COHERENT POTENTIAL APPROXIMATION, AVERAGED T-MATRIX APPROXIMATION AND LLOYD'S MODEL

A. PRASANNA KUMAR
Department of Physics, Central College, Bangalore University, Bangalore-560001, India

AND

G. BASKARAN
Department of Physics, Indian Institute of Science, Bangalore-560012, India

ABSTRACT

In this paper we have shown how the single site Coherent Potential Approximation (CPA) and the Averaged T-Matrix Approximation (ATA) become exact in the calculation of the averaged single particle Green's function of the electron in the Anderson model, when the site energy is distributed randomly with Lorentzian distribution. Thus we reproduce Lloyd's exact result using the above-mentioned approximations.

COHERENT Potential Approximation (CPA) and Averaged T-Matrix Approximation (ATA) (Korringa, 1958 ; Beeby, 1964) are useful approximations in the study of disordered systems. CPA is the simplest self-consistent approximation which gives the first several moments of the density of states correctly (Schwartz and Siggia, 1972). In the present note we wish to point out an interesting observation regarding the exactness of CPA and ATA (from the averaged single particle Green's 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)

$$H = \sum_n \epsilon_n C_n^+ C_n + \sum_{m \neq n} V_{mn} C_m^+ C_n \qquad (1)$$

$$= V + H_0$$

where C_n^+ and C_n are the creation and annihilation operators for the electron in the Wannier orbital centred at the n-th 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.

$$G^0 = \frac{1}{E - H_0} \quad \text{and} \quad G = \frac{1}{E - H_0 - V}$$

are the single particle Green's operators. And $G_{kq}(E)$ and $G_n(E)$ are the Green's functions in the momentum and site representation respectively. The ensemble averaged Green's function

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

$$= G_{kk}^0 (E - U(k, E))$$

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

In the CPA we calculate G self-consistently as follows. Dyson's equation is

$$G = \bar{G} + \bar{G} T \bar{G} \qquad (2)$$

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

$$T = \sum_m T_m$$

$$T_m = t_m (1 + \bar{G}) \sum_{m \neq n} T_n$$

and

$$t_m = \frac{\epsilon_n - U}{1 - (\epsilon_n - U)\bar{G}}$$

is the T-matrix corresponding to the n-th site. We want to find a G self-consistently such that $\langle T \rangle = 0$ (which implies that $G = \langle G \rangle$). In the single site CPA we write

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

$$\therefore \langle T \rangle = \sum \langle T_n \rangle \approx \sum \langle t_n \rangle [(1 + \langle G \rangle) \sum_{m \neq n} T_m]$$

Therefore

$$\langle T \rangle = 0 \Rightarrow \langle t_n \rangle = 0.$$

Choosing the Lorentzian distribution

$$P(\epsilon) = \frac{1}{\pi} \frac{\Gamma}{(\epsilon^2 + \Gamma^2)}$$

for the randomness in energy (centred at the origin) with

$$\langle t_n \rangle = \frac{1}{\pi} \int_{-\infty}^{+\infty} \frac{\Gamma}{\epsilon_n^2 + \Gamma^2} \left[1 - \frac{\epsilon_n - U}{(\epsilon_n - U)\langle G \rangle}\right] \times d\epsilon_n = 0.$$

Performing the integration by using the contour-integration method making use of the general analytic properties of G and U we get

$$U = -i\Gamma S(E)$$

where

$$S(E) = \text{sign}\,(Im\,(G)) = \text{sign}\,(ImE)$$

$$\therefore \langle G(E)\rangle = G^0(E + i\Gamma S(E)). \quad (3)$$

This is exactly the exact (averaged) Green's function got by Lloyd (Lloyd, 1969) for the Anderson Hamiltonian with site energies distributed according to Lorentzian distribution.

In the ATA we do not find U self-consistently. But we just average the T-matrix with the following approximations and find out the self-energy. The Green's function

$$G_{nn}(E) = G^0_{nn}(E) + \sum_{m\neq n} G^0_{nm}(E)\, t_m\, G^0_{mn}(E) + \sum_{\substack{m\neq n\\ m'\neq m}} G^0_{nm}(E)\, t_m\, G^0_{mm'}(E)\, t_{m'}\, G^0_{m'n}(E) + \cdots.$$

Averaging G with the assumption that

$$\langle t_n^m\rangle \approx \langle t_n\rangle^m = \langle t\rangle^m.$$

(Because after averaging t is independent of the site) we find

$$\langle G_{nn}(E)\rangle = G^0_{nn}(E) + \sum_{m\neq n} G^0_{nm}(E)\,\langle t\rangle\, G^0_{mn}(E) + \sum G^0_{nm}(E)\,\langle t\rangle\, G_{mm'}(E)\,\langle t\rangle\, G^0_{m'n}(E) + \cdots.$$

We can also write (with no restriction in the summation) (Ziman, 1968)

$$\langle G_{nn}(E)\rangle = G^0_{nn}(E) + \sum_m G^0_{nm}(E)\, U\, G^0_{mn}(E) + \sum_{m\neq} G^0_{nm}(E)\, U\, G^0_{mm'}(E)\, U\, G^0_{m'm}(E) + \cdots$$

where

$$U = \frac{\langle t\rangle}{1 + \langle t\rangle G^0_{00}(E)} \quad (4)$$

and

$$\langle t\rangle = \frac{1}{\pi}\int_{-\infty}^{\infty} \frac{\Gamma}{\epsilon^2 + \Gamma^2}\,\frac{\epsilon}{1 - \epsilon G^0_{00}(E)}.$$

Performing the integration by contour integration method as mentioned before

$$\langle t\rangle = \frac{i\Gamma S(E)}{1 - i\Gamma S(E)\, G^0_{00}(E)}.$$

Substituting for $\langle t\rangle$ in equation (4) we get $U = -i\Gamma S(E)$

Thus again we get Lloyd's exact result, namely,

$$\langle G_{00}(E)\rangle = G^0_{00}(E + i\Gamma S(E)).$$

In this note we have shown how the single site CPA and ATA become exact in evaluating the averaged single particle Green's 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's function) for materials with cellular disorder with the randomness approximately Lorentzian, CPA and ATA will be good approximations.

The authors wish to thank Dr. N. Kumar and Prof. K. P. Sinha for valuable discussions. One of us (G. B.) thanks the C.S.I.R. (Delhi, India) and the authorities of the Indian Institute of Science (Bangalore, India) for their financial assistance.

1. Anderson, P. W., *Phys. Rev.*, 1928, 109, 1492.
2. Beeby, J. L., *Proc. Roy. Soc.* (London), 1964, 279 A, 82.
3. Korringa, J., *J. Phys. Chem. Solids*, 1958, 1, 252.
4. Lloyd, P., *J. Phys. C. Solid St. Phys.*, 1969, 2, 1717.
5. Schwartz, L. and Siggia, E., *Phys. Rev.*, 1972, 5 B, 383.
6. Soven, P., *Ibid.*, 1967, 156, 809.
7. Ziman, J. M., *J. Phys. C. Solid St. Phys.*, 1969, 2, 1230.