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Published in:
Physical Review B

Link to article, DOI:
[10.1103/PhysRevB.95.045109](https://doi.org/10.1103/PhysRevB.95.045109)

Publication date:
2017

Document Version
Publisher's PDF, also known as Version of record

[Link back to DTU Orbit](#)

Citation (APA):
Olsen, T., Resta, R., & Souza, I. (2017). Metal-insulator transition in disordered systems from the one-body density matrix. *Physical Review B*, 95(4), Article 045109. <https://doi.org/10.1103/PhysRevB.95.045109>

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Metal-insulator transition in disordered systems from the one-body density matrixThomas Olsen,^{1,2,*} Raffaele Resta,^{3,4,†} and Ivo Souza^{1,5,‡}¹*Centro de Física de Materiales, Universidad del País Vasco, 20018 San Sebastián, Spain*²*Center for Atomic-Scale Materials Design, Department of Physics, Technical University of Denmark, 2800, Kgs. Lyngby, Denmark*³*Dipartimento di Fisica, Università di Trieste, 34127 Trieste, Italy*⁴*Donostia International Physics Center, 20018 San Sebastián, Spain*⁵*Ikerbasque Foundation, 48013 Bilbao, Spain*

(Received 4 April 2016; revised manuscript received 5 December 2016; published 6 January 2017)

The insulating state of matter can be probed by means of a ground state geometrical marker, which is closely related to the modern theory of polarization (based on a Berry phase). In the present work we show that this marker can be applied to determine the metal-insulator transition in disordered systems. In particular, for noninteracting systems the geometrical marker can be obtained from the configurational average of the norm-squared one-body density matrix, which can be calculated within open as well as periodic boundary conditions. This is in sharp contrast to a classification based on the static conductivity, which is only sensible within periodic boundary conditions. We exemplify the method by considering a simple lattice model, known to have a metal-insulator transition as a function of the disorder strength, and demonstrate that the transition point can be obtained accurately from the one-body density matrix. The approach has a general *ab initio* formulation and could in principle be applied to realistic disordered materials by standard electronic structure methods.

DOI: [10.1103/PhysRevB.95.045109](https://doi.org/10.1103/PhysRevB.95.045109)**I. INTRODUCTION**

The metal-insulator transition in solid state systems is notoriously difficult to approach from a theoretical point of view. The description of the Mott transition, where the metal-insulator transition is induced by electron-electron interactions, traditionally involves explicitly correlated methods such as dynamical mean field theory (DMFT) [1]. While it is indeed possible to unravel the Mott transition in real materials [2], the application of DMFT is computationally demanding and still restricted to rather simple systems. In the case of the Anderson transition, where a metal-insulator transition is induced by disorder, the calculational probes are invariably specific to model lattice Hamiltonians [3,4], and a first principles treatment seems to be out of reach with the present theoretical tools.

Here we adopt a different and more general approach, stemming from the 1964 seminal paper by W. Kohn [5,6]. According to Kohn, the qualitative difference between insulators and conductors manifests itself in a different organization of the electrons in their many-body *ground state*. A series of more recent papers [7–10] has established Kohn’s pioneering viewpoint on a sound formal and computational basis, rooted in geometrical concepts. These developments followed (and were inspired by) the modern theory of polarization, based on a Berry phase [11,12], and we will refer to these developments altogether as the *modern theory of the insulating state* (MTIS). Its basic ingredient is the quantum metric tensor [13] as we will explain below.

The MTIS has previously been used to address the Mott transition by adopting either lattice models [7,14–16] or first-principle Hamiltonians [17,18]. To the best of our knowledge

it has never been applied to the Anderson transition in three-dimensional (3D) disordered samples. In the latter case, the tools currently in use focus on properties either of the spectrum, or of the individual Hamiltonian eigenstates [4]. In contrast, for the case of independent electrons, the only ingredient of the MTIS is the ground-state density matrix. Moreover, the MTIS unites the concepts of Anderson insulators and Mott insulators into a common framework based on the quantum metric tensor, offering the exciting possibility of studying the metal-insulator transition in cases where both disorder and electronic correlations play an important role in the transition. In principle the framework presented here can be straightforwardly implemented in any first principles electronic structure code. However, the required computations may still be too demanding for any reliable prediction of Anderson transitions in real materials.

