

A Local Representation of the Dielectric Response Function

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The screened dielectric response function (χ) is a fundamental physical quantity that captures the many-electron correlation effect, key to a range of excited state properties formulated in the correlated electron theories. Although χ is non-local by definition, a real space partition of χ onto local structural motifs can help us gain further physical insight into, e.g., effective local screening properties. Because the bare response function, χ_0 , is normally expressed in electron - hole pairs, standard localization procedures for electron wave functions can not be directly applied. In this work, we propose a new method to decompose χ_0 and χ into contributions from local response of Wannier orbitals. We demonstrate that the localization properties of the local dielectric response can be exploited to build a local basis set for χ_0 , which can be used to construct a tight-binding Hamiltonian to perform dielectric band structure interpolation.

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