INTRODUCTION TO MANY BODY PHYSICS: 620. Fall 2003

Questions 4. (Due Mon, Oct 27th)

1. (a) Consider the non-interacting Hubbard model for next nearest neighbor hopping on a two dimensional lattice

$$H - \mu N = -t \sum_{j,\hat{a}=\hat{x},\hat{y},\sigma} [{c^\dagger}_{j+\hat{a}\sigma} c_{j\sigma} + \text{H.c}] - \mu \sum_{j\sigma} {c^\dagger}_{j\sigma} c_{j\sigma}$$

where $n_{j\sigma} = {c^\dagger}_{j\sigma} c_{j\sigma}$ represents the number of electrons of spin component $\sigma = \pm 1/2$ at site j. Show that the dispersion of the electrons in the absence of interactions is given by

$$\epsilon(\vec{k}) = -2t(\cos k_x a + \cos k_y a) - \mu$$

where a is the distance between sites, and $\vec{k} = (k_x, k_y)$ is the wavevector.

(b) Derive the relation between the number of electrons per site n_e and the area of the Fermi surface.

(c) Sketch the Fermi surface when

i. $n_e < 1$.

ii. "half filling" where $n_e = 1$

(d) The corresponding interacting Hubbard model, with an interaction term $U n_\uparrow n_\downarrow$ at each site describes a class of material called "Mott insulators", which includes the mother compounds for high temperature superconductors. What feature of the Fermi surface at half-filling makes the non-interacting ground-state unstable to spin density wave formation and the development of a gap around the Fermi surface ?

(e) Derive the dispersion for the case when, in the one-particle Hamiltonian there is an additional next-nearest neighbor hopping matrix element of strength across the diagonal, $-t'$. (Hint: use the Fourier transform of $t(R)$, given by $t(\vec{k}) = \sum_{\vec{R}} t(\vec{R}) e^{-i\vec{k}\cdot\vec{R}}$). How does this affect the dispersion at half filling?

2. Consider an atom trap where the confining potential is given by a harmonic potential

$$V(x, y, z) = \frac{1}{2} m\omega^2 (x^2 + y^2 + z^2)$$

so that the quantized kinetic energy of an atom in the trap is

$$\begin{aligned} E_{lmn} &= \hbar\omega(l + \frac{3}{2}) \\ l &= n_1 + n_2 + n_3 \end{aligned} \tag{1}$$

where $n_{1,2,3} \geq 0$ are non-negative integers.

(a) Show that in thermal equilibtrium, the total number of particles in the trap is given by

$$N = \frac{z}{1-z} + \sum_{l \neq 0} \frac{1}{z^{-1} e^{\beta \hbar \omega l} - 1}$$

where $z = e^{\beta \mu^*}$, $\mu^* = \mu - \frac{3}{2}\hbar\omega$ and the sum over l, denotes a sum over all values of $n_{1,2,3}$. What is the interpretation of the first term? Why must μ^* be negative? What happens to z when condensation develops?

(b) Show that below the Bose Einstein condensation temperature,

$$N = N_0(T) + \sum_{k=1}^{\infty} \left[\left(\frac{1}{1 - e^{-xk}} \right)^3 - 1 \right], \qquad (x = \beta \hbar \omega)$$

where $N_0(T)$ is the number of atoms condensed in the lowest energy state. (Hint, Taylor expand the second term in (a) and then invert the order of summation.)

(c) Show that when x is small,

$$N = N_o(T) + \frac{T^3}{(\hbar\omega)^3}\zeta(3) + \frac{T^2}{(\hbar\omega)^2}\zeta(2) + O(T)$$

where $\zeta(n) = \sum_{k=1}^{\infty} \frac{1}{k^n}$. Notice that if the first term is of order N, the second term is of order $N^{2/3} << N$, if N is large.

(d) Calculate an expression for the Bose Einstein condensation temperature T_{BE} of the trap, and show that to a good approximation,

$$\frac{N_o(T)}{N} = 1 - \left(\frac{T}{T_{BE}} \right)^3 .$$

(e) Qualitatively: what do you expect to happen to the density profile across the trap, once the atoms start to condense?