In the present work we address a paradigmatic model: a tight-binding Hamiltonian on a 3D simple cubic lattice, with random onsite matrix elements. The Anderson transition for this model has been studied in the previous literature by means of various tools [4,19–22]. Here we show that—according to the MTIS basic tenet—the ground-state density matrix of finite samples within “open” boundary conditions (OBCs) carries the information needed to detect the metal-insulator transition.

II. THEORY

For the sake of simplicity we address isotropic systems only, whose scalar longitudinal conductivity is

$$\sigma(\omega) = \sigma'(\omega) + i\sigma''(\omega); \quad (1)$$

the real and imaginary parts σ' and σ'' obey Kramers-Kronig relationships. In a conductor, the low-frequency real part of σ takes the general form [23]

$$\sigma'(\omega) = D\delta(\omega) + \sigma'_{\text{reg}}(\omega), \quad (2)$$

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where D is the Drude weight, and the regular part $\sigma'_{\text{reg}}(\omega)$ may be nonvanishing for $\omega \rightarrow 0$. The nomenclature owes to the classical Drude theory in the dissipationless limit, where $D = \pi e^2(n/m)$; n is the carrier density and m the corresponding mass. Taking into account the Kramers-Kronig relationships and Eq. (2), we may also rewrite

$$\sigma(\omega) = D \left[\delta(\omega) + \frac{i}{\pi\omega} \right] + \sigma_{\text{reg}}(\omega), \quad (3)$$

whence the alternative definition [5,24]

$$D = \pi \lim_{\omega \rightarrow 0} \omega \sigma''(\omega). \quad (4)$$

The insulating behavior of a material implies both $D = 0$ and $\sigma'_{\text{reg}}(\omega) \rightarrow 0$ for $\omega \rightarrow 0$ at zero temperature, while in conductors one has either $D \neq 0$ (in pristine crystalline metals) or $\sigma'_{\text{reg}}(0) \neq 0$.

The Kubo formula provides the quantum-mechanical expression for $\sigma'_{\text{reg}}(\omega)$, while instead D is a ground-state property. In the special case of a pristine crystal at the independent-particle level D measures the current due to freely accelerating electrons at the Fermi surface, while $\sigma_{\text{reg}}(\omega)$ is due to interband transitions. Both terms in Eq. (3), however, have a more general meaning and are well defined even for an interacting many-body system [25]. In either case a nonvanishing static conductivity requires adopting periodic boundary conditions (PBCs) and choosing the vector-potential gauge for the electric field. Indeed there cannot be any steady-state current in a finite crystallite within OBCs. The Kubo formula for the conductivity is the standard approach for discriminating between insulating and metallic phases. However, the MTIS implies that an alternative approach is possible, as will be shown below. Notably, the difference between an insulator and a metal can be detected within either PBCs or OBCs. We will adopt the latter in the present investigation, stressing the fact that the metallic/insulating behavior is a *ground state* property that can be addressed without reference to the static conductivity.

Consider N interacting electrons in a box of volume V , with Hamiltonian (in atomic units)

$$\hat{H}(\boldsymbol{\kappa}) = \frac{1}{2} \sum_{i=1}^N (\hat{\mathbf{p}}_i + \boldsymbol{\kappa})^2 + \hat{U}, \quad (5)$$

where \hat{U} comprises one- and two-body interactions. At $\boldsymbol{\kappa} = 0$ Eq. (5) is the standard many-body Hamiltonian of the system, while setting $\boldsymbol{\kappa} \neq 0$ amounts to a gauge transformation. Such a transformation within OBCs is trivial, and can be easily “gauged away”: for instance, the ground-state energy is $\boldsymbol{\kappa}$ independent. Matters are instead nontrivial within PBCs, where the ground-state energy $E_0(\boldsymbol{\kappa})$ is in general $\boldsymbol{\kappa}$ dependent. For the sake of clarity we remind that PBCs mean that the wave function at any $\boldsymbol{\kappa}$ is periodic in the supercell of volume V in each electronic coordinate (the coordinates are indeed angles). It has been shown by Kohn [5,24] that within PBCs the Drude weight is given (for isotropic systems) by

$$D = \frac{\pi}{V} \frac{d^2 E_0(\boldsymbol{\kappa})}{d\boldsymbol{\kappa}^2} \Big|_{\boldsymbol{\kappa}=0}. \quad (6)$$

