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Exercises for Computational Methods in Solid State Theory
SS 2013

Exercise Set 8
(Due date: Tuesday, July 9, 2013)

Exercise 8 (**Hartree-Fock (HF) mean field calculations**) (10 points)

The physical properties of κ-(BEDT-TTF)$_2$X charge transfer salts can be described by a Hubbard model on the anisotropic triangular lattice which is given as

$$H = \sum_{\langle ij\rangle,\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} - \mu \sum_{i\sigma} c^\dagger_{i\sigma} c_{i\sigma}, \tag{1}$$

where $c^\dagger_{i\sigma}$ ($c_{i\sigma}$) are creation (annihilation) operators for electrons of spin σ, $n_{i\sigma} = c^\dagger_{i\sigma} c_{i\sigma}$ is the density of σ spin electrons and t_{ij} is the hopping amplitude. We choose to study here the case where $t_{ij} = t$ in two of the directions of the triangular lattice, and $t_{ij} = t'$ in the third direction (see Figure 1).

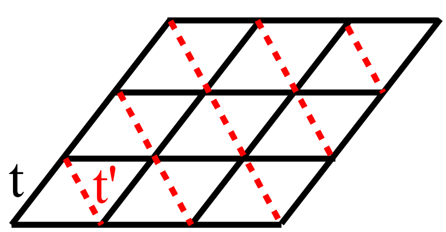

Figure 1: Anisotropic triangular lattice.

To study this model in the Hartree-Fock approximation we can consider two particular mean fields:

(2) $$H^{MF1} = H_\uparrow + H_\downarrow + C,$$

with:

$$\begin{aligned} H_\uparrow &= -t\sum_{\langle i,j\rangle} c^\dagger_{i,\uparrow}c_{j,\uparrow} + U\sum_i n_{i,\uparrow}\langle n_{i,\downarrow}\rangle, \\ H_\downarrow &= -t\sum_{\langle i,j\rangle} c^\dagger_{i,\downarrow}c_{j,\downarrow} + U\sum_i \langle n_{i,\uparrow}\rangle n_{i,\downarrow}, \\ C &= -U\sum_i \langle n_{i,\uparrow}\rangle\langle n_{i,\downarrow}\rangle. \end{aligned}$$

and

(3) $$H^{MF2} = C^\dagger \begin{pmatrix} H^{\uparrow\uparrow} & H^{\uparrow\downarrow} \\ H^{\downarrow\uparrow} & H^{\downarrow\downarrow} \end{pmatrix}_{2N\times 2N} C,$$

with:

$$\begin{aligned} C^\dagger &= (c^\dagger_{1,\uparrow}, ..., c^\dagger_{N,\uparrow}, c^\dagger_{1,\downarrow}, ..., c^\dagger_{N,\downarrow}) \\ H^{\uparrow\uparrow}_{i,j} &= (U\langle n_{i\downarrow}\rangle - \mu)\delta_{i,j} + T_{i,j} \\ H^{\uparrow\downarrow}_{i,j} &= -U\langle S^-_i\rangle\delta_{i,j} \\ H^{\downarrow\uparrow}_{i,j} &= -U\langle S^+_i\rangle\delta_{i,j} \\ H^{\downarrow\downarrow}_{i,j} &= (U\langle n_{i\uparrow}\rangle - \mu)\delta_{i,j} + T_{i,j} \end{aligned}$$

$$\begin{aligned} H^{MF2} &= -t\sum_{\langle i,j\rangle,\sigma} c^\dagger_{i,\sigma}c_{j,\sigma} + U\sum_i \left[\langle n_{i,\downarrow}\rangle n_{i,\uparrow} + \langle n_{i,\uparrow}\rangle n_{i,\downarrow} - \langle n_{i,\uparrow}\rangle\langle n_{i,\downarrow}\rangle\right] \\ &\quad -U\sum_i \left[\langle S^+_i\rangle c^\dagger_{i,\downarrow}c_{i,\uparrow} + \langle S^-_i\rangle c^\dagger_{i,\uparrow}c_{i,\downarrow} - \langle S^+_i\rangle\langle S^-_i\rangle\right] \end{aligned}$$

and in this exercise we will use the particular case where all the spin are in the xz-plane: $\langle S^+_i\rangle = \langle S^-_i\rangle = \langle S^x_i\rangle$

a) Using MF1 compute: the ground state energy per site, the gap and the local magnetization $\langle S^z\rangle$ at $U/t = 1$ and $U/t = 16$ at $t'/t = 0, 0.5$ for a system of size 10×10.

b) Using MF2 compute: the ground state energy, the local magnetizations $\langle S^z\rangle$ and $\langle S^x\rangle$ at $U/t = 16$ at $t'/t = 0.5, 0.8, 1$ for a system of size 10×10 and 12×12.

c) How could you define/describe the phase corresponding to each of the cases of question a) and b)?

d) Discuss the difference between results for the systems of size 10×10 and 12×12.

The computation should be realized in real space and at half-filling for a total magnetization equal to zero.