PHYSICAL MATHEMATICS SEMINAR
Bloch, Wannier, and Berry: don't lose your phase, but do follow your manifold.

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Abstract:

The electronic structure of materials is usually described in terms of extended Bloch orbitals, since the Hamiltonian and translation operators commute. A Wannier representation can also be used, giving rise to orthonormal localized functions spanning the same subspace. The Wannier mapping is strongly non-unique, and so its application has never been straightforward nor universal.

We discuss here an algorithm to determine the "maximally-localized" set of Wannier functions for any given Hamiltonian. We use as a measure of localization the total spread of the Wannier functions in real space, and provide an algorithm that iteratively refines the Wannier mapping, leading to the maximally-localized of all possible sets. We proceed directly from the Bloch functions represented on a mesh of k-points, and a gauge-covariant expression for the position operator in periodic boundary conditions, to carry out the minimization in the space of unitary matrices U_k^{mn}. These account at each point k in the Brillouin zone for all possible unitary transformations between the Bloch bands. A global measure of smoothness is also introduced, to extract from any entangled manifold a submanifold of interest, thus selecting a "maximally-differentiable" set inside an arbitrary energy window (e.g. around the Fermi energy in a metal).

The maximally-localized Wannier representation provides an insightful chemical picture of the hybridization and bonding that occur when a molecule or a crystal is formed, and allows for an optimal and general solution to the inverse tight-binding problem. Moreover, it establishes a discrete mapping of the local polarization field; such information can not be obtained by other means, and it provides a classical, electrostatic description of quantum dielectric properties. Finally, the characteristic localization of the ground state is both of fundamental interest, and of practical importance for the development of linear-scaling electronic-structure algorithms. [Work done in collaboration with David Vanderbilt (Rutgers) and Ivo Souza (Berkeley)]