Wannier Functions: Past, Present, and Future

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In this talk I will give an introduction to the theory of Wannier functions (WFs) and discuss some of the reasons why interest in WFs has expanded rapidly in recent years.

I will briefly introduce WFs, starting with the simplest case of orthonormal WFs for a single isolated band in a periodic crystal and discussing the non-uniqueness associated with the choice of phases. I will then discuss some of the ways in which the definition of WFs can be generalized, including: (i) multiband WFs and their associated gauge freedom; (ii) non-orthonormal WFs; (iii) Wannier-like functions ("localized molecular orbitals") for the occupied states of finite systems (molecules and clusters) and of disordered infinite systems; (iv) "disentangled" or "downfolded" orbitals that can be used as a basis to describe the occupied states and/or the states near ε_F in a metal; and (v) hybrid or "hermaphrodite" WFs that are Bloch-like in one or more Cartesian directions while being Wannier-like in the orthogonal directions(s). Unfortunately the terminology in the field is not well established, and there is little consensus about whether or not such generalized objects still deserve to be called WFs. I will discuss my views on this question and make some modest suggestions about it.

I will then briefly discuss two approaches for resolving the phase or gauge freedom: the use of projection methods, and the generation of maximally localized WFs. I will make several comments about the projection methods, especially concerning how well-localized non-orthonormal WFs are best constructed using a projection method.

I will present only a very brief outline of the types of applications of WF methods that are currently of interest, as these will be well illustrated by other talks in the workshop.

I will devote the last part of the talk to discussing several problems connected with the theory of WFs that have only recently been solved or that remain unsolved. In the former category, a proof of the exponential localization of WFs in the three-dimensional multiband case has recently been given. Among the latter, I will focus mainly on issues relating to the definition of WFs for systems with broken time-reversal symmetry. Most of the work done in the last decade on the theory of electric polarization, finite electric fields, localization, and the nature of the insulating state have been limited, implicitly or explicitly, to the case in which time-reversal symmetry is preserved. However, much remains to be done to bring our understanding of systems with broken time-reversal symmetry up to the same level. For example, is there an appropriate generalization of the concept of WFs for a Chern insulator (that is, an insulator with a non-zero Chern invariant)? Can the recently given derivation for the orbital magnetization of an ordinary insulator be extended to the case of a metal or a Chern insulator using a derivation based on the Wannier representation? If time permits, some tentative and partial steps in these directions may be discussed.