1. Prove that the expectation value of a Hermitean operator $\mathcal{A}$,

$$A = \sum_n f(\varepsilon_n) \langle \varphi_n | \mathcal{A} | \varphi_n \rangle \ , \tag{1}$$

where $f(\varepsilon) = 1/\left(1 + e^{(\varepsilon-\mu)/k_BT}\right)$ is the Fermi distribution, μ is the chemical potential, and $H|\varphi_n\rangle = \varepsilon_n|\varphi_n\rangle$, can be expressed as

$$A = -\frac{1}{\pi} \operatorname{Im} \int_{\curvearrowright} dz\, f(z)\, Tr\left(\mathcal{A}\mathcal{G}(z)\right) - 2k_BT \sum_{\operatorname{Im} z_k > 0} \operatorname{Re} Tr\left(\mathcal{A}\mathcal{G}(z_k)\right) \ , \tag{2}$$

where $\curvearrowright$ denotes a contour in the upper complex semiplane starting end ending at $-\infty$ and ∞, respectively, and $z_k = \mu + i(2k+1)\pi k_BT \quad (k \in \mathbb{Z})$ are the poles of $f(z)$ (fermionic Matsubara poles) lying between the real axis and $\curvearrowright$.

2. Let's consider a solid system described by a tight-binding Hamiltonian matrix, $\underline{\underline{H}} = \left\{\underline{H}_{ij}\right\}$. The atom at site i is replaced by an other atom, characterized by the on-site matrix, $\underline{H}'_i$, while the off-site blocks of the Hamiltonian are supposed to be unchanged.

(a) Prove that the corresponding site-diagonal block of the resolvent matrix is

$$\underline{G}'_{ii}(z) = \underline{G}_{ii}(z) \left(\underline{I} - \Delta\underline{H}_i \underline{G}_{ii}(z)\right)^{-1} \ , \tag{3}$$

where $\Delta\underline{H}_i = \underline{H}'_i - \underline{H}_i$ and $\underline{G}_{ii}(z)$ is the site-diagonal block of the resolvent matrix of the host system.

(b) Show that the single-site CPA condition for the t-matrices is equivalent with the following condition for the resolvent matrices,

$$\underline{G}^c_{ii}(z) = c\underline{G}^A_{ii}(z) + (1-c)\underline{G}^B_{ii}(z) \ , \tag{4}$$

where $\underline{G}^\alpha_{ii}(z)$ denotes the site-diagonal block of the resolvent matrix when a single impurity of type $\alpha \in \{A, B\}$ is embedded into the effective medium at site i.

(The exercize was in part solved during the course.)

3. The nearest neighbor tight-binding Hamiltonian for a single-band system on a simple one-dimensional lattice with lattice constant a is given by

$$H_{ij} = \varepsilon_0 \delta_{ij} + V\left(\delta_{i,j+1} + \delta_{i,j-1}\right) \ , \tag{5}$$

where i and j denote sites of the lattice ($V > 0$). Prove that, for $\operatorname{Im} z > 0$ and $\varepsilon_0 - 2V < \varepsilon \equiv \operatorname{Re} z < \varepsilon_0 + 2V$, the real lattice representation of the resolvent can be expressed as

$$G_{ij}(z) = \frac{\left(\frac{z-\varepsilon_0}{2V} - \sqrt{\left(\frac{z-\varepsilon_0}{2V}\right)^2 - 1}\right)^{|i-j|}}{2V\sqrt{\left(\frac{z-\varepsilon_0}{2V}\right)^2 - 1}} \ , \tag{6}$$

consequently,

$$G_{ii}(z) = \frac{1}{\sqrt{(z-\varepsilon_0)^2 - 4V^2}} \ , \tag{7}$$

and the density of states per lattice site is

$$D(\varepsilon) = \frac{1}{\pi\sqrt{4V^2 - (\varepsilon - \varepsilon_0)^2}} \; ! \tag{8}$$

(The exercize was in part solved during the course.)

4. Show that the single-site CPA condition for the above mentioned system can be written in the form,

$$\varepsilon_c = c\varepsilon_A + (1-c)\,\varepsilon_B - (\varepsilon_A - \varepsilon_c(z))\,(\varepsilon_B - \varepsilon_c(z))\,G_c(z) \;\; , \tag{9}$$

where c is the concentration of component A, ε_A and ε_B are the on-site energies for components A and B, $\varepsilon_c(z)$ is the self-energy for the effective medium and

$$G_c(z) = \frac{1}{\sqrt{(z - \varepsilon_c(z))^2 - 4V^2}} \; ! \tag{10}$$

5. Let us fix the on-site energies in the above example as

$$\varepsilon_A = \varepsilon_0 \quad \varepsilon_B = -\varepsilon_0 \tag{11}$$

and introduce the variables

$$x_0 = \frac{\varepsilon_0}{2V} \;\; , \quad x_c = \frac{\varepsilon_c(z)}{2V} \;\; , \quad \omega = \frac{z}{2V} \;\; . \tag{12}$$

Eq. (9) can then be written as

$$x_c = (2c-1)\,x_0 + \frac{x_0^2 - x_c^2}{\sqrt{(\omega - x_c)^2 - 1}} \;\; . \tag{13}$$

Solve this equation numerically by writing a corresponding computer code!

Important note: from the two possible values of $\sqrt{(\omega - x_c)^2 - 1}$ *the one with negative imaginary part should be chosen!*

(a) An iterative solution can start with $x_c^{(1)} = (2c-1)\,x_0$ (in fact, this is the virtual crystal approximation). Apply a small positive imaginary part for ω ($\mathrm{Im}\,\omega \simeq 0.01 - 0.05$) and use a linear mixing scheme,

$$x_c^{(n+1),in} = \alpha\, x_c^{(n),out} + (1-\alpha)\, x_c^{(n),in} \tag{14}$$

with a suitable value of α ($\alpha \simeq 0.1 - 0.5$)!

(b) More preferably, the iterative process proposed to have a power-like convergence should be used. Start again with $x_c^{(1)} = (2c-1)\,x_0$, then follow the steps:

$$1: \quad G_c^{(n)}(z) = \frac{1}{\sqrt{\left(\omega - x_c^{(n)}\right)^2 - 1}} \tag{15}$$

$$\Downarrow$$

$$2: \quad t_c^{(n)} = \frac{c\left(x_0 - x_c^{(n)}\right)}{1 - \left(x_0 - x_c^{(n)}\right) G_c^{(n)}} - \frac{(1-c)\left(x_0 + x_c^{(n)}\right)}{1 + \left(x_0 + x_c^{(n)}\right) G_c^{(n)}} \tag{16}$$

$$\Downarrow$$

$$3: \quad \Delta x_c^{(n+1)} = \frac{t_c^{(n)}}{1 + t_c^{(n)} G_c^{(n)}} \tag{17}$$

$$x_c^{(n+1)} = x_c^{(n)} + \Delta x_c^{(n+1)}$$

$$\Downarrow$$

$$\text{repeat from step 1 until convergence} \tag{18}$$

After getting the self-consistent solution for x_c, plot the dimensionless densities of states,

$$D_c(\omega) = -\operatorname{Im} \frac{1}{\sqrt{(\omega - x_c)^2 - 1}}\,, \tag{19}$$

for $c = 0.5$ and $x_0 = 1$, for $c = 0.5$ and $x_0 = 2$, and for $c = 0.1$ and $x_0 = 2$!