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LETTER TO THE EDITOR

Coherent potential approximation, averaged T-matrix approximation and Lloyd's model

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Abstract. It is shown how the single-site coherent potential approximation and the averaged T-matrix approximation become exact in the calculation of the averaged single-particle Green function of the electron in the Anderson model when the site energy is distributed randomly with lorentzian distribution. Using these approximations, Lloyd's exact result is reproduced.

The coherent potential approximation (CPA) and averaged T-matrix approximation (ATA) (Korringa 1958, Beeby 1964) are useful approximations in the study of disordered systems. The CPA is the simplest selfconsistent approximation which gives the first several moments of the density of states correctly (Schwartz and Siggia 1972). In this letter we wish to point out an interesting observation regarding the exactness of the CPA and ATA (from the averaged single-particle Green function point of view) for the lorentzian distribution of randomness (diagonal) in the Anderson hamiltonian (Anderson 1958). This, to the best of our knowledge, has not been observed before.

We consider the hamiltonian of an electron in the tight-binding approximation in the Wannier representation (Anderson 1958):

$$H = \sum_n \epsilon_n C_n^\dagger C_n + \sum_{m \neq n} V_{mn} C_m^\dagger C_n = V + H_0 \tag{1}$$

where $C_n^\dagger$ and C_n are the creation and annihilation operators for the electron in the Wannier orbital centred at the nth site, ϵ_n is the corresponding energy which is assumed to be random with a probability distribution $P(\epsilon)$, and V_{mn} is the hopping matrix element which is not random. Since it is essentially a one-body problem, we omit the spin index. $G^0 = 1/(E - H_0)$ and $G = 1/(E - H_0 - V)$ are the single-particle Green operators. And $G_{kq}(E)$ and $G_{mn}(E)$ are the Green functions in the momentum and site representation respectively. The ensemble-averaged Green function

$$\langle G_{kk}(E) \rangle = \frac{1}{E - \epsilon_k - U(k,E)} = G_{kk}{}^0(E - U(k,E)) \tag{2}$$

where ϵ_k is the Fourier transform of V_{mn}, and $U(k,E)$ is the self-energy of the electron which arises because of averaging.

In the CPA we calculate $\langle G \rangle$ selfconsistently as follows. Dyson's equation is (Soven 1967)

$$G = \bar{G} + \bar{G}T\bar{G} \tag{3}$$

where T is the total scattering matrix (T-matrix) defined as

$$T = \sum_m T_m, \qquad T_m = t_m(1 + \bar{G}) \sum_{m \neq n} T_n. \tag{4}$$

Here

$$t_m = \frac{\epsilon_m - U}{1 - (\epsilon_m - U)\bar{G}} \tag{5}$$

is the T-matrix corresponding to the nth site. We want to find a $\bar{G}$ selfconsistently such that $\langle T \rangle = 0$ (which implies that $\bar{G} = \langle G \rangle$). In the single-site CPA we write

$$\langle t_n \sum_{n \neq m} T_m \rangle \approx \langle t_n \rangle \sum_{m \neq n} \langle T_m \rangle.$$

Therefore

$$\langle T \rangle = \sum_m \langle T_m \rangle \approx \sum_n \langle t_n \rangle [(1 + \langle G \rangle) \sum_{m \neq n} T_m] \tag{6}$$

and hence $\langle T \rangle = 0$ implies $\langle t_n \rangle = 0$.

Choosing the lorentzian distribution $P(\epsilon) = \Gamma/[\pi(\epsilon^2 + \Gamma^2)]$ for the randomness in energy (centred at the origin with half-width Γ), we have

$$\langle t_n \rangle = \frac{1}{\pi} \int_{-\infty}^{+\infty} \frac{\Gamma^2}{\epsilon_n^2 + \Gamma^2} \frac{(\epsilon_n - U)\mathrm{d}\epsilon_n}{1 - (\epsilon_n - U)\langle G \rangle} = 0. \tag{7}$$

Performing the integration by using the contour integration method (Lloyd 1969), making use of the general analytic properties of U and $\langle G \rangle$, we get

$$U = -\mathrm{i}\Gamma S(E)$$

where

$$S(E) = \text{sign (Im } E).$$

Therefore

$$\langle G(E) \rangle = G^0(E + \mathrm{i}\Gamma S(E)). \tag{8}$$

This is exactly the exact (averaged) Green function obtained by Lloyd (1969) for the Anderson hamiltonian with site energies distributed according to a lorentzian distribution.

In the ATA we do not find $\langle G \rangle$ selfconsistently; we merely average the T-matrix with the following approximations and find out the self-energy. The Green function

$$G_{nn}(E) = G_{nn}{}^0(E) + \sum_m G_{nm}{}^0(E) t_m(E) G_{mn}{}^0(E) + \sum_{\substack{m \neq n \\ m' \neq m}} G_{nm}{}^0(E) t_m(E) G_{mm'}{}^0(E) t_{m'}(E) G_{m'n}{}^0(E) + \ldots . \tag{9}$$

Averaging G with the assumption that

$$\langle t_n{}^m \rangle \approx \langle t_n \rangle^m = \langle t \rangle^m \tag{10}$$

(because G_{nn} and t_n become independent of the site after averaging), we find

$$\langle G_{nn}(E) \rangle = G_{nn}{}^0(E) + \sum_m G_{nm}{}^0(E) \langle t(E) \rangle G_{mn}{}^0(E) + \sum_{\substack{m \neq n \\ m' \neq m}} G_{nm}{}^0(E) \langle t(E) \rangle G_{mm'}{}^0(E) \langle t(E) \rangle G_{m'n}{}^0(E) + \ldots . \tag{11}$$

We can also write (with no restriction in the summation) (Ziman 1969)

$$\langle G_{nn}(E)\rangle = G_{nn}^{0}(E) + \sum_{m} G_{nm}^{0}(E)UG_{mn}^{0}(E) + \sum_{m,m'} G_{nm}^{0}(E)UG_{mm'}^{0}(E)UG_{m'n}^{0}(E) + \ldots \tag{12}$$

where

$$U = \frac{\langle t\rangle}{1 + \langle t\rangle G_{00}^{0}(E)}, \qquad \langle G_{nn}(E)\rangle \equiv \langle G_{00}(E)\rangle, \qquad G_{nn}^{0}(E) \equiv G_{00}^{0}(E) \tag{13}$$

and

$$\langle t\rangle = \frac{1}{\pi}\int_{-\infty}^{\infty} \frac{\Gamma}{\epsilon^2 + \Gamma^2}\frac{\epsilon \mathrm{d}\epsilon}{1 - \epsilon G_{00}^{0}(E)}. \tag{14}$$

Performing the integration by the contour integration method as mentioned before, we get

$$\langle t\rangle = \frac{\mathrm{i}\Gamma S(E)}{1 - \mathrm{i}\Gamma G_{00}^{0}(E)S(E)}. \tag{15}$$

Substituting for $\langle t\rangle$ in equation (13) we get $U = -\mathrm{i}\Gamma S(E)$. Thus again we get Lloyd's exact result, namely

$$\langle G_{00}(E)\rangle = G_{00}^{0}(E + \mathrm{i}\Gamma S(E)). \tag{16}$$

In this letter we have shown how the single-site CPA and ATA become exact in evaluating the averaged single-particle Green function with lorentzian distribution of energy in Anderson's model. Hence, in the calculation of the single-particle density of states (and properties which can be calculated from the averaged Green function) for materials with cellular disorder with the randomness approximately lorentzian, the CPA and ATA will be good approximations

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