Nearsightedness of Electronic Matter

EMIL PRODAN, University of California at Santa Barbara, WALTER KOHN, UCSB — The concept of “nearsightedness of electronic matter” (NEM) articulates and quantifies the common, qualitative consensus among chemists and also among many physicists, that static, local electronic properties like the density or energy density at a given point r, of a many-atomic covalent or metallic system depend significantly on the external potential v(r′) only for values of r′ near r. NEM provides the physical basis for linear scaling [O(N)] electronic structure calculations. We say that a system of electrons is nearsighted at r, if distant potential perturbations w(r′) [w(r′) vanishing for |r-r′| <D] produce insignificant density changes at r. For non-interacting electrons in 1, 2 and 3 dimensions, we have obtained explicit complete asymptotic (D large) functional behaviors and the pre-factors of the density changes generated by distant perturbing potentials. For periodic or non-periodic metals and insulators, these results show that the density changes at r cannot exceed a maximum value regardless of the shape or magnitude of w(r′). This allows us to introduce a new concept, the nearsightedness range R, defined as the minimum distance for which the density changes at r, due to any potential w(r′) vanishing for |r-r′| <R, are less than a desired accuracy. We present here the dependence of the nearsightedness range on the desired accuracy, for gapped and un-gapped electronic systems. We also discuss the implications for O(N) electronic structure calculations.