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THE LOCALIZATION DICHOTOMY FOR PERIODIC SCHRÖDINGER OPERATORS

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The understanding of transport properties of quantum systems out of equilibrium is a crucial challenge in statistical mechanics. A long term goal is to explain the conductivity properties of solids starting from first principles, as *e.g.* from the Schrödinger equation governing the dynamics of electrons and ionic cores. While the general goal appears to be beyond the horizon, some results can be obtained for specific models, in particular for independent electrons in a periodic or random background.

As a general paradigm, in this case the electronic transport properties are related to the spectral type of the Hamiltonian and to the (de-)localization of the corresponding (generalized) eigenstates. However, when ***periodic systems*** are considered, the Hamiltonian operator has generically purely absolutely continuous spectrum [(1)]. Therefore, one needs a finer notion of localization, which allows for example to predict when a crystal, in the absence of any external magnetic field, exhibits a zero transverse conductivity, as it happens for ordinary insulators, and when a non-vanishing one, as in the case of the recently realized ***Chern insulators*** [BFK, CZK] predicted by Haldane [Hal, HK].

Our main message is that such a finer notion of localization is provided by the rate of decay of ***composite Wannier functions*** (CWF) associated to the gapped periodic Hamiltonian operator. Equipped with this notion of localization, we are able to identify two different regimes:

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(1) A remarkable exception is the well-known Landau Hamiltonian. Notice, however, that if a periodic background potential is included in the model, one is generically back to the absolutely-continuous setting.

(i) whenever the system is time-reversal (TR) symmetric, there exist exponentially localized composite Wannier functions which are associated to the Bloch bands below the Fermi energy, assuming that the latter is in a spectral gap; correspondingly, the Hall conductivity vanishes;
(ii) viceversa, as soon as the Hall conductivity is non-zero, as it happens for Chern insulators, the composite Wannier functions are delocalized.

Moreover, the relevant information to discriminate between the tworegimes is of topological nature, being provided by the the triviality of the ***Bloch bundle*** associated to the occupied states, that is, the vector bundle over the Brillouin torus whose fiber over k is spanned by the occupied Bloch states at fixed crystal momentum k.

We rigorously prove a ***Localization–Topology Correspondence***. We consider a gapped periodic (magnetic) Schrödinger operator, and we assume that the Fermi projector corresponds to a *non-trivial* (magnetic) Bloch bundle, as it may happen when TR-symmetry is broken. For example, one might think of the operators modeling Chern insulators or Quantum Hall systems. The rate of decay of composite Wannier functions changes drastically in this case, from exponential to polynomial. We prove that the ***optimal decay*** for a system $w = (w_1, \dots, w_m)$ of CWFs in a non-trivial topological phase is characterized by the divergence of the second moment of the position operator, defined as

$$\langle X^2 \rangle_w \equiv \sum_{a=1}^{m} \int_{\mathbb{R}^d} |x|^2 |w_a(x)|^2 \mathrm{d}x.$$

Heuristically, this corresponds to a power-law decay $|w_a(x)| \asymp |x|^{-\alpha}$, with $\alpha = 2$ for $d = 2$ and $\alpha = 5/2$ for $d = 3$. The former exponent was foreseen by Thouless [Th], who also argued that the exponential decay of the Wannier functions is intimately related to the vanishing of the Hall current. More precisely, we prove – under suitable technical hypothesis – the following statement:

Localization–Topology Correspondence: *Consider a gapped periodic (magnetic) Schrödinger operator. Then it is always possible to construct a system $w = (w_1, \dots, w_m)$ of CWFs for the occupied states such that*

$$\sum_{a=1}^{m} \int_{\mathbb{R}^d} |x|^{2s} \, |w_a(x)|^2 \mathrm{d}x < +\infty \qquad \textit{for every } s < 1. \tag{0.1}$$

Moreover, the following statements are equivalent:

(a) **Finite second moment:** *there exists a choice of Bloch gauge such that the corresponding CWFs $w = (w_1, \dots, w_m)$ satisfy*

$$\langle X^2 \rangle_w = \sum_{a=1}^{m} \int_{\mathbb{R}^d} |x|^2 \, |w_a(x)|^2 \mathrm{d}x < +\infty;$$

(b) **Exponential localization:** *there exists $\alpha > 0$ and a choice of Bloch gauge such that the corresponding CWFs $\widetilde{w} = (\widetilde{w}_1, \dots, \widetilde{w}_m)$ satisfy*

$$\sum_{a=1}^{m} \int_{\mathbb{R}^d} \mathrm{e}^{2\beta|x|} \, |\widetilde{w}_a(x)|^2 \mathrm{d}x < +\infty \qquad \text{for every } \beta \in [0, \alpha);$$

(c) **Trivial topology:** *the Bloch bundle associated to the occupied states is trivial.*

In case (a) holds, then there exist a sequence $\{w^{(\ell)}\}$ of systems of exponentially localized *CWFs such that $w^{(\ell)} \to w$ in $L^2(\mathbb{R}^d, \langle x \rangle^2 \mathrm{d}x)^m$ as $\ell \to \infty$.*

Our result can be reformulated in terms of the localization functional introduced by Marzari and Vanderbilt [MV, MYSV], which with our notation reads
(0.2)

$$F_{\mathrm{MV}}(w) = \sum_{a=1}^{m} \int_{\mathbb{R}^d} |x|^2 |w_a(x)|^2 \, \mathrm{d}x - \sum_{a=1}^{m} \sum_{j=1}^{d} \left(\int_{\mathbb{R}^d} x_j |w_a(x)|^2 \, \mathrm{d}x \right)^2 =: \langle X^2 \rangle_w - \langle X \rangle_w^2 .$$

In view of the first part of the statement, there always exists a system of CWFs satisfying (0.1) for fixed $s = 1/2$, so that the first moment $\langle X \rangle_w$ is finite. Hence, the Marzari–Vanderbilt functional is finite if and only if $\langle X^2 \rangle_w$ is. By the second part of the Localization–Topology Correspondence, the latter condition is equivalent to the triviality of the Bloch bundle. The result is in agreement with previous numerical and analytic investigations on the Haldane model [TV]. As a consequence, the minimization of F_{MV} is possible only in the topologically trivial case, and numerical simulations in the topologically non-trivial regime should be handled with care: we expect that the numerics become unstable when the mesh in k-space becomes finer and finer.

Further possible applications of the Localization–Topology Correspondence go beyond the realm of crystalline solids, including superfluids and superconductors [PT, TPTH], and tensor network states [Rd]. In view of that, we hope that our results will trigger new developments in the theory of superconductors and of many-body systems, and possibly in other realms of solid-state physics.

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