

## Electron Localization in the Insulating State

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The insulating state of matter is characterized by the excitation spectrum, but also by qualitative features of the electronic ground state. The insulating ground wave function in fact (i) sustains macroscopic polarization, and (ii) is *localized*. We give a sharp definition of the latter concept and we show how the two basic features stem from essentially the same formalism. Our approach to localization is exemplified by means of a two-band Hubbard model in one dimension. In the noninteracting limit, the wave function localization is measured by the spread of the Wannier orbitals. [S0031-9007(98)08159-9]

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In a milestone paper that appeared in 1964 [1], W. Kohn investigated the very basic features which discriminate between an insulator and a metal: he gave evidence that *localization* of the electronic ground wave function implies zero dc conductivity, and therefore characterizes the insulating state. In this Letter, we provide a definition of localization which is deeply rooted into the modern theory of polarization [2–5], and rather different from Kohn's. Indeed, besides zero dc conductivity, the property which obviously discriminates between insulators and metals is dielectric polarization: whenever the bulk symmetry is low enough, an insulator displays nontrivial static polarization. Here, we show that the whole information needed for describing *both* localization and polarization is embedded into the same many-body expectation value, namely, the complex number  $z_N$  defined in Eq. (10) below. It was previously shown [5] that macroscopic polarization is essentially the *phase* of  $z_N$ : here we show that the *modulus* of  $z_N$  yields a definition of localization length which is sharper and more meaningful than the available ones. In our formalism a vanishing  $z_N$  implies a delocalized wave function *and* an ill-defined polarization: this characterizes the metallic state. Our definition is first demonstrated for a one-dimensional crystalline system of independent electrons, in which case our localization length coincides (for insulators) with the spread of the Wannier orbitals. We then study a two-band Hubbard model undergoing a Mott-like transition: both in the band regime (below the transition) and in the highly correlated regime (above the transition) the wave function turns out to be localized, while the localization length diverges at the transition point, thus indicating a metallic ground state. Our approach to localization in a many-electron system sharply discriminates between a conducting and nonconducting ground state, yet avoids any reference to the excitation spectrum.

Let us start with a single one-dimensional electron: the distinction between localized (bound) and delocalized (scattering) states is a clearcut one when the usual boundary conditions are adopted; much less so when periodic Born–von Kàrmàn boundary conditions (BvK) are adopted, implying a ring topology for the one-dimensional system. Within the latter choice—which is almost mandatory in condensed matter physics—all states appear in a sense as “delocalized” since all wave functions  $\psi(x)$  are periodic over the BvK period:  $\psi(x + L) = \psi(x)$ . We show that the key parameter to study localization of an electronic state within BvK is the dimensionless complex number  $z$ , defined as

$$z = \int_0^L dx e^{i(2\pi/L)x} |\psi(x)|^2, \quad (1)$$

whose modulus is no larger than 1. In the case of extreme delocalization, one has  $|\psi(x)|^2 = 1/L$  and  $z = 0$ , while in the case of extreme localization,

$$|\psi(x)|^2 = \sum_{m=-\infty}^{\infty} \delta(x - x_0 - mL), \quad (2)$$

and we get  $z = e^{i(2\pi/L)x_0}$ . In the most general case, depicted in Fig. 1, the electron density  $|\psi(x)|^2$  can always be written as a superposition of a function  $n_{\text{loc}}$ , normalized over  $(-\infty, \infty)$ , and of its periodic replicas:

$$|\psi(x)|^2 = \sum_{m=-\infty}^{\infty} n_{\text{loc}}(x - x_0 - mL). \quad (3)$$

Both  $x_0$  and  $n_{\text{loc}}(x)$  have a large arbitrariness: we restrict it a little bit by imposing that  $x_0$  is the center of the distribution, in the sense that  $\int_{-\infty}^{\infty} dx x n_{\text{loc}}(x) = 0$ .

