V_{cell}), $\varepsilon_{j\mathbf{k}}$ are the band energies, μ is the Fermi level, the integration is over $[d\,\mathrm{k}] = d\mathbf{k}/(2\pi)^d$, and d is the dimension. We recast eqn. (58) in terms of Bloch projectors $\mathcal{P}_{\mathbf{k}}$ as

$$\langle\mathbf{r}|\mathcal{P}|\mathbf{r}'\rangle = V_{\text{cell}} \int_{\text{BZ}} [d\,\mathrm{k}]\, \mathrm{e}^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}\langle\mathbf{r}|\mathcal{P}_{\mathbf{k}}|\mathbf{r}'\rangle, \qquad \mathcal{P}_{\mathbf{k}} = \sum_j \theta(\mu - \varepsilon_{j\mathbf{k}}) |u_{j\mathbf{k}}\rangle\langle u_{j\mathbf{k}}|, \tag{59}$$

and we choose a gauge which makes $|u_{j\mathbf{k}}\rangle$ smooth on the whole BZ: this is always possible, even in topologically nontrivial materials. The Bloch projectors $\mathcal{P}_{\mathbf{k}}$ are gauge-invariant in the generalized Marzari-Vanderbilt sense [30, 31], i.e., they are invariant for any unitary transformation of the occupied $|u_{j\mathbf{k}}\rangle$ at the given $\mathbf{k}$.

The BZ integrand is smooth in insulators, and only piecewise continuous in metals. In the latter case, the sharpness of the Fermi surface is responsible for the power-law decay of $\langle\mathbf{r}|\mathcal{P}|\mathbf{r}'\rangle$ for $|\mathbf{r} - \mathbf{r}'| \to \infty$; the decay is instead quasi-exponential (i.e. exponential times a power) in insulators [32].

The ground-state projector is lattice-periodic, i.e.,

$$\langle\mathbf{r}|\mathcal{P}|\mathbf{r}'\rangle = \langle\mathbf{r} + \mathbf{R}|\mathcal{P}|\mathbf{r}' + \mathbf{R}\rangle, \tag{60}$$

where $\mathbf{R}$ is a lattice translation. Therefore in the large-N limit the crystalline form of eqn. (57) is

$$\tilde{g}_{\alpha\beta} = \frac{1}{N_{\text{c}}} \int_{\text{cell}} d\mathbf{r} \int_{\text{all space}} d\mathbf{r}'\, (\mathbf{r} - \mathbf{r}')_\alpha (\mathbf{r} - \mathbf{r}')_\beta\, |\langle\mathbf{r}|\mathcal{P}|\mathbf{r}'\rangle|^2, \tag{61}$$

where N_{c} is the number of electrons per crystal cell.

Next we are going to address the PBCs metric $g_{\alpha\beta}$, starting with the insulating case, where it coincides with the OBCs metric $\tilde{g}_{\alpha\beta}$ and obeys the SWM sum rule in the form of eqn. (40). The number of occupied bands is $N_{\text{c}}/2$, independent of $\mathbf{k}$. A well known result, first shown in Ref. [33], is

$$g_{\alpha\beta} = \frac{2}{n} \int_{\text{BZ}} [d\,\mathrm{k}]\, \mathrm{Re}\, \mathcal{F}_{\alpha\beta}(\mathbf{k}), \tag{62}$$

where n is the electron density and $\mathcal{F}_{\alpha\beta}(\mathbf{k})$ is the $\mathbf{k}$-dependent metric-curvature tensor [22, 30, 31, 33]:

$$\mathcal{F}_{\alpha\beta}(\mathbf{k}) = \sum_{j=1}^{N_c/2} \langle \partial_{k_\alpha} u_{j\mathbf{k}} | \partial_{k_\beta} u_{j\mathbf{k}} \rangle - \sum_{j,j'=1}^{N_c/2} \langle \partial_{k_\alpha} u_{j\mathbf{k}} | u_{j'\mathbf{k}} \rangle \langle u_{j'\mathbf{k}} | \partial_{k_\beta} u_{j\mathbf{k}} \rangle. \tag{63}$$

The BZ integral in the r.h.s. of eqn. (62) made its first appearance in the Marzari-Vanderbilt theory of maximally localized Wannier function, where it provides the gauge-invariant term in the quadratic spread, universally indicated as Ω_I in the literature. The relationship is [30, 31]:

$$\Omega_\mathrm{I} = V_\mathrm{cell} \int_\mathrm{BZ} [d\,\mathbf{k}] \; \sum_\alpha \mathcal{F}_{\alpha\alpha}(\mathbf{k}) = \frac{N_c}{2} \sum_\alpha g_{\alpha\alpha}. \tag{64}$$

Notice that the original definition of Ω_I is not intensive.

