INTRODUCTION TO MANY BODY PHYSICS: 620. Fall 2004

Answers to Questions 4. (Mon, Nov 1)

1. (a) If we insert the Fourier transformed operator

$$c_{j\sigma} = \frac{1}{\sqrt{N}} \sum_{\vec{k}} c_{\vec{k}\sigma} e^{-i\vec{k}\cdot\vec{R}_j} \tag{1}$$

into the kinetic part of the Hamiltonian

$$H = -t \sum_{\hat{a}=\hat{x},\hat{y},j\sigma} [c^{\dagger}{}_{j+\hat{a}\sigma} c_{j\sigma} + \text{H.c}] \tag{2}$$

we obtain

$$\begin{aligned} H &= -t \sum_{\vec{k},\vec{k}'\sigma} [c^{\dagger}{}_{\vec{k}\sigma} c_{\vec{k}'\sigma} e^{i(k_x+k_y)} \overbrace{\frac{1}{N}\sum_j e^{iR_j\cdot(\vec{k}-\vec{k}')}}^{\delta_{\vec{k},\vec{k}'}} + \text{H.c}] \\ &= \sum_{\vec{k}\sigma} [-2t(\cos k_x + \cos k_y)]\, c^{\dagger}{}_{\vec{k}\sigma} c_{\vec{k}\sigma}. \end{aligned}$$

Combining this with the chemical potential term $-\mu N = -\mu \sum_{\vec{k}\sigma} c^{\dagger}{}_{\vec{k}\sigma} c_{\vec{k}\sigma}$, we obtain

$$H = \sum_{\vec{k}\sigma} \epsilon_{\vec{k}} c^{\dagger}{}_{\vec{k}\sigma} c_{\vec{k}\sigma} \tag{3}$$

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

(b) The total number of particles is given by

$$N_e = \sum_{\vec{k}\sigma} \langle c^{\dagger}{}_{\vec{k}\sigma} c_{\vec{k}\sigma} \rangle \tag{4}$$

In the thermodynamic limit, we can replace $\sum_{\vec{k}} \to V \int_{\vec{k}}$, where $A = Na^2$ is the area of the system. Thus

$$N_e = Na^2 \sum_{\sigma} \int \frac{d^2k}{(2\pi)^2} n_{\vec{k}\sigma} \tag{5}$$

Now in the ground-state, $n_{\vec{k}\sigma} = \theta(-\epsilon_{\vec{k}})$ so that

$$N_e = 2Na^2 \int \frac{d^2k}{(2\pi)^2} \theta(-\epsilon) \tag{6}$$

We can identify the integral as $A_{FS}/(2\pi)^2$, where A_{FS} is the area of the Fermi surface. Thus the number of particles per unit area is

$$n_e = \frac{N_e}{Na^2} N_e = 2\frac{A_{FS}}{(2\pi)^2}. \tag{7}$$

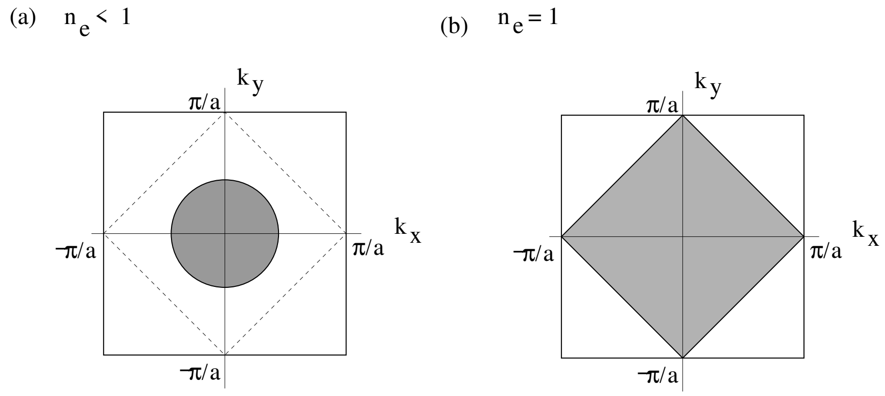


Figure 1:

(c) (a) When $\mu < 0$, the band is less than half filled, with $n_e < 1$. In this case, the Fermi surface is centered around $k = 0$ and for small filling, approximates a circle. (See below) (b) When $\mu = 0$, the band is "half filled" and $n_e = 1$. The Fermi surface is now a square, rotated through 45^0, occupying one half of the Brillouin zone, as shown in Fig. 1.

