The insulating state of matter: A geometrical theory

R. Resta

Dipartimento di Fisica Teorica, Università di Trieste,
and CNR-INFM DEMOCRITOS National Simulation Center, Trieste

The insulating vs. conducting behavior of condensed matter is usually addressed in terms of excitation spectra. At variance with such wisdom, W. Kohn showed in 1964 that the insulating state of matter also reflects a peculiar organization of the electrons in their *ground state* [1]. Nowadays we are able to relate the two features by means of a fluctuation-dissipation theorem.

The modern developments of the "theory of the insulating state" started in 1999, and continue to these days. The many-body ground wavefunction of an insulator is sharply characterized by means of geometrical concepts.

We consider an N-electron system, whose most general Hamiltonian includes both a "twist" (alias "flux"), and a vector potential $\mathbf{A}$ of magnetic origin:

$$\hat{H}(\mathbf{k}) = \frac{1}{2m}\sum_{i=1}^{N}[\mathbf{p}_i + \frac{e}{c}\mathbf{A}(\mathbf{r}_i) + \hbar\mathbf{k}]^2 + \hat{V},$$

where the potential $\hat{V}$ includes a one-body term (the external potential) and a two-body one (the electron-electron interaction). For any $\mathbf{k}$ the ground wavefunction obeys periodic (toroidal) boundary conditions over a $3N$-dimensional hypercube of size L. The Provost-Vallee quantum metric tensor [2], is in our case:

$$g_{\alpha\beta}(\mathbf{k}) = \mathrm{Re}\ \langle\partial_\alpha\Psi_0(\mathbf{k})|\partial_\beta\Psi_0(\mathbf{k})\rangle - \langle\partial_\alpha\Psi_0(\mathbf{k})|\Psi_0(\mathbf{k})\rangle\langle\Psi_0(\mathbf{k})|\partial_\beta\Psi_0(\mathbf{k})\rangle,$$

where Greek symbols are 3-dimensional Cartesian coordinates and $\partial_\alpha = \partial/\partial k_\alpha$. The corresponding many-body Berry curvature is

$$\Omega_{\alpha\beta}(\mathbf{k}) = i[\,\langle\partial_\alpha\Psi_0(\mathbf{k})|\partial_\beta\Psi_0(\mathbf{k})\rangle - \langle\partial_\beta\Psi_0(\mathbf{k})|\partial_\alpha\Psi_0(\mathbf{k})\rangle\,],$$

and vanishes for time-reversal invariant systems.

The metric g at $\mathbf{k}=0$ sharply determines the insulating/conducting behavior. More precisely, the insulating state of matter is characterized by having $g_{\alpha\beta}(0)/N$ finite in the thermodynamic limit, at variance with metals where it diverges [3]. This applies to *any kind* of insulator; in the simple case of a crystalline system of noninteracting electrons, this same quantity sets a lower bound for the quadratic spread of the Wannier functions (which, again, diverges in the metallic case).

The curvature Ω at $\mathbf{k}=0$, instead, has to do with the Hall effect [4].

[1] W. Kohn, *Theory of the insulating state*, Phys. Rev. **133**, A171 (1964)

[2] J. P. Provost and G. Vallee, *Riemaniann structure on manifolds of quantum states*, Commun. Math Phys. **76**, 289 (1980).

[3] R. Resta, *Why are insulators insulating and metals conducting?*, J. Phys.: Condens. Matter **14**, R625 (2002).

[4] R. Resta, *Electron Localization in the Quantum-Hall Regime*, Phys. Rev. Lett. **95**, 196805 (2005).