Following Ref. [23] the PBCs metric of a band insulator, eqn. (62), can be recast in a compact trace form, which has the virtue of showing gauge invariance explicitly. A tedious calculation shows that

$$\mathcal{F}_{\alpha\beta}(\mathbf{k}) = \mathrm{Tr}\left\{ \mathcal{P}_\mathbf{k} (\partial_{k_\alpha} \mathcal{P}_\mathbf{k})(\partial_{k_\beta} \mathcal{P}_\mathbf{k}) \right\}. \tag{65}$$

We may extend the definition of eqns. (62) and (65) to the metallic case as well, noticing that the $\mathbf{k}$-derivative of the Bloch projector acquires a singular δ-like term at the Fermi level:

$$\partial_{k_\alpha} \mathcal{P}_\mathbf{k} = -\sum_j \delta(\mu - \varepsilon_{j\mathbf{k}}) \partial_{k_\alpha} \varepsilon_{j\mathbf{k}} \, |u_{j\mathbf{k}}\rangle\langle u_{j\mathbf{k}}| + \sum_j \theta(\mu - \varepsilon_{j\mathbf{k}})(|u_{j\mathbf{k}}\rangle\langle \partial_{k_\alpha} u_{j\mathbf{k}}| + |\partial_{k_\alpha} u_{j\mathbf{k}}\rangle\langle u_{j\mathbf{k}}|). \tag{66}$$

In the insulating case the singularity vanishes, and we thus retrieve the previous result, while the squared δ, when inserted into eqn. (62), provides the sought for divergence.

The second term in eqn. (66) is smooth in insulators; instead it is only piecewise continuous— and therefore integrable—in metals. If eqn. (62) is evaluated using this term *only*, we retrieve the nondivergent SWM sum rule in the PBCs form of eqn. (39).

Noncrystalline systems

The OBCs metric, eqn. (58), has been implemented to study the metal-insulator (Anderson) transition in disordered systems. It is well known that in $1d$ any amount of (uncorrelated) disorder yields an insulating ground state. OBCs simulations over a lattice model in $1d$ have shown that the system has no spectral gap but eqn. (58) converges nonetheless to a finite value in the large-N limit [28].

In $3d$ matters are different: a genuine metal-insulator transition may occur. The integral in eqn. (57) converges whenever $\langle \mathbf{r} | \mathcal{P} | \mathbf{r}' \rangle$ is exponential in $|\mathbf{r} - \mathbf{r}'|$ (as in crystalline insulators), as well as when $|\langle \mathbf{r} | \mathcal{P} | \mathbf{r}' \rangle|^2$ decays as $|\mathbf{r} - \mathbf{r}'|^{-a}$, with $a > 5$. A detailed study of the Anderson transition on a paradigmatic lattice model, based on eqn. (57), has recently appeared [34]. This confirms that the OBCs metric is an alternative tool with respect to the ones currently adopted in the literature. The standard computational methods to address the Anderson transition are often peculiar to lattice models (recursive methods and the like) [35], while our approach has a

general ab-initio formulation and could in principle be applied to realistic disordered materials by standard electronic structure methods.

A novel approach to disordered and macroscopically inhomogeneous systems (such as hetero-junctions) has been proposed in Ref. [23]. We recast here the PBCs metric in trace form, i.e.,

$$g_{\alpha\beta} = \frac{2}{n} \operatorname{Re} \int_{\mathrm{BZ}} [d\,\mathrm{k}] \operatorname{Tr} \{ \mathcal{P}_{\mathbf{k}} (\partial_{k_\alpha} \mathcal{P}_{\mathbf{k}}) (\partial_{k_\beta} \mathcal{P}_{\mathbf{k}}) \}. \tag{67}$$

We are going to show that eqn. (67) can be equivalently cast in a form where any explicit reference to lattice periodicity disappears.

