VARIATIONAL FORMULATION FOR FINDING WANNIER FUNCTIONS WITH ENTANGLED BAND STRUCTURE

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Wannier function representation of Kohn-Sham orbitals is part of the essential toolset for modern electronic structure calculations. However, the construction of the Wannier functions may strongly depend on the initial guess and thus human input, which makes it difficult for high throughput material computation. This issue becomes particularly noticeable for systems with entangled band structure, where the disentanglement procedure is needed.

Recently we have developed the selected columns of the density matrix (SCDM) method. SCDM is a deterministic procedure and can provide a robust initial guess for the Wannier localization procedure even for metallic systems, and hence facilitates high throughput calculations.

We further develop a variational formulation to optimize the Wannier functions, under which the disentanglement procedure can be interpreted as an alternating minimization method performed by a single step. We demonstrate the effectiveness of our method using real materials including silicon, copper, and aluminum, and compare with the results obtained from the disentanglement procedure. We also present interesting numerical observations for the variationally optimized Wannier functions for the uniform electron gas. (Joint work with Anil Damle and Antoine Levitt).