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Exercises for Computational Methods in Solid State Theory SS 2012

Exercise Set 6

(Due date: Monday, June 11, 2012)

Exercise 6 (**Semiclassical approximation**) (10 points)

The Hamiltonian of the single-band Hubbard model with frustration is given as

$$H = -t \sum_{<i,j>\sigma} c^\dagger_{i\sigma} c_{j\sigma} - t' \sum_{<i,j'>\sigma} c^\dagger_{i\sigma} c_{j'\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}, \tag{1}$$

where $c_{i\sigma}$ ($c^\dagger_{i\sigma}$) is the annihilation (creation) operator of an electron with spin σ at the i-th site, and U represents the Coulomb repulsion. The first two sums run over nearest and next nearest neighbours, respectively. The primitive vectors $\vec{a}_1$ and $\vec{a}_2$ on the triangular lattice are given as $\vec{a}_1 = (1, 0)$ and $\vec{a}_2 = (1/2, \sqrt{3}/2)$, respectively.

a) Calculate the non-interacting Green's function $G(i\omega_n)$ as a function of Matsubara frequency at half-filling for $T/t = 0.2$ and $t = t' = 1.0$.

b) Using single-site dynamical mean field theory (DMFT) with the semiclassical approximation as impurity solver, calculate the impurity Green's function $G(i\omega_n)$ and $G(\omega)$ as a function of Matsubara frequency ω_n and real frequency ω, respectively, at half-filling for $T/t = 0.2$, $t = t' = 1.0$ and $U/t = 12.0$.

c) Calculate $G(\omega)$ using the Padé approximation from $G(i\omega_n)$ and compare it with $G(\omega)$ from b) calculated directly with the semiclassical approximation.