Using Eq. (3),  $z$  can be expressed in terms of the Fourier transform of  $n_{\text{loc}}$  as

$$z = e^{i(2\pi/L)x_0} \tilde{n}_{\text{loc}}\left(-\frac{2\pi}{L}\right). \quad (4)$$

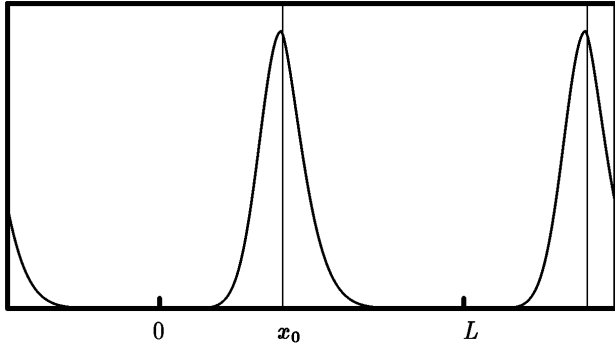


FIG. 1. The distribution  $|\psi(x)|^2$  of a localized state within periodic Born-von Kärman boundary conditions (schematic).

The distinction between a localized and a delocalized state becomes clear if one studies the behavior of  $z$  when the BvK periodicity  $L$  is varied. For a localized state, in fact, the shape of  $n_{\text{loc}}(x)$  is essentially  $L$  independent (exponentially with  $L$  for large  $L$ ), while the opposite is true for a delocalized state. If the electron is localized in a region of space much smaller than  $L$ , its Fourier transform is smooth over reciprocal distances of the order of  $L^{-1}$  and can be expanded as

$$\tilde{n}_{\text{loc}}\left(-\frac{2\pi}{L}\right) = 1 - \frac{1}{2}\left(\frac{2\pi}{L}\right)^2 \int_{-\infty}^{\infty} dx x^2 n_{\text{loc}}(x) + \mathcal{O}(L^{-3}). \quad (5)$$

Therefore at the increase of  $L$ ,  $|z|$  tends to 1 for a localized state, while it vanishes in the delocalized case.

A very natural definition of the center of a localized periodic distribution  $|\psi(x)|^2$  is provided by the phase of  $z$  through the formula

$$\langle x \rangle = \frac{L}{2\pi} \text{Im} \ln z, \quad (6)$$

first proposed by Selloni *et al.* in Ref. [6] to track the adiabatic time evolution of a single quantum particle in a disordered condensed system within BvK. The expectation value  $\langle x \rangle$  is defined modulo  $L$ , as expected since  $|\psi(x)|^2$  is periodic: the previous equations imply indeed  $\langle x \rangle \approx x_0 \text{ mod } L$ . The modulus of  $z$  can be used to measure the localization length  $\lambda$ . Using Eq. (5), we get

$$\ln|z| \approx -\frac{1}{2}\left(\frac{2\pi}{L}\right)^2 \int_{-\infty}^{\infty} dx x^2 n_{\text{loc}}(x), \quad (7)$$

and the spread of the electronic distribution can be defined through

$$\lambda^2 = \langle x^2 \rangle - \langle x \rangle^2 = -\left(\frac{L}{2\pi}\right)^2 \ln|z|^2, \quad (8)$$

which for large  $L$  goes to a constant limit for a localized state, and diverges for a delocalized one. Equation (8) provides an alternative measure of localization with respect to the usual participation ratio [7].

We now switch from the one-body case to the many-body one, and we consider a finite density of electrons  $n_0$ :  $N$  particles in a periodic box of size  $L$ . Eventually, the thermodynamic limit is taken:  $N \rightarrow \infty$ ,  $L \rightarrow \infty$ ,  $N/L =$

$n_0$  constant. Even for a system of independent electrons, our approach takes a simple and compact form if a many-body formulation is adopted. In this case, the ground state obeys BvK in each electronic variable separately:

$$\Psi(x_1, \dots, x_i, \dots, x_N) = \Psi(x_1, \dots, x_i + L, \dots, x_N). \quad (9)$$

Spin variables are omitted (here and in the following formulas), while they of course are taken care of in the calculations. In analogy with the one-particle case, we define the many-body multiplicative operator  $\hat{X} = \sum_{i=1}^N x_i$ , and the complex number

$$z_N = \langle \Psi | e^{i(2\pi/L)\hat{X}} | \Psi \rangle, \quad (10)$$

which will be used to discriminate between a localized many-body ground eigenstate (where  $|z_N| \rightarrow 1$  for large  $N$ ) and a delocalized one, where  $z_N$  vanishes. Ergo, following Kohn's viewpoint [1], the modulus of  $z_N$  will be used here to discriminate between insulators and metals. We start with the dimensionless quantity

$$D = -\lim_{N \rightarrow \infty} N \ln|z_N|^2, \quad (11)$$

which is finite in insulators and divergent in metals: we define the localization length as  $\lambda = \sqrt{D}/(2\pi n_0)$ . We emphasize that our definition of localization—as well as the definition of polarization given in Ref. [5]—deals on the same ground with a general system, either ordered or disordered, either independent-electron or correlated.

