Revisiting the NLCPA: insight from non-site-diagonal observables

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We re-examine the non-local coherent potential approximation (NLCPA) from the point of view of actual unicity in its effective medium construction.
This method extends the originally single-site theory [1] with the ability of modelling different forms of short-range ordering (SRO) [2]. Characteristically with respect to other extension proposals [3], in this approach to the study of disordered systems on-average translational invariance is retained. This derives from a self-consistent prescription which couples extended treatment in direct space (i.e. a $N_c \geq 1$ -sites wide 'cavity' carved from the bulk) with a Brillouin zone partitioning in reciprocal space (i.e. $N_c \geq 1$ 'tiles' $\mathbf{\Omega}_{BZ}^{(cav)}(\vec{K}_n)$ such that: $\bigcup_{n=1}^{N_c} \mathbf{\Omega}_{BZ}^{(cav)}(\vec{K}_n) = \mathbf{\Omega}_{BZ}$).
After iterating between both descriptions until convergence, results can be used for the actual calculation of all desired observables. As in the original theory [4], it is convenient to distinguish in particular among site-diagonal (SD) and non-site-disagonal (NSD) quantities. Essential examples of these can be the electronic density of states, as opposed to the electronic Bloch's spectral function which corresponds to its $\vec{k} \in \mathbf{\Omega}_{BZ}$ derivative.
We show how proper deployment of the general formalism to calculate the latter at a Korringa, Kohn, Rostocker (KKR) -DFT level for real materials [5] confirms previous insight from 1D tight-binding calculations [6]. The role of a "free" phase factor in the above lattice Fourier transformations definition becomes in particular apparent, with noticeable consequences in both SD and NSD observables. This requires in general an extra averaging step for recovery of a fully physical effective medium. We review this additional aspect of the theory and re-look at previous case studies in the physics of substitutional alloys, as well as disordered local moment simulations of the paramagnetic phase of metals, for different forms of spectroscopy [7-9] are available

References

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