In order to arrive at such a transformation, we start noticing that the integrand in eqn. (58) is periodical over the reciprocal lattice, and therefore the BZ integral of its $\mathbf{k}$-gradient vanishes:

$$i(\mathbf{r} - \mathbf{r}')\langle \mathbf{r}|\mathcal{P}|\mathbf{r}'\rangle + V_{\mathrm{cell}} \int_{\mathrm{BZ}} [d\,\mathrm{k}] \, \mathrm{e}^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')} \langle \mathbf{r}|\partial_{\mathbf{k}}\mathcal{P}_{\mathbf{k}}|\mathbf{r}'\rangle = 0; \tag{68}$$

we remind that eqn. (68) is a well behaved expression only in insulators. The first term therein is i times $[\mathbf{r}, \mathcal{P}]$: a lattice periodic operator (unlike $\mathbf{r}$ itself). The trace of eqn. (68) can therefore be cast as

$$\int_{\mathrm{BZ}} [d\,\mathrm{k}] \operatorname{Tr} \{ \partial_{k_\alpha} \mathcal{P}_{\mathbf{k}} \} = -\frac{i}{V_{\mathrm{cell}}} \int_{\mathrm{cell}} d\mathbf{r} \, \langle \mathbf{r}| \, [r_\alpha, \mathcal{P}] \, |\mathbf{r}\rangle = -i \operatorname{Tr}_V \{ [r_\alpha, \mathcal{P}] \}, \tag{69}$$

where Tr_V indicates the trace per unit volume in the Schrödinger representation.

Using similar arguments it is not difficult to prove that, for an unbounded sample within PBCs,

$$g_{\alpha\beta} = \frac{2}{n} \operatorname{Re} \int_{\mathrm{BZ}} [d\,\mathrm{k}] \operatorname{Tr} \{ \mathcal{P}_{\mathbf{k}} (\partial_{k_\alpha} \mathcal{P}_{\mathbf{k}}) (\partial_{k_\beta} \mathcal{P}_{\mathbf{k}}) \} = -\frac{2}{n} \operatorname{Re} \operatorname{Tr}_V \{ \mathcal{P} \, [r_\alpha, \mathcal{P}] \, [r_\beta, \mathcal{P}] \}. \tag{70}$$

The second expression on the r.h.s. has two outstanding virtues: (i) it is expressed directly in the Schrödinger representation, making no reference to reciprocal space, and (ii) it can be adopted as such for supercells of arbitrarily large size, thus extending the concept of PBCs metric to noncrystalline systems, such as alloys and liquids. We have not proved yet that such form can be adopted as it stands even for bounded samples within OBCs.

If we evaluate the trace per unit volume over the whole sample of volume V, eqn. (70) yields

$$g_{\alpha\beta} = -\frac{2}{N} \operatorname{Re} \operatorname{Tr} \{ \mathcal{P} \, [r_\alpha, \mathcal{P}] \, [r_\beta, \mathcal{P}] \} = \frac{2}{N} \operatorname{Tr} \{ \mathcal{P} r_\alpha r_\beta \mathcal{P} \} - \frac{2}{N} \operatorname{Tr} \{ \mathcal{P} \alpha \mathcal{P} r_\beta \mathcal{P} \}. \tag{71}$$

We have stated above that in insulators the PBCs metric $g_{\alpha\beta}$ is finite and coincides with the OBCs metric $\tilde{g}_{\alpha\beta}$: a simple calculation confirms that eqn. (71) is indeed identical to eqn. (57). Our novel approach reconciles the PBCs metric with the OBCSs one: both metrics yield the same message even in the metallic case. Looking at eqn. (70), the first expression on the r.h.s. diverges because of the sharpness of the Fermi surface embedded in eqn. (66), while the divergence of the second expression has been discussed in Sec. 7.

The next issue is whether one may adopt eqn. (70) *locally*, in order to address inhomogeneous systems: preliminary results indicate that the answer is affirmative [36]. For an isotropic system the local marker for the insulating state is the real function

$$\mathcal{L}_{\alpha\alpha}(\mathbf{r}) \propto \operatorname{Re} \langle \mathbf{r}| \, \mathcal{P} \, [r_\alpha, \mathcal{P}] \, [r_\alpha, \mathcal{P}] \, |\mathbf{r}\rangle : \tag{72}$$

when averaged locally in a homogenous region of the sample it detects the insulating vs. metallic character of that region. For instance in a metal/insulator heterojunction it diverges on the metallic side and converges to a finite value on the insulating side. It therefore provides a marker complementary to the (commonly used) local density of states; at variance with it, $\mathcal{L}_{\alpha\alpha}(\mathbf{r})$ probes locally the organization of the electrons in the *ground state*, the main property that—according to the outstanding Kohn's message [5]—discriminates insulators from metals.

