

Frankfurt, May 7, 2013

Exercises for Computational Methods in Solid State Theory
SS 2013

Exercise Set 3

(Due date: Tuesday, May 21, 2013)

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

Consider the one-band tight binding model that you determined for $\text{Sr}_2\text{CuO}_2\text{Cl}_2$ in Exercise 2¹.

a) Calculate the noninteracting retarded Matsubara Greens functions

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

and determine the local Greens function

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

by explicitly performing the \vec{k} summation. $\varepsilon(\vec{k})$ is the tight binding dispersion. Consider a temperature $\beta = 40 \text{ eV}^{-1}$.

b) Use the Hilbert transformation which is given as

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

where the density of states $\rho(\varepsilon)$ for the Cu $3d_{x^2-y^2}$ band crossing the Fermi level was determined by 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).

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 $\rho(\omega) = -1/\pi \text{Im } G_0(\omega)$ and compare to the tight binding result.

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

¹Suggestion: $\mu = 0.170664 \text{ eV}$, $t_1 = -0.409348 \text{ eV}$, $t_2 = 0.0793483 \text{ eV}$, $t_3 = -0.0566522 \text{ eV}$.