If we define the projector

$$\hat{Q}(\boldsymbol{\kappa}) = \hat{1} - |\Psi_0(\boldsymbol{\kappa})\rangle\langle\Psi_0(\boldsymbol{\kappa})|, \quad (7)$$

the quantum metric tensor [13] is

$$G_{\alpha\beta}(\boldsymbol{\kappa}) = \frac{1}{N} \text{Re} \langle \partial_{k_\alpha} \Psi_0(\boldsymbol{\kappa}) | \hat{Q}(\boldsymbol{\kappa}) | \partial_{k_\beta} \Psi_0(\boldsymbol{\kappa}) \rangle, \quad (8)$$

where we have divided by N in order to obtain an *intensive* quantity. This tensor has the dimensions of a squared length, and is a scalar in isotropic systems, where we define the MTIS localization length as

$$\lambda^2 = G_{\alpha\alpha}(0) \quad (9)$$

in the thermodynamic limit. We note in passing that the imaginary part of $\langle \Psi_0(\boldsymbol{\kappa}) | \hat{Q}(\boldsymbol{\kappa}) | \partial_{k_\beta} \Psi_0(\boldsymbol{\kappa}) \rangle$ is closely related to the Berry curvature of the system, thus emphasizing the geometric interpretation of the MTIS localization length. The MTIS basic tenet is that λ is the main marker for the insulating state of matter: λ is finite in any insulator, while it diverges in any metal [7–10]. For the sake of clarity, we stress that the MTIS localization length λ bears *no relationship* to the Anderson localization length [4]: The former is a property of the many-body ground state, while the latter is a property of the one-body eigenstates in an independent-electron system. In Appendix B we demonstrate the relationship between λ and the regular part of the conductivity, from which it follows that a finite static regular conductivity implies a diverging MTIS localization length.

The convergence/divergence of λ has been often used to address the Mott transition in correlated systems [7,14–18]; the present paper is about adopting the same viewpoint to address the Anderson transition in a 3D disordered system. The metal-insulator transition in the presence of both disorder and electron-electron interaction has received much interest as well [26]. Here we only quote two very recent simulations based on 1D model Hamiltonians within PBCs: Ref. [16] adopts the MTIS, while Ref. [27] proposes a marker based on the one-body density matrix ρ . The two approaches are not equivalent, since in the correlated case λ cannot be evaluated from a knowledge of ρ only.

One of the virtues of the MTIS is that Eqs. (8) and (9) can be equally well implemented within either PBCs or OBCs. In this work we adopt OBCs, where the metric assumes a very transparent meaning. If we define the many-body operator

$$\hat{\mathbf{r}} = \sum_{i=1}^N \hat{\mathbf{r}}_i, \quad (10)$$

then the $\boldsymbol{\kappa}$ dependence of the ground eigenstate is very simple within OBCs:

$$|\Psi_0(\boldsymbol{\kappa})\rangle = e^{-i\boldsymbol{\kappa} \cdot \hat{\mathbf{r}}} |\Psi_0(0)\rangle = e^{-i\boldsymbol{\kappa} \cdot \hat{\mathbf{r}}} |\Psi_0\rangle, \quad (11)$$

with an obvious simplification of notations. From this we easily get

$$\partial_{k_\alpha} |\Psi_0(\boldsymbol{\kappa})\rangle |_{\boldsymbol{\kappa}=0} = -i \hat{r}_\alpha |\Psi_0\rangle \quad (12)$$

$$G_{\alpha\beta}(0) = \frac{1}{N} \text{Re} (\langle \Psi_0 | \hat{r}_\alpha \hat{r}_\beta | \Psi_0 \rangle - \langle \Psi_0 | \hat{r}_\alpha | \Psi_0 \rangle \langle \Psi_0 | \hat{r}_\beta | \Psi_0 \rangle), \quad (13)$$