9 Geometry in the anomalous Hall effect

On the theory side, the anomalous Hall effect (in both insulators and metals) is closely related to the theory of the insulating state. In this section we remain at the independent-particle level. Furthermore, in agreement with the literature on the topic, we adopt a spinless-electron formalism: factors of two here will differ from the previous sections. The metric-curvature tensor for a band insulator, eqn. (63), is rewritten as

$$\mathcal{F}_{\alpha\beta}(\mathbf{k}) = \sum_{j=1}^{N_c} \langle \partial_{k_\alpha} u_{j\mathbf{k}} | \partial_{k_\beta} u_{j\mathbf{k}} \rangle - \sum_{j,j'=1}^{N_c} \langle \partial_{k_\alpha} u_{j\mathbf{k}} | u_{j'\mathbf{k}} \rangle \langle u_{j'\mathbf{k}} | \partial_{k_\beta} u_{j\mathbf{k}} \rangle. \tag{73}$$

So far, we have addressed the real symmetric part of $\mathcal{F}_{\alpha\beta}(\mathbf{k})$, i.e., the $\mathbf{k}$-space metric first introduced by Marzari and Vanderbilt in the theory of maximally localized Wannier functions [30, 31]. The imaginary antisymmetric part (times -2) is the Berry curvature of the occupied manifold:

$$\Omega_{\alpha\beta}(\mathbf{k}) = -2\,\mathrm{Im}\,\mathcal{F}_{\alpha\beta}(\mathbf{k}) = i \sum_{j=1}^{N_c} \left(\langle \partial_{k_\alpha} u_{j\mathbf{k}} | \partial_{k_\beta} u_{j\mathbf{k}} \rangle - \langle \partial_{k_\beta} u_{j\mathbf{k}} | \partial_{k_\alpha} u_{j\mathbf{k}} \rangle \right). \tag{74}$$

From eqn. (65) we equivalently get

$$\Omega_{\alpha\beta}(\mathbf{k}) = i\,\mathrm{Tr}\,\{ \mathcal{P}_\mathbf{k} [\, \partial_{k_\alpha} \mathcal{P}_\mathbf{k}, \partial_{k_\beta} \mathcal{P}_\mathbf{k} \,] \}. \tag{75}$$

While this form was used in the past for the insulating case only, we stress that it holds for the metallic case as well: in fact, the singular term in eqn. (66) disappears after antisymmetrization. The key difference is that the Berry curvature of the occupied manifold is smooth in insulators and only piecewise continuous in metals: its BZ integral is well defined and finite in both cases. The anomalous Hall conductivity (AHC) is by definition the Hall conductivity in zero magnetic field; it can be nonvanishing only if the Hamiltonian lacks time-reversal symmetry. When expressed in klitzing^{-1} it is dimensionless for $d = 2$, while it has the dimensions of an inverse length for $d = 3$. The known expression for the $\omega = 0$ AHC in both metals and insulators is

$$\sigma_{\alpha\beta}^{(-)}(0) = \frac{4\pi e^2}{h} \int_{\mathrm{BZ}} [d\,\mathrm{k}]\ \mathrm{Im}\,\mathcal{F}_{\alpha\beta}(\mathbf{k}) = -\frac{e^2}{h}\frac{1}{2\pi} \int_{\mathrm{BZ}} d\mathbf{k}\ \Omega_{\alpha\beta}(\mathbf{k}), \tag{76}$$

and this expressions holds for both $d = 2$ and $d = 3$; notice the two equivalent forms, where the integral is either in $[d\,\mathrm{k}] = d\mathbf{k}/(2\pi)^d$ or in $d\mathbf{k}$.

We address the insulating case first: the AHC is quantized, and in natural units it equals minus the Chern invariant C_γ, usually defined as

$$C_\gamma = \frac{1}{4\pi} \varepsilon_{\gamma\alpha\beta} \int_{\text{BZ}} d\mathbf{k} \; \Omega_{\alpha\beta}(\mathbf{k}). \tag{77}$$

In $2d$ the Chern invariant is a dimensionless integer $\in \mathbb{Z}$. The definition of eqn. (77) coincides indeed with the Chern number C_1, as defined in Sec. 6 for a many-body wavefunction [26].

