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Exercise 5:
Quantum Phase Transition in the Bose-Hubbard Model

In this exercise, we will return to the Bose-Hubbard model and study the quantum phase transition that arises from the competition between the kinetic and potential energy terms that favor a superfluid or Mott insulating phase, respectively. The Bose-Hubbard model is defined by the Hamiltonian

$$H_{BH} = -t \sum_{\langle ij \rangle} \left(b_i^\dagger b_j + b_j^\dagger b_i \right) + \frac{U}{2} \sum_i n_i(n_i - 1) - \mu \sum_i n_i$$

where the b_i ($b_i^\dagger$) are bosonic annihilation (creation) operators and $n_i = b_i^\dagger b_i$ is the onsite occupation. The parameter t is the hopping strength, U the strength of the onsite interaction, and μ the chemical potential.

We want to study this model via a world-line **quantum Monte Carlo** technique, and turn to the open-source ALPS project for an implementation of the so-called worm algorithm (where "worm" refers to the peculiarities of the construction of non-local updates of the world-line configuration).

Let's get started by taking a look at the ALPS project at: http://alps.comp-phys.org
Go to the *Download and Installation* section and install ALPS on your computer – you can either use the binary package for your system (Windows, Linux, OS X) or you may build ALPS from the source (Linux, OS X).

Once you have installed ALPS, you are almost ready to run a simulation of the Bose-Hubbard model above. Here is what needs to be done:

1. *Set up the model and define simulation parameters.* An example parameter file which allows you to set up the quantum Bose-Hubbard model will be discussed in the exercise class. We want to start with a simulation for a square lattice with $L \times L$ sites and periodic boundary conditions. Setting $U = 1$ we will vary the hopping strength $0 < t/U < 0.12$. From your simulations can you tell whether the system undergoes a phase transition in this parameter regime?

2. *Identifying the quantum phase transition.* To estimate the location of the quantum phase transition rather accurately we will to turn to the so-called superfluid stiffness ρ_s and its finite-size scaling in the vicinity of the transition.

- Extract the superfluid stiffness from your simulation output. Plot both ρ_s as well as $L \cdot \rho_s$ versus the hopping strength t – how does this help to locate the phase transition?
- Do you find agreement with the location of the transition $(t/U)_c = 0.05974...$ reported in the literature?
- Why do your current simulations overestimate the critical point of the transition?

3. *Further variations.* One of the strengths of the ALPS package is that you can easily change the setup of your simulations. In this spirit, redo the above analysis for the honeycomb lattice instead of the square lattice.