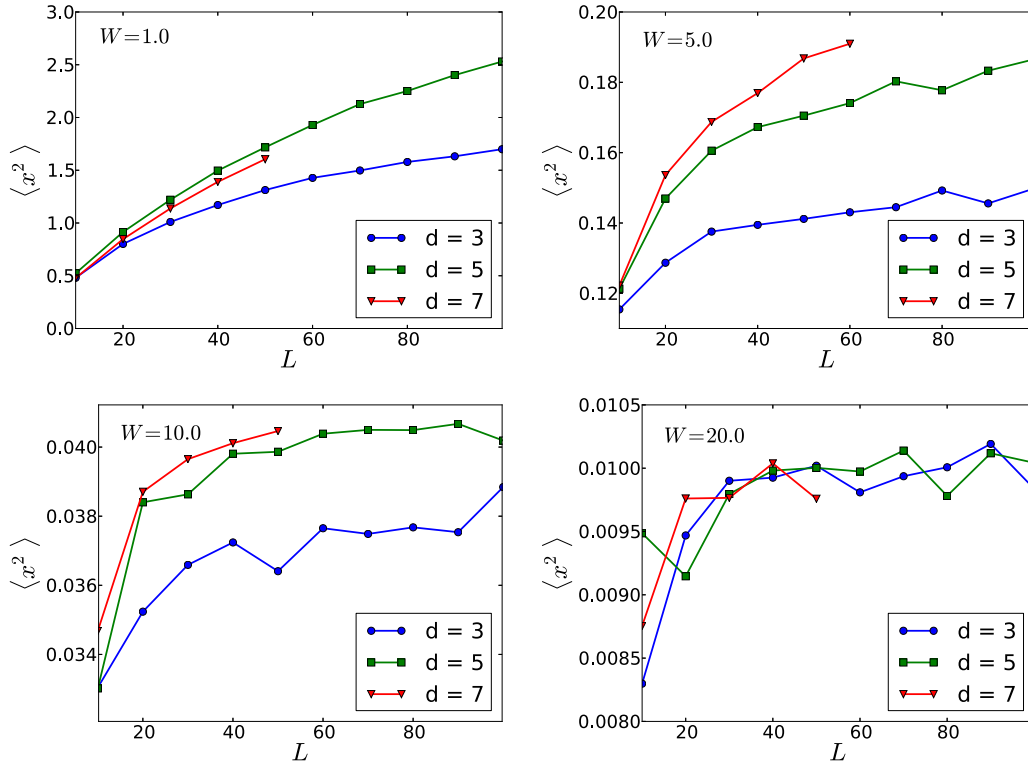


FIG. 1. Localization length $\lambda^2 = \langle x^2 \rangle$ as a function of rod length L . λ diverges for small values of W and saturates to a finite value for large values of W .

i.e., the metric tensor is the second cumulant moment of the electron distribution in the many-electron system. From Eq. (13) it is clear that within OBCs the MTIS localization length is a function of the *two-body* density matrix [9]. In the case of noninteracting particles Eq. (13) can be expressed in terms of the one-body density matrix as

$$G_{\alpha\beta}(0) = \frac{1}{2N} \int d\mathbf{r} \int d\mathbf{r}' (\mathbf{r} - \mathbf{r}')_{\alpha} (\mathbf{r} - \mathbf{r}')_{\beta} |\rho(\mathbf{r}, \mathbf{r}')|^2. \quad (14)$$

Here we have adopted a “spinless electron” formulation, which we will use throughout the present work. The scaling behavior of $|\rho(\mathbf{r}, \mathbf{r}')|$ for $|\mathbf{r} - \mathbf{r}'| \rightarrow \infty$ determines whether the integral in Eq. (14) converges or diverges in the large-system limit. The crystalline case is well known [28]: $|\rho(\mathbf{r}, \mathbf{r}')|$ decays exponentially in insulators and as a power-law in metals, resulting in convergence in the former case, and typically divergence in the latter.

In a disordered system $|\rho|^2$ in Eq. (14) has to be replaced with its configurational average $\langle |\rho|^2 \rangle_c$. A very crucial point is that $\langle |\rho|^2 \rangle_c$ is in general *different* from the squared modulus of the configurational average of $|\rho|$. Thus, knowing the decay of $|\rho|$ is in general not sufficient to determine whether a disordered system is insulating or metallic. This is closely related to the so-called vertex corrections in the well established transport theories based on Green’s functions [23,29]. We discuss this point in detail in Appendix B.

III. RESULTS

Our case study is a paradigmatic system displaying the metal-insulator transition. We consider the half-filled 3D tight-

binding model

$$H = t \sum_{\langle ij \rangle} c_i^{\dagger} c_j + \text{H.c.} + W \sum_i \varepsilon_i c_i^{\dagger} c_i, \quad (15)$$

where i, j denote sites on a simple cubic lattice, $\langle ij \rangle$ are pairs of nearest neighbor sites, and the onsite energies ε_i are randomly picked from the interval $[-1, 1]$. W is the disorder strength and the model has previously been shown to exhibit an Anderson transition at $W_c/t = 8.25$ [19–22]. We set $t = 1$ in the following.