For a crystalline system of independent electrons, the many-body wave function  $\Psi$  can be written as a Slater determinant of Bloch orbitals and  $z_N$  factors. Using the same algebra as in Ref. [5], Eq. (14) onwards, one can easily prove that for a metal  $z_N$  vanishes, while for an insulator  $D$  converges to the Brillouin-zone (BZ) integral:

$$D = 4m_b \frac{2\pi}{a} \int_{\text{BZ}} dk \left[ \sum_{m=1}^{m_b} \langle u'_{m,k} | u'_{m,k} \rangle - \sum_{l,m=1}^{m_b} \langle u'_{m,k} | u_{l,k} \rangle \langle u_{l,k} | u'_{m,k} \rangle \right]. \quad (12)$$

In Eq. (12) we assume a linear system of lattice constant  $a$  with  $m_b$  occupied bands and density  $n_0 = 2m_b/a$ ;  $u_{m,k}$  is the periodic factor in the Bloch orbital (chosen to be a differentiable function of  $k$ ), and the prime indicates the  $k$  derivative. The integral in Eq. (12) is a “geometric distance” [8] and measures the spread  $\lambda^2 = \langle x^2 \rangle - \langle x \rangle^2$  of the optimally localized Wannier orbitals [9,10]: our  $\lambda^2$  coincides in fact with  $\Omega_I/m_b$ , where  $\Omega_I$  is the quantity defined by Marzari and Vanderbilt [11] (in one dimension).

Next, we study a one-dimensional model of a correlated polar crystal. We focus on the centrosymmetric case where  $z_N$  is real and its phase is either 0 or  $\pi$ . We choose a two-band Hubbard model at half filling, whose Hamiltonian is

$$\sum_{j\sigma} [(-1)^j \Delta c_{j\sigma}^\dagger c_{j\sigma} - t(c_{j\sigma}^\dagger c_{j+1\sigma} + \text{H.c.})] + U \sum_j n_{j\uparrow} n_{j\downarrow}, \quad (13)$$

and depends on two parameters besides the Hubbard  $U$ : the hopping  $t$ , and the difference in site energies  $2\Delta$ .

In the special case  $U = 0$  we recover a system of independent electrons and the model describes an insulator whenever  $\Delta \neq 0$ . As discussed above,  $D$  is finite [Eq. (12)] in the insulating case and formally infinite (even at *finite*  $N$ ) in the metallic one. We show in Fig. 2 the convergence of  $D$  for several values of  $\Delta/t$ : the localization length diverges upon approaching the metallic state ( $\Delta = 0$ ), and a large system size  $N$  is needed for evaluating  $D$  if  $\Delta/t$  is small. Approximating  $D$  with its finite- $N$  value is exactly equivalent to a discretization of the BZ integral in Eq. (12): if we further replace the logarithm in Eq. (11) with its leading expansion, we recover the same discretization proposed in Ref. [10]. While one gets the same limiting value, our logarithm form converges much faster: this is also shown in Fig. 2, for a selected value of  $\Delta/t$ .

The case of  $U > 0$  is much more interesting, since no Wannier functions or single-particle orbitals can be defined. Notwithstanding, our  $\lambda$  maintains its value of a meaningful measure of the localization of the many-body wave function as a whole, even in the highly correlated regime. The model Hamiltonian of Eq. (13) has been thoroughly studied by several authors [12–14]: when  $U$  is increased to large values, the system undergoes an interesting transition from a band insulator to a Mott insulator. The real number  $z_N$  changes sign at the transition: this fact has an important physical meaning, since it indicates a swapping of roles between anion and cation. In the low- $U$  regime, the anion is the ion having the lowest on-site energy (odd  $j$  for positive  $\Delta$ ), while the opposite is true in the highly correlated regime. We have shown in Ref. [13] that the anion-cation swap manifests itself in a discontinuous change of the *dynamical* (or Born) ionic charge, while instead the static charge is *continuous* and carries no information about the transition.

