1 Computation of Green function of 1d Anderson model

Let $G(E) = (E - i\eta - H_0 - V)^{-1}$ (with $\eta > 0$ and $\eta \searrow 0$) the Green operator for the Anderson 1d model with $(H_0)_{nm} = -t(\delta_{n,m+1} + \delta_{n,m-1}$ (with periodic boundary conditions : $n, m \in \{0, \ldots, N-1\}$ and $n = N \quad \Leftrightarrow \quad n = 0$) and $V_{nm} = \varepsilon_n \, \delta_{nm}$ with random $\varepsilon_n \in [-W/2, W/2]$ (W =disorder strength and $t = 1$ hopping parameter). Let $\bar{G}(E) = \langle G(E) \rangle$ the average of $G(E)$ with respect to all random diagonal energies ε_n. According to the resummation of the 1d simple disorder diagramms one can shown that in a very good approximation :

$$\bar{G}(E) = \frac{1}{E - H_0 - \Sigma(E)}$$

where the (complex) self energy is determined by the implicit equation :

$$\Sigma(E) = \left\langle V \bar{G}(E) V \right\rangle = \left\langle V \frac{1}{E - H_0 - \Sigma(E)} V \right\rangle \quad \Rightarrow$$

$$\Sigma(E)_{nm} = \left\langle \varepsilon_n \left(\frac{1}{E - H_0 - \Sigma(E)} \right)_{nm} \varepsilon_m \right\rangle = \delta_{nm} \sigma^2 < n | \frac{1}{E - H_0 - \Sigma(E)}) | m > \tag{1}$$

where $\sigma^2 = \langle \varepsilon_n^2 \rangle = W^2/12$ and $\langle \varepsilon_n \varepsilon_m \rangle = 0$ if $n \neq m$. Note in principle the diagrammatic argument requires a gaussien distributed energy ε_n but it also works well for the box distribution $\varepsilon_n \in [-W/2, W/2]$ if we use the correct value of the variance $\sigma^2 = W^2/12$. Here $|n>$ are the states of the lattice basis. Furthermore, in principle $\Sigma(E)$ is a matrix but the above formula shows it is diagonal and in addition its diagonal matrix elements $\Sigma(E)_{nn} = \Sigma(E)$ do not depend on n due to translational invariance (once the ensemble ε_n-average is done), i.e. $\Sigma(E) = \Sigma(E) \mathbb{1}$ (it is proportional to the unit matrix).

We denote by $|k>$ the eigenstates of H_0 which are $< n|k >= e^{ikn}/\sqrt{N}$ with $k = 2\pi l/N$ for $l = 0, 1, \ldots, N-1$. Then we have $H_0|k> = -2t\cos(k)|k>$ and also $\bar{G}(E)|k> = 1/(E + 2t\cos(k) - \Sigma(E))|k>$, i.e. the average green function $\bar{G}(E)$ is also diagonal in the $|k>$ basis. Then we can rewrite :

$$\Sigma(E) = \sigma^2 \sum_k < n|k > \frac{1}{E + 2t\cos(k) - \Sigma(E)} < k|n >= \frac{\sigma^2}{N} \sum_k \underbrace{e^{-ikn} e^{ikn}}_{=1} \frac{1}{E + 2t\cos(k) - \Sigma(E)}$$

$$\Rightarrow \quad \Sigma(E) = \frac{\sigma^2}{N} \sum_k \frac{1}{E + 2t\cos(k) - \Sigma(E)} \equiv F_1(\Sigma(E)) \tag{2}$$

$$\Rightarrow \quad \Sigma(E) = \frac{\sigma^2}{2\pi} \int_0^{2\pi} \frac{dk}{E + 2t\cos(k) - \Sigma(E)} \equiv F_2(\Sigma(E)) \; , \tag{3}$$

Here we have replaced $1/N \sum_k (\ldots) \to 1/(2\pi) \int_k dk (\ldots)$ since $k = 2\pi l/N \quad \Rightarrow \quad dk = 2\pi/N$ (because $l = 0, 1, \ldots, N-1$ is integer).

