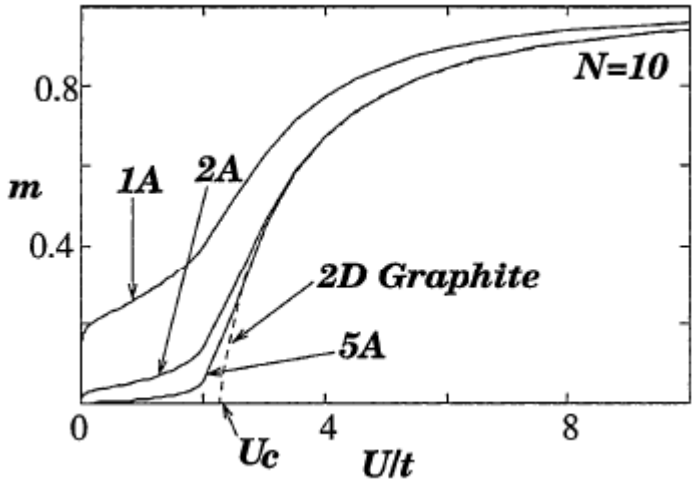
Graphene: Mean-field Hubbard model (For this project, you will need your own laptop computer and environment for numerical simulation and data visualization.)

We will discuss the mean-field Hubbard model during the lecture. Based on our discussion, do the following tasks.

(1) Solve self-consistently the mean-field Hubbard model for graphene (considering only the p_z orbitals and assuming that the overlap matrix is the identity matrix). More specifically, reproduce the dashed curve in the figure below [taken from Fujita et al., J. Phys. Soc. Jpn. 65, 1920 (1996)] within mean-field Hubbard scheme and show that magnetism appears only at U/t higher than a critical value (find this value). For the mean-field calculation, you will need to converge your calculation with respect to the number of k points. (Note that pristine graphene is not magnetic since U/t is not high enough. If graphene is strained, however, this ratio can be increased and graphene may have magnetism.)

At several distinct values of U/t (including 0 and U_c), draw the energy band structure. When m is not zero, what kind of magnetism do you see?



(2) Now repeat (1) for several non-zero charge density values.

In addition, describe how the phase diagram (like the figure above) changes as a function of charge density.