We have calculated the localization length λ , Eq. (9), within OBCs for various values of W using rods of size $L \times d \times d$ where $L = 100$ and $d = 3, 5, 7$. To obtain the configurational average we used 100 configurations, and for each configuration the component of the localization tensor, Eq. (14), along the length of the rod was obtained by averaging over the two short dimensions. The results for various values of W are shown in Fig. 1 for different rod widths d . We clearly observe a tendency for λ to saturate when W becomes large. For small W , instead, λ appears to be increasing monotonically with the rod length L . Within the MTIS, the Anderson transition would emerge as a transition from a divergent λ to a finite λ in the limit of large L . While it seems plausible that this may happen around $W_c = 8.25$, it is very difficult to extract a quantitative estimate of W_c from λ alone. For example, for $W = 10$, the localization length appears to be saturated at a finite value for $L \sim 100$, but it is hard to verify if this is really the case, or if λ is merely increasing too slowly to be observable at the size of our simulations.

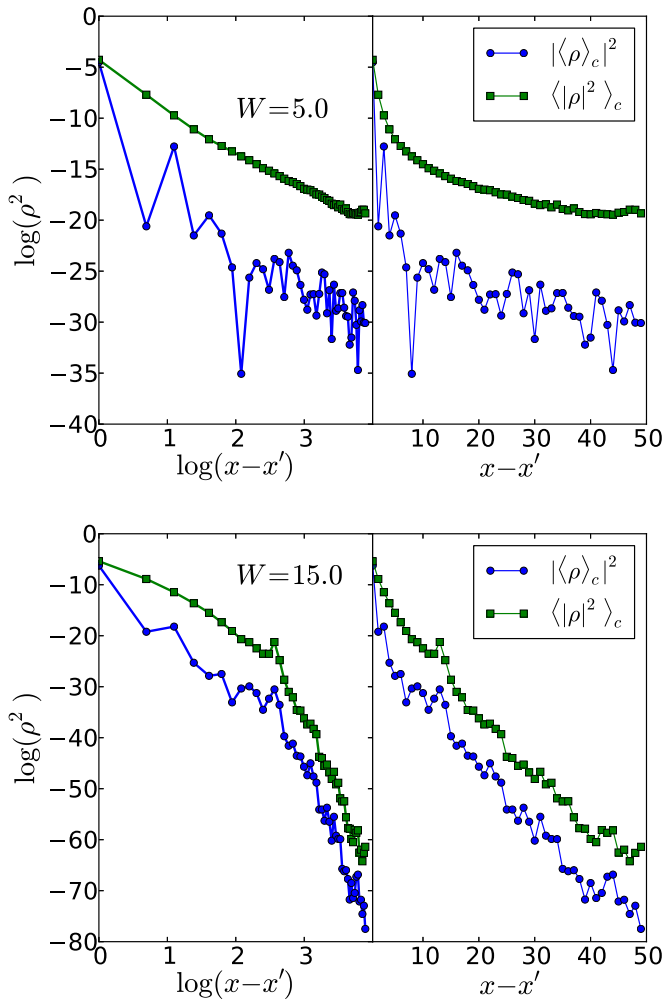


FIG. 2. Configurational averaged density matrix. Top: density matrix with $W = 5.0$ in log-log scale to the left and in semilog scale to the right. Bottom: same as top, but with $W = 15.0$. The norm-squared density matrix is seen to be well approximated by power-law decay for $W = 5.0$ and exponential decay for $W = 15.0$.

In the following we will analyze the density matrix directly, showing that the Anderson transition can be indeed detected from the long range behavior of $\langle |\rho^2| \rangle_c$. As discussed above (and in Appendix B) it is essential to take the square of the density matrix *before* the configurational average, and not the reverse. In Fig. 2 we show the result of our computer experiments, performed for $W = 5$ (in the conducting regime) and $W = 15$ (in the Anderson-insulating regime), after averaging over 300 random configurations; both options— $\langle |\rho^2| \rangle_c$ and $\langle |\rho_c|^2 \rangle_c$ —are shown, and both are plotted in semilogarithmic and double logarithmic scales. The panels in Fig. 2 show first of all that $\langle |\rho^2| \rangle_c$ is a much smoother quantity: This property will allow us (see below) to locate the critical disorder strength W_c . The top left panel in Fig. 2 clearly indicates a power-law behavior at $W = 5$, while the bottom right panel indicates an exponential behavior at $W = 15$: This is indeed qualitatively consistent with Fig. 1 and also with analytical results in the literature [30]. It should be noted, however, that exponential decay is a sufficient, but not a necessary condition for the finiteness of λ . For example, in a homogeneous system it can

