EQUIVALENCE OF PROPAGATOR AND LOCATOR APPROACH FOR THE AVERAGE-t-MATRIX APPROXIMATION

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It is shown that propagator and locator formalism agree for the average-t-matrix approximation.

The recently developed theory of disordered substitutional alloys [1] is centered around the average-t-matrix approximation (ATA) and the coherent-potential approximation (CPA) as methods for dealing with the tight-binding single-band model Hamiltonian

$$H = \sum_n |n\rangle E_n \langle n| + \sum_{n \neq m} |n\rangle W_{nm} \langle m| = D + W , \quad (1)$$

where the site energy E_n depends upon the nature of the atom at site n and W is independent of the alloy configuration [2]. It has been emphasized [3–5] that the CPA result for the configurationally averaged Green's function $\langle G(E)\rangle$ may be obtained both by a locator and a propagator approach. In this letter it is shown that the same is true for the ATA if one starts the calculation from the same reference system in both approaches.

With respect to a periodic reference medium with propagator $P_M(E) = (EI - W - V_M)^{-1}$ the equation for G is

$$G = P_M + P_M(D - V_M)G = P_M + P_M T P_M , \quad (2)$$

which defines T. If we take a site-diagonal $V_M = E_M I$ the perturbation $D - V_M$ is a sum of single-site contributions $V_n = |n\rangle (E_n - E_M)\langle n|$, and

$$T = \sum_n T_n [I + P_M^{OD} T] \quad (3a)$$

$$= \sum_n T_n + \sum_n T_n P_M \sum_{m(\neq n)} T_m + \dots , \quad (3b)$$

where $T_n = [I - V_n P_M]^{-1} V_n$ and P_M^{OD} is the off-diagonal part of P_M. Approximation procedures for averaging (3) lead via (2) to approximations for $\langle G\rangle$.

In the τ-matrix formalism [4] of the locator approach the renormalized interactor $U = W + WGW$ is determined with respect to the interactor $U_M = (W^{-1} - \sigma_M)^{-1}$ of a reference medium by

$$U = U_M + U_M(g - \sigma_M)U = U_M + U_M \mathcal{T} U_M , \quad (4)$$

where $g(E) = (EI - D)^{-1}$. Again, for a site-diagonal σ_M the perturbation $g - \sigma_M$ is a sum of $\mathcal{V}_n$ and

$$\mathcal{T} = \sum_n \mathcal{T}_n [I + U_M^{OD} \mathcal{T}] \quad (5a)$$

$$= \sum_n \mathcal{T}_n + \sum_n \mathcal{T}_n U_M \sum_{m(\neq n)} \mathcal{T}_m + \dots , \quad (5b)$$

where $\mathcal{T}_n = [I - \mathcal{V}_n U_M]^{-1} \mathcal{V}_n$.

If U_M and P_M refer to the same reference medium they are related through either of the equations

$$U_M = W + W P_M W , \quad (6)$$

$$P_M = \sigma_M + \sigma_M U_M \sigma_M . \quad (7)$$

If we insert the definition of U and eq. (6) into the defining relation for $\mathcal{T}$, eq. (4), and multiply from both sides by W^{-1}, we obtain after some algebra

$$G = P_M + W^{-1} U_M \mathcal{T} U_M W^{-1} = P_M + P_M(\sigma_M^{-1} \mathcal{T} \sigma_M^{-1}) P_M . \quad (8)$$

Comparison of this equation with (2) shows that

$$T = \sigma_M^{-1} \mathcal{T} \sigma_M^{-1} , \quad (9)$$

$$\langle T\rangle = \sigma_M^{-1} \langle \mathcal{T}\rangle \sigma_M^{-1} . \quad (10)$$

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These equations are still exact. Now if an approximation is made, the results of locator and propagator formalism will be equivalent (i.e. give the same $\langle G \rangle$) if (10) still holds for the *approximations* to $\langle T \rangle$ and $\langle \mathcal{T} \rangle$.

For a site-diagonal σ_M the off-diagonal part of (7) is $P_M^{OD} = \sigma_M U_M^{OD} \sigma_M$. Substitution into (3a) followed by multiplication from both sides by σ_M gives

$$\sigma_M T \sigma_M = \sum_n \sigma_M T_n \sigma_M \, [I + U_M^{OD} \sigma_M T \sigma_M] \, . \qquad (11)$$

Comparing this with (5a) we find, because of (9), $\Sigma_n \sigma_M T_n \sigma_M = \Sigma_n \mathcal{T}_n$. Taking the nn-matrix element of this equation shows that

$$\sigma_M T_n \sigma_M = \mathcal{T}_n \, . \qquad (12)$$

From this equation we infer that the multiple-scattering expansion (3b) for T and the corresponding expansion (see (5b)) for $\sigma_M^{-1} \mathcal{T} \sigma_M^{-1}$ are term-by-term and factor-by-factor equal. Therefore *any* formal procedure for averaging these expansions in an approximate way produces approximations to $\langle T \rangle$ and $\langle \mathcal{T} \rangle$ that satisfy (10). This statement in particular applies to the single-site approximation, where one decouples averages over products of t-matrices completely, and we conclude that propagator and locator approach are equivalent for this approximation. We have seen that in order to obtain this result it is of no importance whether the reference medium is determined self-consistently (CPA) or not (ATA). Note also that our proof holds for any probability distribution of site energies, either discrete or continuous. The fact that both propagator and locator formalism yield the ATA implies that, irrespective of the choice of E_M, the ATA describes both the virtual crystal limit and the atomic limit correctly.

Essential in arriving at our result are the following points. First, the possibility to decompose, in either formalism, the perturbation into non-overlapping contributions leading to the occurrence of only the off-diagonal part of P_M and U_M in the expansions of T and $\mathcal{T}$. Second, the absence of mixing between diagonal and off-diagonal part of P_M and U_M in going from one formalism to the other. Both characteristics arise from the particular structure of the Hamiltonian and the choice of a site-diagonal σ_M (or V_M). Similar arguments apply to the molecular extension of the ATA [6], the non-self-consistent analogue of Tsukada's molecular CPA [7], characterized by non-overlapping contributions from molecular clusters and a cluster-diagonal σ_M. With slight modifications our proof shows that the propagator-locator equivalence holds not only for the molecular CPA [8] but also for the molecular ATA.

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