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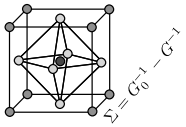
Computational Methods in Solid State Theory SS2016



Frankfurt, May 6, 2016

Exercise Set 3

(Due date: Monday, May 30, 2016)

Exercise 3 (**Matsubara Greens functions and Padé method**) (10 points)

Consider the two-band tight binding model that you determined for linarite in Exercise 2[1]. For calculations on the imaginary frequency axis use 500 positive Matsubara frequencies ω_n starting at index $n = 0$.

a) Calculate the non-interacting retarded Matsubara Greens functions

$$G(i\omega_n, \vec{k}) = \frac{1}{i\omega_n - \varepsilon(\vec{k})} \tag{1}$$

and determine the local Greens function

$$G_0(i\omega_n) = \sum_{\vec{k}} G(i\omega_n, \vec{k}) \tag{2}$$

by explicitly performing the summation over $\vec{k}$. $\varepsilon(\vec{k})$ is the tight binding dispersion. Consider a temperature $\beta = 40$ eV^{-1}. Mind that the unit cell of linarite contains two equivalent Cu atoms.

b) The Hilbert transformation is given by

$$G_0(i\omega_n) = \int_{-\infty}^{\infty} d\epsilon \frac{\rho(\epsilon)}{i\omega_n - \epsilon}, \tag{3}$$

where the density of states $\rho(\epsilon)$ for the Cu $3d_{x^2-y^2}$ bands crossing the Fermi level was determined from the tight binding fit in Exercise 2. Calculate $G_0(i\omega_n)$ via Hilbert transformation and compare to $G_0(i\omega_n)$ obtained from a). Again mind that the unit cell of linarite contains two equivalent Cu atoms.

c) Implement the method of Padé approximants and continue $G_0(i\omega_n)$ of Eq. (2) analytically to the real frequency axis. Plot the density of states $\rho(\omega) = -1/\pi \operatorname{Im} G_0(\omega)$ and compare to the tight binding result.

d) Use your tight binding density of states $\rho(\omega)$ from Exercise 2 to determine $\operatorname{Re} G_0(\omega)$ on the real frequency axis via Kramers-Kronig relations. Compare the result to $\operatorname{Re} G_0(\omega)$ from c).

[1] Suggestion: $\mu = 0.025409$ eV, $t_1 = 0.068275$ eV, $t_2 = 0.035080$ eV, $t_3 = 0.003569$ eV, $t_4 = 0.076800$ eV.