QCM : practical exercices

June 20, 2012

Problem 1 : CPT and model building

Construct the cluster and model files representing a one-dimensional Hubbard model with dimerization : The hopping terms are between nearest neighbors only, but they alternate between the value t and the value t'. Plot the spectral function for the case $t = 1.1$ and $t' = 0.9$, at $U = 0$ and then $U = 4$, at half-filling. Compare the $U = 0$ case with the analytic solution to the problem.

Problem 2 : VCA for antiferromagnetism

A Find the VCA solution for Néel antiferromagnetism in the nearest-neighbor, particle-hole symmetric Hubbard model at half-filling, using **two** 3×3 clusters embedded in a two-dimensional square lattice. Use only one variational parameter : the Weiss field M. Plot the order parameter $\langle M \rangle$ as a function of U, from $U = 10$ to $U = 0$, in steps of $\Delta U = 0.5$.

B Refine your solution by adding to the list of variational parameters the hopping t on the cluster. Use the quasi-Newton method. Just find the solution for $U = 8$, still at half-filling. Is the ground state energy lower that in the simpler solution above ? What about the order parameter ?

C Refine your solution further by defining an additional operator on the cluster, that describes the hopping terms along the boundary of the cluster only (i.e. over 8 links). Add this operator to the list of variational parameters. Has the ground state energy still improved ? What about the order parameter ?

Problem 3 : CDMFT and the Mott transition in graphene

A Construct a model file that describes graphene, based on a single, two-site cluster with a bath of 4 sites (file `L2-4b.cluster` provided). Check that the correct dispersion relation is found at $U = 0$ by plotting the spectral function.

B At half filling, find de CDMFT solution (normal state) as a function of U, from $U = 10$ to $U = 0$ in steps of $\Delta U = 0.2$. Can you identify the Mott transition ? Stay at half-filling, using particle-hole symmetry.