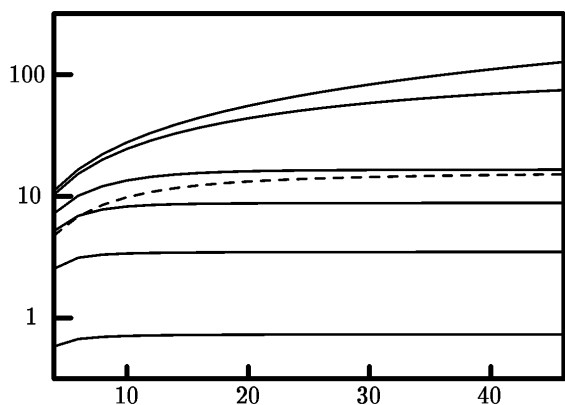


FIG. 2. Solid lines:  $-N \ln|z_N|^2$  as a function of  $N$  at several values of  $\Delta/t$  for independent electrons ( $U = 0$ ). From bottom to top,  $\Delta/t$  assumes the values 5, 2, 1, 0.5714, 0.1, and 0.01, respectively. The dashed line is obtained replacing the logarithm with its leading expansion at  $\Delta/t = 0.5714$ .

The many-body wave function is explicitly needed for detecting the transition, and the relevant information is indeed embedded in  $z_N$ . We adopt in the following the value of  $\Delta/t = 0.5714$ , previously used in Refs. [13,14]: the Mott transition occurs then at  $U = 2.27t$ .

We perform exact diagonalizations for  $N = 8$  via the Lanczos algorithm, as described in Ref. [13]. The results are shown in Fig. 3 (dashed line) and would indicate an increase of the localization length until the transition point, where a discontinuous drop occurs; in the high- $U$  region the wave function is strongly localized. However, upon performing the calculations in this way, the finite size effects are clearly very relevant: this depends on the chosen value of  $\Delta/t$ . Even at  $U = 0$  (where we can afford exact diagonalizations at arbitrarily large sizes) the value of  $D$  calculated at  $N = 8$  differs from the fully converged value by 27% (see Fig. 2): in the correlated case, the situation is expected to worsen. We have performed a few calculations at different sizes, up to  $N = 12$ : The convergence turns out to be slow and oscillatory, with  $N = 4n$  and  $N = 4n + 2$  following different trends.

We overcome this drawback upon building approximate wave functions for much larger sizes. At a fixed size  $N$ , we perform *several* independent calculations, using skew (quasiperiodic) boundary conditions with Bloch vector  $k$  over each electronic variable separately:

$$\Phi_k(x_1, \dots, x_i + L, \dots, x_N) = e^{ikL} \Phi_k(x_1, \dots, x_i, \dots, x_N). \quad (14)$$

We choose  $M$  equally spaced value of  $k$  in the interval  $[0, 2\pi/L)$ :

$$k_s = \frac{2\pi}{ML} s, \quad s = 0, 1, \dots, M-1. \quad (15)$$

Each of the  $\Phi_{k_s}$  is therefore BvK periodical over a period  $L' = ML$ , and we build an ansatz wave function for  $N' = MN$  electrons as the antisymmetrized product of the  $M$  different  $N$ -particle wave functions  $\Phi_{k_s}$ . In the simple case of  $N = 1$  this construction yields the Slater determinant of  $M$  orbitals, and is therefore the exact wave function for a system of  $N' = M$  noninteracting electrons. Upon choosing  $N > 1$ , one allows the  $MN$  electrons to correlate, but only in clusters of  $N$  at a time: of course, our ansatz wave function has restricted variational freedom. At any given  $M$ , and for even  $N$ , the number  $z_N$ , factorizes as [15]

$$\begin{aligned} z_{N'} &= z_{MN} = \langle \Psi | e^{i(2\pi/ML)\hat{X}} | \Psi \rangle \\ &= \prod_{s=0}^{M-1} \langle \Phi_{k_{s+1}} | e^{i(2\pi/ML)\hat{X}} | \Phi_{k_s} \rangle. \end{aligned} \quad (16)$$

