Why are insulators insulating and metals conducting?

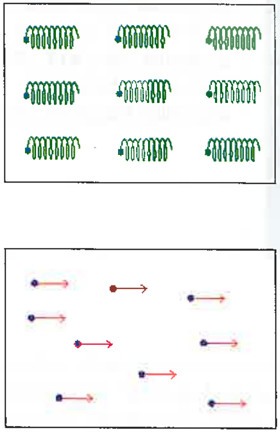
Raffaele Resta, University of Trieste, Italy

An insulator is distinguished from a metal by its vanishing dc conductivity at low temperature. In contrast to what happens in metals, the electronic charge in insulators (and quite generally nonmetals) cannot flow freely under an applied dc field, but instead undergoes static polarization. Within classical physics, this qualitative difference is attributed to the nature of the electronic charge, as sketched in Fig. 1: either "bound" (Lorentz model for insulators) or "free" (Drude model for metals). In other words, electrons are *localized* in insulators and *delocalized* in metals. Switching to quantum physics, this clearcut distinction is apparently lost. In most textbooks [1], the insulating/metallic behaviour is explained by means of band structure theory, focussing on the position of the Fermi level of the given material: either in a band gap (insulators), or across a band (metals), as in Fig. 2.

Why do we need a theory of the insulating state different-and formally more complex-than the familiar one sketched in Fig. 2? The point is that such a picture applies only to a crystalline material, within the independent-electron approximation [1]: a very limited class of insulators indeed. In some materials the insulating behaviour is dominated by disorder (Anderson insulators), in some it is dominated by electron correlation (Mott insulators): therefore, for a large number of insulators, the band picture is grossly inadequate. The present theory of the insulating state [2, 3, 4] deals with *all* kinds of insulators on the same basis: either crystalline or disordered, either independent-electron or correlated.

The insulating/metallic state of matter is characterized by the excitation spectrum, but the qualitative difference in dc conductivity must also reflect a qualitative difference in the organization of the electrons in their *ground state*: a concept first emphasized by W. Kohn in a milestone 1964 paper [5]. Its outstanding message is that even within quantum mechanics the *cause* for insulating behaviour is electron localization. Such localization, however, manifests itself in a very subtle way: in fact the electrons in a condensed system appear, from several viewpoints, about equally delocalized in nonmetals and metals. For instance, the Bloch orbitals in either crystalline silicon or crystalline aluminum are similarly delocalized, and do not reveal any sharp difference. The challenge is to show how electron localization can be detected and measured in the ground wavefunction of a condensed many-electron system. The difference between localized and delocalized must be, in the thermodynamic limit, a sharp one. A solution to this problem was provided by Kohn in his original 1964 paper. In 1999 the problem was reconsidered and a solution different from Kohn's-and in many respects simpler-was found [3].

There is an outstanding phenomenological link between macroscopic polarization and the insulating state of matter. Suppose we expose a finite macroscopic sample to an electric field, say



◀ **Fig. 1:** Schematic view of insulators and metals in classical physics. Top sketch: Lorentz model for insulators, where each electron is tied (by an harmonic force) to a particular center. Bottom sketch: Drude model for metals, where electrons roam freely over macroscopic distances, hindered only by atomic scattering potentials.

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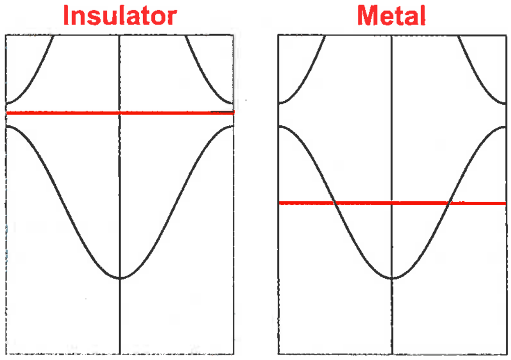