(d) When the band is half filled, the edges of the Fermi surface are parallel, and are said to be "nested". In this situation, the susceptibility of the metal towards the formation of a spin-density wave is logarithmically enhanced, which leads to a spin-density wave instability the moment a finite Hubbard U interaction is introduced into the system.

(e) If we introduce a second neighbor coupling t' across the diagonal, then the Fourier transform of the bond-hopping $t(\vec{R})$ becomes

$$t_{\vec{k}} = -2t(c_x + c_y) + 4t' c_x c_y$$

where $c_{x,y} \equiv \cos k_{x,y} a$. The dispersion is now

$$\epsilon_{\vec{k}} = t_{\vec{k}} = -2t(c_x + c_y) + 4t' c_x c_y - \mu \tag{8}$$

The next-neighbor coupling suppresses hopping along the diagonals, causing the Fermi surface to bulge along the diagonals at half-filling.

2. (a) The number of particles in the "$l - th$" level is given by the Einstein formula

$$n_l = \frac{1}{e^{\beta E_l} - 1} = \frac{1}{e^{\beta \hbar \omega_l} z^{-1} - 1} \tag{9}$$

where $z = e^{\beta(\mu - \hbar\omega 3/2}$. The total number of particles is then

$$N_e = \sum_l n_l = n_0 + \sum_{l \neq 0} \frac{1}{e^{\beta l \hbar \omega} z^{-1} - 1} = N_0(T) + \sum_{l \neq 0} n_l \tag{10}$$

where $N_0 \equiv n_0 = \frac{z}{(1-z)}$.

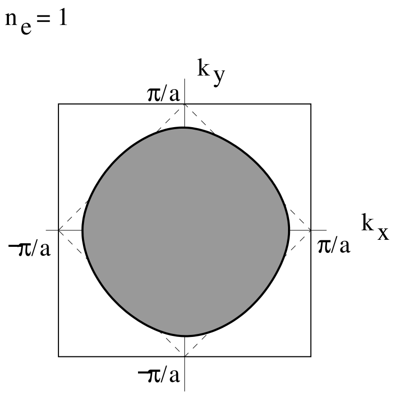


Figure 2:

(b) Beneath the Bose-Einstein condensation temperature $z \to 1$ and the number of bosons in the $l = 0$ state becomes quasi-macroscopic. In this case, we can write

$$N = \sum_l n_l = N_0 + \sum_{l \neq 0} \frac{1}{e^{\beta\hbar l\omega} - 1} \tag{11}$$

If we expand the Bose function as a power-series in $e^{-\beta\hbar\omega l}$, we obtain

$$\begin{aligned}
N &= N_0 + \sum_{l \neq 0} \sum_{k=1}^{\infty} e^{-k(\beta\hbar l\omega)} \\
&= N_o(T) + \sum_{k=1}^{\infty} \sum_{l \neq 0} e^{-k(\beta\hbar l\omega)} \\
&= N_o(T) + \sum_{k=1}^{\infty} \left(\sum_{n_1, n_2, n_3 \geq 0} e^{-k(\beta\hbar\omega(n_1+n_2+n_3))} - 1 \right) \\
&= N_o(T) + \sum_{k=1}^{\infty} \left(\left[\sum_{n \geq 0} e^{-k(\beta\hbar n\omega)} \right]^3 - 1 \right) \\
&= N_o(T) + \sum_{k=1}^{\infty} \left(\left[\frac{1}{1 - e^{-k\beta\hbar\omega}} \right]^3 - 1 \right)
\end{aligned} \tag{12}$$

(c) For small $x = \beta\hbar\omega$ we can expand

$$\frac{1}{(1 - e^{-kx})^3} = \frac{1}{(xk - \frac{1}{2}(xk)^2)^3} = \frac{1}{(xk)^3} + \frac{3}{2} \frac{1}{(xk)^2} + \ldots \tag{13}$$

so that The equation for the total number of particles then becomes

$$N = N_0 + \frac{T^3}{(\hbar\omega)^3} \zeta(3) + \frac{3}{2} \frac{T^2}{(\hbar\omega)^2} \zeta(2) + \ldots \tag{14}$$

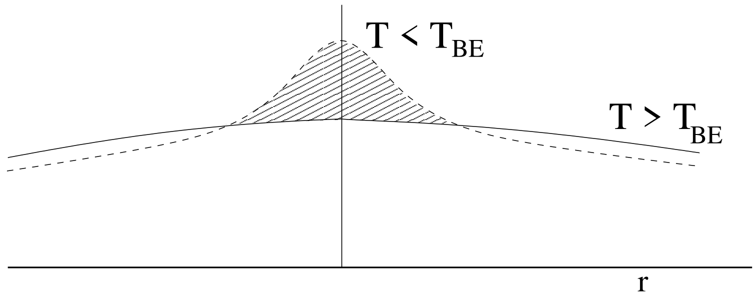


Figure 3: Sketching change in density profile below the condensation temperature.

