Spectral and Fermi Surface Properties from Wannier Interpolation

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We describe a widely-applicable Wannier function (WF) based scheme for interpolating both the energy bands and any given one-electron operator. This provides an efficient first-principles approach for calculating Fermi surface averages and spectral properties of solids [1].

The first step is to perform a conventional first-principles calculation and store the low-lying Bloch functions evaluated on a uniform grid of k-points in the Brillouin zone. We then map those states onto a set of maximally-localized Wannier functions, and evaluate the matrix elements of the Hamiltonian and the other needed operators between the Wannier orbitals, thus setting up an "exact tight-binding model." In this compact representation the k-space quantities are evaluated inexpensively using a generalized Slater-Koster interpolation. Because of the strong localisation of the Wannier orbitals in real space, the smoothness and accuracy of the k-space interpolation increases rapidly with the number of grid points originally used to construct the Wannier functions. This allows k-space integrals to be performed with *ab-initio* accuracy at low cost. In the Wannier representation, band gradients, effective masses, and other k-derivatives needed for transport and optical coefficients can be evaluated analytically, producing numerically stable results even at band crossings and near weak avoided crossings.

We present its application to the calculation of the spontaneous anomalous Hall conductivity [2] and magnetic circular dichroism [1] of ferromagnets. The possibility of similar field-induced effects in paramagnets, including an anomalous contribution to the low-field Hall effect, is discussed.

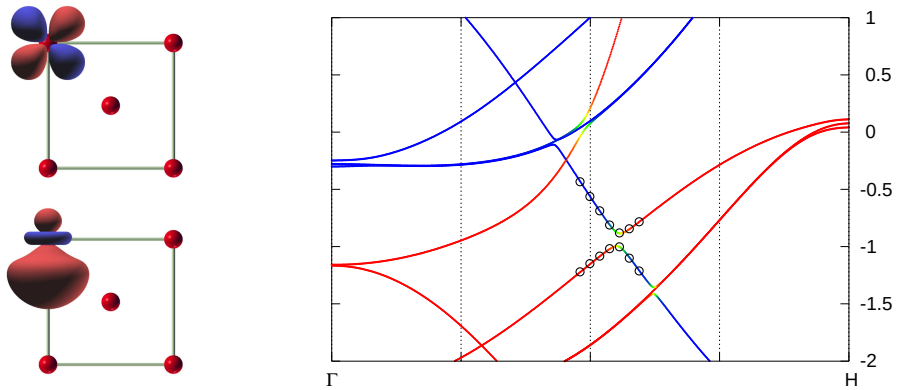

Figure 1: Left: WFs for bcc Fe. Right: Wannier-interpolated bands of bcc Fe along Γ–H. The bands are color-coded according to the value of $\langle S_z \rangle$: red for spin up and blue for spin down. The energies are given in eV and the Fermi level is at 0 eV. The vertical dashed lines indicate k-points on the *ab-initio* mesh used for constructing the WFs. For comparison, points from a full *ab-initio* calculation are shown as open circles.

[1] J. R. Yates, X. Wang, D. Vanderbilt, and I. Souza, cond-mat/0702554.

[2] X. Wang, J. R. Yates, I. Souza, and D. Vanderbilt, Phys. Rev. B **74**, 195118 (2006).