4th Exercise 10.7.2015

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Greens functions an self-energies

Consider a "molecule" described by a (2 × 2) Hamiltonian matrix

$$H = \begin{bmatrix} \varepsilon_0 & \tau \\ \tau & \varepsilon_1 \end{bmatrix}$$

1. Create the corresponding Green's function
$$G(E) = [EI - H + i\eta I]^{-1}$$
with a given η and I denotes the identity matrix. Hint: imaginary numbers in python are e.g. `z=5+4j` and the inverse of a matrix can be obtained with `numpy.linalg.inv()`. Use G to calculate the (2 × 2) spectral function $A(E)$ with
$$A = i[G - G^+].$$
Hint: The transpose of a `numpy` matrix `A` is `A.T`, the complex conjugate `A.conj()` and the real part of a complex number by `z.real`. Use $A(E)$ to calculate the local density of states where the diagonal elements are interpreted as local density of states (LDOS) on the two sites (why ?).
Use $\varepsilon_0 = -0.25$ eV, $\varepsilon_1 = 0.25$ eV, $\tau = 0.5$ eV and find a reasonable value for η to plot the LDOS at the two sites in the energy range [-1, 1]. How does a change of parameters influence the LDOS ?
2. Now we use the equivalent formulation using the self-energy that is induced to site 0 through the presence of site 1
$$\Sigma = \tau g_1 \tau = \frac{|\tau|^2}{E - \varepsilon_1 + i\eta}$$
leading to the Green's function of site 0
$$g = \frac{1}{E - \varepsilon_0 + i\eta - \Sigma}$$
from which we can obtain the LDOS of site 0 through
$$a = i(g - g^*).$$
Show that this leads to the same result as above.