The self energy energy $\Sigma(E)$ can be computed numerially from either (2) or (3) as solution of an implicit equation. Here it is important to use a complex value of $\Sigma(E) = \Sigma_1(E) + i\Sigma_2(E)$. For example, one can choose some initial value for $\Sigma(E)$ (e.g. $\Sigma(E)_{\text{initial}} = i\sigma^2/2$) and then iterate $\Sigma(E) = F_j(\Sigma(E))$ for $j = 1$ or $j = 2$. This method converges but quite slowly. To have faster convergence, one can use the secant method to find the (complex) zero of the function $\tilde{F}_j(x) \equiv F_j(x) - x$. For the case $j = 1$ one can directly evaluate the k-sum in a computer code (Python or C/C++ etc.) but if W is too small one needs a large value of N to have a better continuous limit (e.g. $N = 1000$ for $W = 1$ but $N = 100000$ for $W = 0.1$). This method is "easy" to implement in a code.

For the case $j = 2$ (with the integral) one needs first to evaluate (analytically) the integral (as **exercice !**). For this one can replace $z = e^{ik} \quad \Rightarrow \quad dz = ie^{ik} dk \quad \Rightarrow \quad dk = dz/(iz)$ which gives a closed complex integral over the unit cercle which can be evaluated by the residuum theorem. Here the integrand function will be of the form $1/[(z - z_1)(z - z_2)]$ where e.g. z_1 is inside the unit cercle and z_2 is outside the unit cercle ($z_{1,2}$ have to expressed in E and $\Sigma(E)$). Once the formula for the integral $F_2(\Sigma(E))$ is known, one has to do numerics (fix point iteration or secant method) to compute $\Sigma(E)$.

Once $\Sigma(E)$ is computed for many E-values one can compute the density of states :

$$\rho(E) = \frac{1}{\pi}\Im(\mathrm{Tr}\bar{G}(E)) = \frac{1}{\pi}\Im\left(\sum_n < n|\bar{G}(E)|n >\right) = \frac{N}{\pi\sigma_2}\Sigma_2(E)$$

where $\Sigma_2(E) = \Im(\Sigma(E))$ is the imaginary part of $\Sigma(E)$. For the last identity, we have used (1) and the fact that $< n|\bar{G}(E)|n >$ does not depend on n.

The above density of states is normalized such that $\int dE\rho(E) = N$. If one wants the normalization to be 1 one has to divide $\rho(E)$ by N. To have the full intervall of E one should compute $\rho(E)$ for all $E \in [-E_{\max}, E_{\max}]$ where $E_{\max}$ should be a bit larger than $2 = 2t$ for small W but for larger W one should choose something like $E_{\max} = 2 + W/2$ (or similar).

If E is outside the spectral interval of H, the methods works also very well. In this case the found solution of $\Sigma(E)$ will be real and $\Sigma_2(E) = 0$ such that $\rho(E) = 0$. For E inside the spectral interval one finds $\Sigma_2(E) > 0$ and $\rho(E) > 0$.

Note : if one uses the method with discrete sum (2) and if W is very small and N not large enough one may also find $\Sigma_2(E) = 0$ even if E is inside the spectral interval. Increasing N will then give $\Sigma_2(E) > 0$ as it should be.

Of course, the best method is to use the analytical formula which can be obtained from (3) by evaluating the integral by the residuum method. Then, one has no problem with a too small value of N.

Remark : If one uses the other convention of the Green function : $G = 1/(E + i\eta - H_0 - V)$ (with a different sign for η one will have $\Sigma_2(E) < 0$ and the density of state formula will be $\rho(E) = -1/(\pi\sigma^2)\Im(\Sigma(E) = -1/(\pi\sigma^2)\Sigma_2(E) = 1/(\pi\sigma^2)|\Sigma_2(E)|$.

In this case one needs to compute the solution with $\Sigma_2(E) < 0$ (of Eqs. (2) or (3)) by choosing an initial value with negative imaginary part.