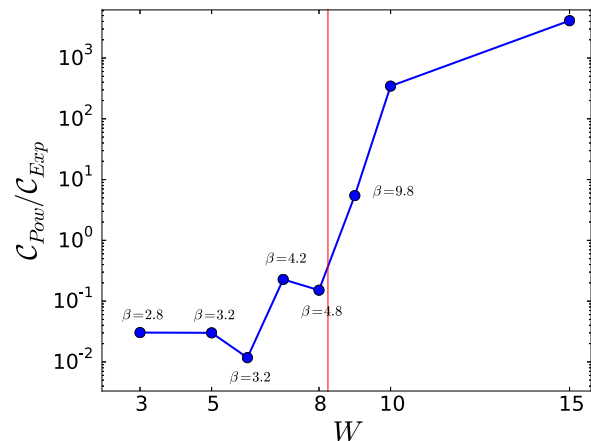


FIG. 3. Ratio of the two cost functions, Eq. (19), from a least-square fit using both power-law and exponential formulas. The displayed values of β are the fitted exponents. The vertical red line is at the value $W_c = 8.25$, taken from the literature [19–22]. Our best estimate of the metal insulator transition from the present method is where $C_{\text{pow}}/C_{\text{exp}}$ becomes unity. This happens at $W \approx 8.5$.

be seen from Eq. (14) that λ stays finite if $\langle |\rho^2| \rangle_c \sim |\mathbf{r} - \mathbf{r}'|^{-\beta}$ and $\beta > 5$.

In order to get a quantitative estimate for the Anderson transition, we consider two alternative formulas for representing the scaling of $y(x) = \langle |\rho(x)|^2 \rangle_c$, where we set $x = |\mathbf{r} - \mathbf{r}'|$. The two formulas have either power-law or exponential decay:

$$\tilde{y}_{\text{pow}}(x) = ae^{-bx}, \quad (16)$$

$$\tilde{y}_{\text{exp}}(x) = \alpha x^{-\beta}. \quad (17)$$

We indicate with \tilde{y}_X any of the two. Then, assuming constant Gaussian noise, the probability of obtaining the data displayed in Fig. 2 using each of the two formulas is

$$P_X \sim e^{-C_X}, \quad (18)$$

where the “cost” function is

$$C_X = \sum_i \frac{(\tilde{y}_X(x_i) - y_i)^2}{2\sigma^2}. \quad (19)$$

Here the index i labels lattice sites along L and y_i are configuration-averaged values of $\langle |\rho(x_i)|^2 \rangle_c$.

We can then obtain the parameters in the two formulas by a least-square fit and compute the resulting cost function for either formula. In Fig. 3 we show the cost-function ratio, as obtained from a fit to the two formulas: We observe a very steep increase (two orders of magnitude) between $W = 8$ and $W = 9$. The transition is therefore very sharp using our indicator, which switches from nearly vanishing to one in a narrow W interval. The present approach yields a critical disorder parameter $W_c \approx 8.5$. It should also be noted that the fitted exponents in the W region where power-law decay is most likely satisfy $\beta < 5$, i.e., all yield a divergent λ .

IV. CONCLUSION

In conclusion we have proved that the modern theory of the insulating state, adopted so far in the previous literature

for band insulators and Mott insulators, successfully applies even to a paradigmatic Anderson insulator. The standard computational methods to address the Anderson transition are often peculiar to lattice models (recursive methods and the like), while the MTIS approach adopted here is quite general. The present methodology could thus in principle be applied to *ab initio* studies, although the actual computations required may still be too demanding. Another merit of the present method is that the expression Eq. (13) is valid for generic many-body systems, and thus it provides a general framework to include interactions in the study of the Anderson transition. The general framework can in principle treat cases where disorder and correlations play equally important roles in the metal-insulator transition.

We stress that the present approach should still be regarded as complementary to the standard treatments of the Anderson transition based on lattice models. For example, it is not simple to derive the critical exponents characterizing the localization length in the vicinity of the transitions from the MTIS. Furthermore, for specific lattice models the well-established methods may provide a more accurate prediction of critical disorder strength at which the Anderson transition emerges. For example, in the present work we studied the simple cubic lattice with random onsite disorder and found $W_c = 8.5$, which compares well, but not exactly, with the established value of $W_c = 8.25$ from the literature. Nevertheless, we believe that the present methodology comprises a promising path that may lead to first principles predictions of the Anderson transition in real materials.