▲ **Fig. 2:** Traditional textbook view of the qualitative difference between insulators and metals. The plots show the energy band structures of crystalline (i.e. ordered) materials, chosen one-dimensional for the sake of simplicity. The insulating/metallic behaviour depends on the position of the Fermi level, which in turn is determined by the number of electrons per cell. A filled band results in insulating behaviour, while an half-filled one results in metallic behaviour. For many insulating materials (e.g. disordered and/or correlated) such a band picture is inappropriate. The present theory of the insulating state is based on quite different concepts, and applies on the same grounds to *any* insulator.

inserting it in a capacitor and applying a voltage. Then the induced macroscopic polarization is qualitatively different in metals and insulators. In the former materials polarization is trivial: universal, material-independent, due to surface phenomena only (screening by free carriers). Therefore polarization in metals is *not* a bulk phenomenon. The opposite is true for insulators: macroscopic polarization is a nontrivial, material-dependent, bulk phenomenon.

On the theoretical side, the concept itself of macroscopic polarization in quantum physics has long evaded even a correct definition: most textbooks contain incorrect statements [1]. The modern theory of polarization [2, 6], based on a Berry phase [7], was developed a decade ago: it revolutionizes both the very definition of the relevant bulk observable, and the ways to compute it in real solids. This theory has been the subject of a previous article in this journal [8], and starts making its way in elementary textbooks [9]. The recent advances about the insulating state of matter [3, 4] are deeply rooted in the modern theory of polarization: in fact polarization and localization can be regarded as two aspects of the same phenomenon, and stem from the same formalism.

In order to provide an oversimplified treatment, here I only deal with a system of N one-dimensional electrons, chosen spinless (or parallel-spin) for the sake of simplicity. The many-body ground wavefunction is then $\Psi(x_1,x_2,\dots x_j,\dots x_N)$, and all the electrons are confined to a segment of length L. Eventually, we will be interested in the thermodynamic limit, defined as the limit $N \to \infty$ and $L \to \infty$, while the density N/L is kept constant. For practical purposes, this limit is well approximated when L is much larger than a typical atomic dimension. A crucial role in our treatment is played by the boundary conditions chosen for the wavefunction: we adopt here-as almost mandatory in condensed matter physics [1]—Born-von Kàrmàn periodic boundary conditions, which amount to imposing that the wavefunction Ψ is periodic, with period L, over each electronic variable x_j separately. Equivalently, one can imagine the electrons to be confined in a circular rail of length L: the coordinates x_j are then proportional to the angles $2\pi x_j/L$, defined modulo 2π.

Following Refs. [2, 3], the key quantity needed to deal with both polarization and localization is the ground-state expectation value

$$z_N = \langle\Psi|U|\Psi\rangle = \int_0^L dx_1 \dots \int_0^L dx_N |\Psi(x_1,\dots x_N)|^2 U(x_1,\dots x_N), \qquad (1)$$

where the unitary operator U, called the "many-body phase operator" or "twist operator", is defined as

$$U(x_1,\dots x_N) = \exp\left(i\frac{2\pi}{L}\sum_{j=1}^{N} x_j\right), \qquad (2)$$

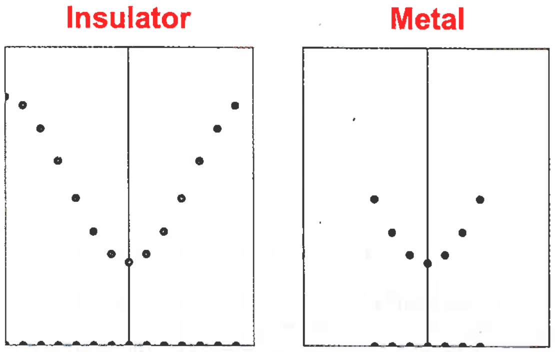
and clearly obeys periodic boundary conditions. The expectation value z_N is a dimensionless complex number, whose modulus is no larger than one.