(d) Since the second term is of order $N^{2/3}$, we can neglect it for large N. At the Bose Einstein condensation temperature, $N_0 = 0$, so that

$$N = \frac{T_{BE}^3}{(\hbar\omega)^3}\zeta(3)$$

from which we deduce that

$$N = N_0 + N\left(\frac{T}{T_{BE}}\right)^3$$

so that the condensate fraction is given by

$$\frac{N_0}{N} = \left[1 - \left(\frac{T}{T_{BE}}\right)^3\right]$$

where

$$T_{BE} = \hbar\omega\left(\frac{N}{\zeta(3)}\right)^{\frac{1}{3}}$$

(e) At temperatures $T > T_{BE}$, the density profile is determined by the sum of densities associated with the occupancy of all the higher states,

$$\rho(x) = \sum_{n_1,n_2,n_3} p_{n_1,n_2,n_3}|\psi_{n_1,n_2,n_3}|^2$$

whereas below the condensation temperature, the occupancy of the $l = 0$ state becomes macroscopic, and now

$$\rho(x) = \frac{N_0(T)}{N}|\psi_0(x)|^2 + \sum_{n_1,n_2,n_3} p_{n_1,n_2,n_3}|\psi_{n_1,n_2,n_3}|^2$$

The wavefunction of the lowest state is given by

$$\psi(x) \sim e^{-(x^2+y^2+z^2)/(4(\Delta x)^2)} \tag{15}$$

where $\Delta x \sim \sqrt{\frac{\hbar}{m\omega}}$. Now at T_{BE}, the characteristic size of the normal state wavefunction is given by $\Delta\tilde{x}^2 \sim T_{BE}/(\hbar\omega) \sim N^{1/3}/(\zeta_3)^{1/3} >> 1$. While the power of 1/3 doesn't make this a huge number, it does mean that the condensate fraction is much more tightly distributed about the origin than the normal state. Thus as the system is cooled through the Bose-Einstein condensation temperature, the density profile develops a bulge at short distances from the center of the trap. (See Fig. 3 above)

3. (a) If we take the expression for the Free energy

$$F(\lambda) = -T\ln Z(\lambda) = -T\ln \mathrm{Tr}[e^{-\beta[H_o+\lambda V]}] \tag{16}$$

and differentiate it, we obtain

$$\frac{\partial F}{\partial \lambda} = -\frac{T}{Z}\frac{\partial Z}{\partial \lambda}. \tag{17}$$

Now

$$\frac{\partial Z}{\partial \lambda} = \mathrm{Tr}[\frac{\partial e^{-\beta[H_o+\lambda V]}}{\partial \lambda}] = -\beta \mathrm{Tr}[Ve^{-\beta[H_o+\lambda V]}]] \tag{18}$$

so that

$$\frac{\partial F}{\partial \lambda} = \frac{\mathrm{Tr}[Ve^{-\beta[H_o+\lambda V]}]]}{Z} = \langle V\rangle = \langle V_{int}\rangle/\lambda. \tag{19}$$

(b) By integrating the result of part (a) over λ, we obtain

$$\Delta F = \int_0^1 d\lambda \frac{\partial F}{\partial \lambda} = \int_0^1 \frac{d\lambda}{\lambda}\langle V_{int}(\lambda)\rangle \tag{20}$$

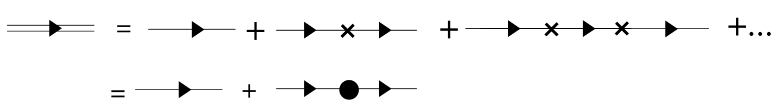
(c) If the interaction energy has an expansion $\langle V_{int}(\lambda)\rangle = \lambda V_1 + \lambda^2 V_2 + \lambda^3 V_3 + \ldots$, then

$$\Delta E = \int_0^1 \frac{d\lambda}{\lambda}\langle\phi|V_{int}(\lambda)|\phi\rangle = V_1 + \frac{1}{2}V_2 + \frac{1}{3}V_3 + \ldots \tag{21}$$

(d) When we turn on the interaction, the change in the ground-state energy involves the contributions from both the change in the Hamiltonian <u>and</u> the change in the ground-state. The factors of $\frac{1}{n}$ appearing in front of the n-th order terms reflect the fact that the ground-state relaxes in response to the change in hamiltonian, so that the change in the ground-state energy from each term is less than the corresponding change in the expectation value of the interaction.