For instance, taking  $N = 4$  and  $M = 3$ , the ansatz reproduces the exact 12 sites result (at  $U/t = 1$ ) within 3%. We then approximate the thermodynamic limit upon studying the large  $M$  limit at fixed  $N$ :

$$D = - \lim_{M \rightarrow \infty} NM \ln|z_{NM}|^2. \quad (17)$$

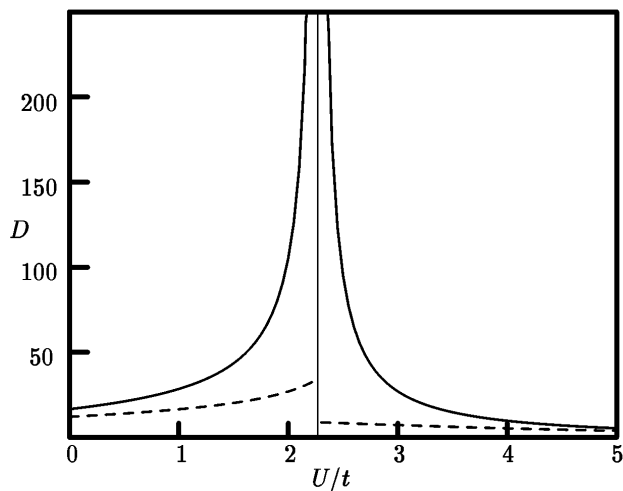


FIG. 3. Dimensionless localization parameter  $D$  [Eq. (11)] as a function of  $U/t$ , where  $\Delta/t = 0.5714$ . Dashed line: Calculations at  $N = 8$ , which are not converged since the size is too small. Solid line: Values of  $D$ , where the thermodynamic limit is achieved by means of the ansatz wave functions (see text); the divergence of the Mott transition is perspicuous.

The values of  $D$  calculated for  $M = 100$  and  $N = 8$  are plotted in Fig. 3 (solid line): one clearly sees a divergence of the localization length at the Mott transition, while the wave function becomes localized again in the highly correlated regime.

The many-dimensional generalization of the present formulation is not straightforward: its presentation is outside the scope of the present Letter. We mention here only a few main features. (i)  $\lambda$  is essentially a unidimensional quantity, in the sense that one fixes a direction and defines a localization length in that given direction: say,  $\lambda_{xx}$  if we choose  $z_N$  identical to form to Eq. (10). For anisotropic crystals, different  $\lambda$ 's coexist: for instance, in graphite we expect  $\lambda$  to be finite in the direction normal to the basal plane, and divergent in the planar direction. (ii) For a  $d$ -dimensional system of  $N$  electrons in a cubic box of volume  $L^d$  the factor  $N$  appearing in Eq. (11) must be replaced with  $N^{2/d-1}$  in order to define the dimensionless  $D_{xx}$ , and the localization length becomes  $\lambda_{xx}^2 = D_{xx}/(2\pi n_0^{1/d})^2$ . (iii) For a crystalline system of independent electrons  $\lambda_{xx}$  can be expressed as a BZ integral. In three dimensions, for a cubic lattice and  $m_b$  occupied bands, we can prove that

$$\lambda_{xx}^2 = -\frac{1}{(2\pi n_0^{1/3})^2} \lim_{N \rightarrow \infty} N^{-1/3} \ln|z_N|^2 = \frac{1}{3m_b} \Omega_1, \quad (18)$$

where  $\Omega_1$  is the BZ integral of Ref. [11].

In conclusion, we have shown how to unambiguously measure localization in the ground state of a many-electron system. We have shown examples of how to

discriminate between an insulator and a metal without actually looking at the excitation spectrum, simply scrutinizing electron localization in the ground eigenstate. For the special case of an insulating crystal of noninteracting electrons, we measure nothing other than the localization of the Wannier functions, whereas in the correlated and/or disordered case our approach to localization is not related—to our best knowledge—to any previously known theory [16]. Our work opens the way to further advances and leaves several important issues open. We mention just a few of them: effects (possibly qualitative) of long-range interaction upon  $\lambda$ ; use of different approximate many-body wave functions (such as, e.g., quantum Monte Carlo); role of  $\lambda$  in the context of Anderson localization in disordered systems.

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