The electronic contribution to the macroscopic polarization of the system can be expressed in the very compact form [2, 4]:

$$P_{\rm el} = \frac{e}{2\pi} \lim_{N\to\infty} \operatorname{Im} \log z_N, \qquad (3)$$

where e is the electron charge. Notice that, for a one-dimensional system, the polarization has the dimensions of a charge (dipole per unit length). The essential ingredient in Eq. (3) is Im logz_N, i.e. the *phase* of the complex number z_N. This phase, which is a rather peculiar kind of Berry phase [7], is ill defined whenever z_N vanishes. And here comes the key message [3, 4]: what differentiates very sharply metals from insulators is the behaviour of the modulus of z_N in the thermodynamic limit: in the former materials it goes to zero, while in the latter it goes to one. We find therefore, in agreement with the above phenomenological considerations, that macroscopic polarization is well defined in insulators and ill defined in metals.

The modulus of z_N can be used to measure the localization of the many-body wavefunction, thus providing a quantitative



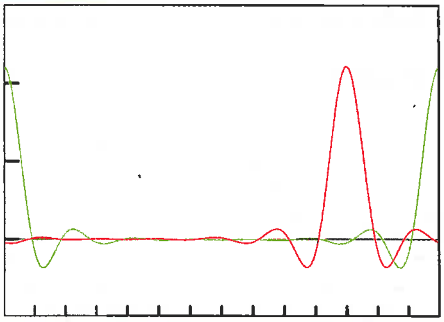
▲ **Fig. 3:** Same energy band structure as in Fig. 2, for a *finite* one-dimensional system with periodic boundary conditions. In drawing the figure, the period *L* has been taken as 14 times the lattice constant. In the insulating case the band is filled, and the ground wavefunction Ψ is the antisymmetrized product (Slater determinant) of 14 Bloch orbitals, whose *k*-vectors and corresponding energies are indicated by dots. Notice that only one of the states at the Brillouin-zone boundaries must be occupied to avoid double counting. In the metallic case the band is half-filled, and the ground wavefunction is the antisymmetrized product of the 7 Bloch orbitals whose energy is below the Fermi level, indicated by dots.

assessment of Kohn's [5] main idea. To this aim, we have introduced [3] the intensive quantity

$$\langle x^2\rangle_c = -\lim_{N\to\infty}\frac{1}{N}\left(\frac{L}{2\pi}\right)^2 \log|z_N|^2, \qquad (4)$$

having the dimensions of a squared length. It can be proved [4] that, in insulators, the modulus of z_N differs from one by the order of $1/N$, hence $\langle x^2\rangle_c$ is finite, while in metals it is divergent: this finding clearly vindicates the classical viewpoint of Fig. 1.

I stress that $\langle x^2\rangle_c$ is an intensive property characterizing the localization of the many-body wavefunction Ψ as a whole, which applies on the same grounds to ordered/disordered and correlated/uncorrelated many-electron systems. It is now expedient to focus on a special case: ordered and uncorrelated, i.e. a crystalline system of independent electrons, as in the band-structure picture of Fig. 2, where a single band is considered. In this case the ground many-body wavefunction $\Psi(x_1,x_2,\ldots x_N)$ is a Slater determinant (i.e. antisymmetrized product) of N single-particle orbitals, which are usually chosen in the Bloch form both for metals and insulators. But there is an outstanding difference, illustrated in Fig. 3: only one half of the band is used to build the Slater determinant for the metal, while the whole band is used for the insulator. These two Slater determinants are therefore qualitatively very different, despite the fact that both are built of (delocalized) Bloch orbitals. Their difference is probed very sharply by the many-body phase operator U, Eq. (2): in fact it can be proved [3, 4] that in the metallic case the expectation value z_N, Eq. (1), vanishes, thus leading to a formally infinite value of $\langle x^2\rangle_c$, while in the insulating case $\langle x^2\rangle_c$ assumes a finite value. Actual values of $\langle x^2\rangle_c$ in nonmetallic materials, as computed e.g. for the III-V semiconductors, are of the order of a few bohr^2. I stress that, in the present analysis, no use is made of the *spectrum* of the system: the metallic/insulating behaviours reflect a different organization of the electrons in the *ground state*.



