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UNIVERSITÄT
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10th Exercise Sheet Many-Body Physics

Will be discussed in the week of July 1-5.

Exercise 1: Bose-Hubbard Hamiltonian

Consider the Bose-Hubbard Hamiltonian on a cubic lattice (with coordination number $z = 2d = 6$),

$$H = -t \sum_{\langle i,j \rangle} b_i^\dagger b_j + \frac{U}{2} \sum_i n_i(n_i - 1) - \mu \sum_i n_i. \tag{1}$$

It has three phases: at high temperatures there is a normal liquid, which may turn into a superfluid at low enough temperature. At strong enough U/T and commensurate filling $n = 1, 2, \ldots$ only, a transition to a Mott insulator may occur however ($T = 0$ only).

a. Perform a Fourier transformation and the Bogoliubov prescription. Keep all terms to quadratic order, and diagonalize the effective Hamiltonian by means of a Bogoliubov transformation.

b. Compute the total density (at finite temperature)

c. We expect the transition to the Mott insulator to occur when we solve for n_0 at interger n and are unable to find a finite n_0. When do you get a transition? (the resulting equation has to be solved numerically, or you need to perform an asymptotic expansion for $U/t \to \infty$. Work with constant chemical potential for convenience).

d. We will now look at an alternative mean-field theory. For this, we first need the ground state in the strong coupling limit: In the limit $t = 0$ and commensurate densities, write down the ground state wave functions which are product wave functions. What do the Green functions look like in this limit?

e. Perform the decoupling approximation $b_i^\dagger b_j \to \langle b_i^\dagger \rangle b_j + b_i^\dagger \langle b_j \rangle - \langle b_i^\dagger \rangle \langle b_j \rangle$, and introduce the order parameter $\psi = \langle b_i^\dagger \rangle = \langle b_i \rangle$, taken uniformly on each lattice site.

f. Perform second order perturbation theory in ψ around the product wave functions ($T = 0$), and compute the second order correction to the energy.

g. The phase boundary can be found by setting the coefficient of the ψ^2 term equal to zero. By doing so, you get equations $\mu(U)$ for the phase boundaries.

h. Plot the resulting $T = 0$ phase diagram in the $(U/zt), (\mu/zt)$ plane.