ACKNOWLEDGMENTS

T.O. acknowledges support from the Danish Council for Independent Research, Sapere Aude Program; R.R. acknowledges support from the ONR (USA) Grant No. N00014-12-1-1041; I.S. acknowledges support from Ministerio de Economía y Competitividad (Spain) Grant No. FIS2016-77188-P, and from the European Commission Grant No. CIG-303602.

APPENDIX A: PURE STATE

We start by considering a pure state of our system. The one-body density matrix thus coincides with the projector over the occupied single-particle states:

$$\rho(\mathbf{r}, \mathbf{r}') = \langle \mathbf{r} | \hat{P} | \mathbf{r}' \rangle = \sum_n f_n \langle \mathbf{r} | n \rangle \langle n | \mathbf{r}' \rangle, \quad (\text{A1})$$

where f_n is the Fermi occupancy factor (either 0 or 1 for spinless electrons). If we then define the complementary projector $\hat{Q} = 1 - \hat{P}$ it is easy to cast Eq. (14) of the main text into the equivalent trace form

$$\begin{aligned} G_{\alpha\beta}(0) &= \frac{1}{N} \text{Re Tr} \{ \hat{r}_\alpha \hat{P} \hat{r}_\beta \hat{Q} \} \\ &= \frac{1}{N} \sum_{m,n} f_m (1 - f_n) \text{Re} [\langle m | \hat{r}_\alpha | n \rangle \langle n | \hat{r}_\beta | m \rangle]. \end{aligned} \quad (\text{A2})$$

For isotropic systems the MTIS localization length is then

$$\lambda^2 = \frac{1}{N} \sum_{m,n} f_m (1 - f_n) | \langle m | \hat{x} | n \rangle |^2. \quad (\text{A3})$$

The MTIS localization length is related to the real part of longitudinal conductivity $\text{Re } \sigma(\omega)$ by an integral sum rule, due to Souza, Wilkens, and Martin (SWM) [8]:

$$\lambda^2 = \frac{\hbar V}{N \pi e^2} \int_0^\infty \frac{d\omega}{\omega} \text{Re } \sigma(\omega), \quad (\text{A4})$$

which we are going to prove below.

The Kubo formula for conductivity can be cast in several equivalent ways; a useful expression is in terms of the velocity operator \hat{v} and of the advanced and retarded Green's functions $\tilde{\mathcal{G}}^\pm = (\epsilon - \hat{H} \pm i\eta)^{-1}$, where the $\eta \rightarrow 0^+$ limit is understood [23,29,31–33]. If we define $\tilde{\mathcal{G}}(\epsilon) = \tilde{\mathcal{G}}^+(\epsilon) - \tilde{\mathcal{G}}^-(\epsilon) = -2\pi i \delta(\epsilon - \hat{H})$ the real part of the conductivity can be cast as a trace:

$$\begin{aligned} \text{Re } \sigma(\omega) &= -\frac{e^2}{4\pi V \omega} \int_{-\infty}^\infty d\epsilon f(\epsilon) \text{Tr} \{ \tilde{\mathcal{G}}(\epsilon) \hat{v}_x \tilde{\mathcal{G}}(\epsilon + \hbar\omega) \hat{v}_x \\ &\quad - \tilde{\mathcal{G}}(\epsilon) \hat{v}_x \tilde{\mathcal{G}}(\epsilon - \hbar\omega) \hat{v}_x \} \\ &= -\frac{e^2}{4\pi V \omega} \int_{-\infty}^\infty d\epsilon [f(\epsilon) - f(\epsilon + \hbar\omega)] \\ &\quad \times \text{Tr} \{ \tilde{\mathcal{G}}(\epsilon) \hat{v}_x \tilde{\mathcal{G}}(\epsilon + \hbar\omega) \hat{v}_x \}. \end{aligned} \quad (\text{A5})$$

The latter form clearly shows that the static limit—whenever nonvanishing—is a Fermi-surface integral. The integrand is singular and needs to be regularized; a standard approach is to start with a finite η , with $\hbar\omega \gg \eta$, taking the $\eta \rightarrow 0^+$ limit first and then the $\omega \rightarrow 0$ limit [32]. Nonetheless here we are not focusing on the static limit, since the full ω integral enters the SWM sum rule, Eq. (A4), which reads

$$\begin{aligned} \lambda^2 &= -\frac{\hbar}{4\pi^2 N} \int_0^\infty \frac{d\omega}{\omega^2} \int_{-\infty}^\infty d\epsilon [f(\epsilon) - f(\epsilon + \hbar\omega)] \\ &\quad \times \text{Tr} \{ \tilde{\mathcal{G}}(\epsilon) \hat{v}_x \tilde{\mathcal{G}}(\epsilon + \hbar\omega) \hat{v}_x \}. \end{aligned} \quad (\text{A6})$$