▶ **Fig. 4:** The ground wavefunction Ψ of an insulator can be equivalently written as an antisymmetrized product of either Bloch orbitals (Fig. 3, left panel) or Wannier orbitals. Both Bloch and Wannier orbitals obey periodic boundary conditions over the period L, which we have taken as 14 times the lattice constant (same as in Fig. 3). For the sake of clarity, we have plotted (red and green) only 2 of the 14 Wannier orbitals which are needed to build Ψ. In the thermodynamic ($L \longrightarrow \infty$) limit the Wannier orbitals are exponentially localized and the second cumulant moment of their distribution $\langle x^2\rangle - \langle x\rangle^2$ is finite: in fact it is equal to $\langle x^2\rangle_c$, Eq. (4). The situation is completely different in the metallic case (Fig. 3, right panel): one *cannot* write Ψ as an antisymmetrized product of orbitals whose second moment is finite in the thermodynamic limit. Notice that such a sharp qualitative difference reflects a different organization of the electrons *in the ground state*, and makes no reference to either the excitation spectrum or conductivity properties.

The intensive quantity $\langle x^2\rangle_c$, measuring electron localization in the many-body wavefunction, has the meaning of a second cumulant moment. Once more, it is expedient to illustrate this for the special case of a crystalline system of independent electrons, as in Figs. 2 and 3. Since a determinant is invariant under unitary transformations, we can perform any unitary transformation on the N single-particle occupied orbitals without affecting the ground N-particle wavefunction Ψ, and therefore leaving z_N and $\langle x^2\rangle_c$ invariant. Starting from orbitals of the Bloch form, hence delocalized throughout the crystal, we may look for a unitary transformation leading to orbitals which are localized around some crystalline sites. One such transformation, namely, the Wannier transformation, is well known in solid-state physics: this is illustrated in Fig. 4. According to our theory, $\langle x^2\rangle_c$ is the minimum possible value for the averaged second cumulant moment $\langle x^2\rangle$ - $\langle x^2\rangle$ of the electron distribution of the localized orbitals, in the $N \longrightarrow \infty$ limit. One outstanding implication is that, for insulators, the many-body wavefunction *can* be written as a Slater determinant of localized single-particle orbitals, whose distributions have *finite* second moments. More precisely, the averaged second moment of the single-particle orbitals can be made as small as $\langle x^2\rangle_c$ with a suitable choice of the unitary transformation. Suppose, instead, that we attempt a localizing transformation on the occupied Bloch orbitals of a metal. Then, since $\langle x^2\rangle_c$ diverges, it is impossible that all of the transformed orbitals have a finite second moment in the thermodynamic limit.

In conclusion, the present theory of the insulating state sharply discriminates between an insulator and a metal *without* actually looking either at the excitation spectrum or at conductivity properties. Instead, it is enough to probe-with an elegant tool, the many-body phase operator of Eq. (2)-the organization of the electrons *in the ground state*. Once our simple definition of localization is adopted, electrons are localized in any insulator and delocalized in any metal. Localization in the ground electronic wavefunction is the key reason why insulators sustain bulk dielectric polarization. In the present treatment, localization and polarization appear as two aspects of the same phenomenon, and are naturally described by the same formalism.

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About the author

Raffaele Resta is professor of *Struttura della Materia*, University of Trieste, and a coordinator in the INFM DEMOCRITOS National Simulation Centre in Trieste. Previously, he was a professor at the University of Pisa and at SISSA, Trieste. He has also worked for many years at EPFL (Swiss Institute of Technology, Lausanne).