Goethe-Universität Frankfurt
Fachbereich Physik

Institut für Theoretische Physik
Dr. Harald O. Jeschke
Daniel Guterding

GOETHE
UNIVERSITÄT
FRANKFURT AM MAIN

Frankfurt, May 13, 2014

Exercises for Computational Methods in Solid State Theory
SS 2014

Exercise Set 3
(Due date: Monday, May 19, 2014)

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

Consider the one-band tight binding model that you determined for $Sr_2CuO_2Cl_2$ 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

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

and determine the local Greens function

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

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

b) The Hilbert transformation is given by

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

where the density of states $\rho(\epsilon)$ for the Cu $3d_{x^2-y^2}$ band 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).

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).

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[1]Suggestion: $\mu = 0.170664$ eV, $t_1 = -0.409348$ eV, $t_2 = 0.0793483$ eV, $t_3 = -0.0566522$ eV.