4. (a) The crosses represent the scattering amplitude $V_{k,k'}$ and the lines represent the propagators.

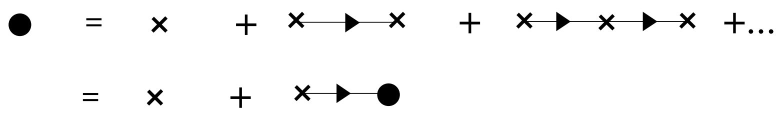
(b) Diagrammatically, we have:



or

$$G_{\vec{k},\vec{k}'}(E) = G^{(0)}_{\vec{k}}(E)\delta_{\vec{k},\vec{k}'} + G^{(0)}_{\vec{k}}(E)t_{\vec{k},\ \vec{k}'}(E)G^{(0)}_{\vec{k}'}(E) \tag{22}$$

where the "blob" is the t-matrix, represented by the following sum of diagrams



Written algebraically, this becomes

$$t_{\vec{k},\vec{k}'}(E) = U(\vec{k}-\vec{k}') + \int \frac{d^d q}{2\pi}^d \frac{U(\vec{k}-\vec{q})}{E - E(q) + i\delta} t_{\vec{q},\vec{k}'}(E) \tag{23}$$

(c) If $U(x) = U\delta^{(d)}(x)$, then $U(q) = U$ and the t-matrix is now momentum independent. We may immediately solve (23) to obtain

$$t(\omega) = \frac{U}{1 - U\int \frac{d^dk}{(2\pi)^d} G^{(0)}(k,\omega)} \tag{24}$$

(d) Let us examine how the integral in the denominator of the t-matrix scales with energy at low energies:

$$\begin{aligned} \int \frac{d^dk}{(2\pi)^d} G^{(0)}(k,\omega) &\propto \int d\epsilon \epsilon^{(\frac{d}{2}-1)} \frac{1}{\omega - \epsilon + i\delta} \\ &\propto -\omega^{(\frac{d}{2}-1)} \\ &\propto -\ln\left(\frac{\Lambda}{\omega}\right), \qquad (d=2). \end{aligned} \tag{25}$$

Thus in dimensions $d \leq 2$, if $U < 0$, the denominator of the t-matrix will develop a pole. To see that this means the development of a bound-state, consider the density of one-particle states

$$\rho(\omega) = \sum_\lambda \delta(\omega - E_\lambda) \tag{26}$$

where E_λ is the energy of the eigenstate $|\lambda\rangle$. We may rewrite this in the form

$$\begin{aligned} \rho(\omega) &= -\frac{1}{\pi}\mathrm{Im}\sum_\lambda \frac{1}{(\omega - E_\lambda + i\delta)} \\ &= -\frac{1}{\pi}\mathrm{Im}\sum_\lambda \langle\lambda|\hat{G}(\omega)|\lambda\rangle \\ = &= -\frac{1}{\pi}\mathrm{Im}\mathrm{Tr}\Big[\hat{G}(\omega)\Big], \end{aligned} \tag{27}$$

where $\hat{G}(\omega) = (\omega - H + i\delta)^{-1}$. We may also take the trace by summing over the momentum eigenstates, rather than energy eigenstates, so that

$$\rho(\omega) = -\frac{1}{\pi}\sum_{\vec{k}} \mathrm{Im}\langle\vec{k}|\hat{G}(\omega)|\vec{k}\rangle$$

$$= -\frac{1}{\pi}\sum_{\vec{k}} \mathrm{Im} G_{\vec{k},\vec{k}}(\omega) \tag{28}$$

Writing the Green-function in terms of the t-matrix, the change in the density of states due to scattering is then

$$\Delta\rho(\omega) = -\frac{1}{\pi}\mathrm{Im}\left[\left(\int \frac{d^d k}{(2\pi)^d} G^{(0)}(k,\omega)\right)^2 t(\omega)\right] \tag{29}$$

Near the pole at negative energies, we may write this in the form

$$\Delta\rho(\omega) = -\frac{1}{U^2\pi}\mathrm{Im}\left[t(\omega)\right] \tag{30}$$

Thus a pole in $t(\omega)$ implies a pole at negative energies in the density of states, indicating a bound-state.