Why are insulators insulating and metals conducting?

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

$$P_{\alpha} = \frac{e}{2\pi L} \lim_{N \to \infty} \text{Im} \log z_N,$$

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 $\text{Im} \log z_N$, 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

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

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

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

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 $\Psi(x_1, x_2, \ldots, x_N)$, 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 $\text{Nil}$ 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 Kármán periodic boundary conditions, which amount to imposing that the wavefunction $\Psi$ is periodic, with period $L$, over each electronic variable $x_i$ separately. Equivalently, one can imagine the electrons to be confined in a circular

1. 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 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.

2. 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 $\Psi$ 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.
The intensive quantity \((x^2)_c\) 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 \(\Psi\), and therefore leaving \(z_n\) and \((x^2)_c\) 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, \((x^2)_c\) is the minimum possible value for the averaged second cumulant moment \((x^2) - \langle x^2 \rangle\) of the electron distribution of the localized orbitals, in the \(N \to \infty\) 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 \((x^2)_c\) 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 \((x^2)_c\) 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.

References


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