In the metallic case eqn. (76) is nonquantized: the difference owes to the fact that the Berry curvature of the occupied manifold $\Omega_{\alpha\beta}(\mathbf{k})$ is smooth in insulators and only piecewise continuous in metals.

In the metallic case eqn. (76) yields only the intrinsic (or geometric) contribution to the AHC; extrinsic contributions, known as "skew scattering" and "side jump" must be added [37]. We stress that, instead, extrinsic contributions have no effect in insulators, owing to the robustness of topological observables.

The same transformation as in eqn. (70) can be carried over for the antisymmetric imaginary part of $\mathcal{F}_{\alpha\beta}(\mathbf{k})$, leading to

$$\sigma_{\alpha\beta}^{(-)}(0) = -\frac{4\pi e^2}{h} \text{Im Tr}_V \{\mathcal{P}[r_\alpha, \mathcal{P}] [r_\beta, \mathcal{P}]\}, \tag{78}$$

where we address a possibly disordered sample, although still unbounded within PBCs. If we try to proceed analogously to what we did for the real symmetric part, by adopting eqn. (78) even for a bounded sample within OBCs and evaluating the trace over the whole sample, we get a vanishing result: the tensor entering eqns. (70) and (78) is obviously real symmetric. This stems from the fact that even the original definition of $\tilde{g}_{\alpha\beta}$, eqn. (48), is *not* endowed with an antisymmetric term.

The solution of the paradox was found in Ref. [38]. The real function

$$\mathfrak{C}(\mathbf{r}) = 4\pi \, \text{Im} \, \langle \mathbf{r} | \, \mathcal{P}[r_\alpha, \mathcal{P}] [r_\beta, \mathcal{P}] \, | \mathbf{r} \rangle \tag{79}$$

carries indeed the information which allows evaluating the AHC *locally*; but its average has to be evaluated using an inner region of the bounded sample and *not* the whole sample. The boundary provides a compensating contribution. When the bounded sample is a crystallite, one may integrate $\mathfrak{C}(\mathbf{r})$ over the central cell; this integral, divided by the cell volume (area in $2d$), provides the AHC value in the large-sample limit.

In the insulating case the function $\mathfrak{C}(\mathbf{r})$ samples the topological nature of the ground state *locally*: it has therefore been dubbed "topological marker" [38]. Simulations on a paradigmatic lattice model in $2d$ for bounded samples (crystalline and disordered) and for heterojunctions have shown that $\mathfrak{C}(\mathbf{r})$ samples indeed the local Chern number (equal to minus the Hall conductivity in natural units).

The metallic case differs from the insulating one in two important respects: (i) the macroscopic current flows across the whole sample, while it only flows at the boundaries in topological insulators; (ii) the ground-state projector entering eqn. (79) is power-law in $|\mathbf{r} - \mathbf{r}'|$, while it

is quasi-exponential in insulators (including topological insulators). Despite these differences, simulations reported in Ref. [39] demonstrate that $\mathfrak{C}(\mathbf{r})$, eqn. (79), provides in the metallic case a "geometrical marker", which allows to evaluate the geometrical contribution to the AHC locally in both homogenous and inhomogeneous samples.

The homogeneous case of a "dirty" metal deserves a comment. The trace per unit volume of $\mathfrak{C}(\mathbf{r})$ clearly includes some geometrical effects due to the impurities. It is argued that the AHC evaluated in this way may yield the sum of the intrinsic and side-jump contributions to the AHC, while instead it may not include the skew scattering [37, 40].

Ref. [39] also provides a convergence study. Therein, a metallic crystallite is addressed vs. an insulating one, and the AHC of the material is evaluated, as said above, by averaging the respective $\mathfrak{C}(\mathbf{r})$ over the central cell. The convergence to the bulk value is—as expected— exponential in the insulating case. In the metallic case the convergence is instead of the order L^{-3}, where L is the linear dimension of the sample. While the actual simulations are in $2d$, it is conjectured that the convergence is of order L^{-3} in any dimension, in analogy with what happens to the large-sample metallic divergence of the metric (of order L in any d).

Acknowledgments

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