We then replace $\tilde{\mathcal{G}}(\epsilon)$ with its spectral decomposition

$$\tilde{\mathcal{G}}(\epsilon) = -2\pi i \sum_n \delta(\epsilon - \epsilon_n) |n\rangle \langle n|, \quad (\text{A7})$$

which yields

$$\begin{aligned} \lambda^2 &= \frac{\hbar}{N} \sum_{m,n} \int_0^\infty \frac{d\omega}{\omega^2} \int_{-\infty}^\infty d\epsilon [f(\epsilon) - f(\epsilon + \hbar\omega)] \\ &\quad \times \delta(\epsilon - \epsilon_m) \delta(\epsilon - \epsilon_n + \hbar\omega) | \langle m | \hat{v}_x | n \rangle |^2 \\ &= \frac{\hbar^2}{N} \sum_{m,n} \frac{f_m - f_n}{(\epsilon_m - \epsilon_n)^2} \theta(\epsilon_n - \epsilon_m) | \langle m | \hat{v}_x | n \rangle |^2 \\ &= \frac{\hbar^2}{N} \sum_{m,n} \frac{f_m (1 - f_n)}{(\epsilon_m - \epsilon_n)^2} | \langle m | \hat{v}_x | n \rangle |^2. \end{aligned} \quad (\text{A8})$$

(A2) Using then $\hat{v}_x = i[\hat{H}, \hat{x}]/\hbar$ we finally arrive at Eq. (A3).

APPENDIX B: CONFIGURATION AVERAGE AND VERTEX CORRECTIONS

Ideally the conductivity of a disordered system can be addressed via the pure state formulation, because all bulk quantities are self-averaged in the large system limit. When instead working with finite-size disordered samples, one has to take the statistical average of the relevant quantity over many random configurations. The real part of the conductivity, Eq. (A5), then becomes [23,29,31–33]

$$\begin{aligned} \text{Re } \sigma(\omega) = & -\frac{e^2}{4\pi V\omega} \int_{-\infty}^{\infty} d\epsilon [f(\epsilon) - f(\epsilon + \hbar\omega)] \\ & \times \langle \text{Tr} \{ \tilde{\mathcal{G}}(\epsilon) \hat{v}_x \tilde{\mathcal{G}}(\epsilon + \hbar\omega) \hat{v}_x \} \rangle_c, \end{aligned} \quad (\text{B1})$$

where $\langle \dots \rangle_c$ denotes the configurational average. This is not the same as separately averaging the two Green's functions entering Eq. (A5): The difference goes under the name of vertex corrections.

The above derivation makes clear that the SWM sum rule, Eq. (A4), holds if we define the MTIS localization length as

the configurational average of Eq. (A2), i.e.,

$$\begin{aligned} \lambda^2 = & \frac{1}{N} \langle \text{Tr} \{ \hat{x} \hat{P} \hat{x} \hat{Q} \} \rangle_c \\ = & \frac{1}{NN_c} \sum_{i=1}^{N_c} \sum_{m_i, n_i} f_{m_i} (1 - f_{n_i}) |\langle m_i | x | n_i \rangle|^2, \end{aligned} \quad (\text{B2})$$

where we average over N_c random configurations, and i is a configuration label. This clearly corresponds to using $\langle |\rho^2| \rangle_c$ in Eq. (14) of the main text. If we adopt the alternative—and incorrect—choice of $\langle |\rho \rangle_c \rangle_c^2$, we instead get

$$\begin{aligned} \tilde{\lambda}^2 = & \frac{1}{N} \text{Tr} \{ \hat{x} \langle \hat{P} \rangle_c \hat{x} \langle \hat{Q} \rangle_c \} \\ = & \frac{1}{NN_c^2} \sum_{i,j=1}^{N_c} \sum_{m_i, m_j} f_{m_i} (1 - f_{n_j}) |\langle m_i | x | n_j \rangle|^2, \end{aligned} \quad (\text{B3})$$

which corresponds to the no-vertex-correction case since the off-diagonal information is lost in $\tilde{\lambda}^2$. It is well known—within the Green's functions formulation of conductivity [23,29]—that off-diagonal information is essential to distinguish localized from delocalized states.

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