INTRODUCTION TO MANY BODY PHYSICS: 620. Fall 2024

Answers to Questions III. Oct. 11th

1. (a) The eigenvalues are as follows:

$$\begin{aligned} |1_{\mathbf{k}}\rangle &= b^{\dagger}{}_{\mathbf{k}}|0\rangle, & \mathcal{E}_{1_{\mathbf{k}}} &= \epsilon_{\mathbf{k}} \\ |2_{\mathbf{k}}\rangle &= \frac{1}{\sqrt{2!}} b^{\dagger}{}_{\mathbf{k}}|0\rangle, & \mathcal{E}_{2_{\mathbf{k}}} &= 2\epsilon_{\mathbf{k}} \\ |3_{\mathbf{k}}\rangle &= \frac{1}{\sqrt{3!}} b^{\dagger}{}_{\mathbf{k}}|0\rangle, & \mathcal{E}_{3_{\mathbf{k}}} &= 3\epsilon_{\mathbf{k}} + U \end{aligned} \tag{1}$$

Notice that the excitation energies are $\epsilon_{\mathbf{k}} = \mathcal{E}_{1_{\mathbf{k}}} = \mathcal{E}_{2_{\mathbf{k}}} - \mathcal{E}_{1_{\mathbf{k}}}$ and $\epsilon_{\mathbf{k}} + U = \mathcal{E}_{3_{\mathbf{k}}} - \mathcal{E}_{2_{\mathbf{k}}}$.

(b) If we can ignore occupancies higher than three, then the partition function is

$$Z = \prod_{\mathbf{k}} (1 + e^{-\beta\epsilon_{\mathbf{k}}} + e^{-2\beta\epsilon_{\mathbf{k}}} + e^{-\beta(3\epsilon_{\mathbf{k}}+U)})$$

so that the free energy is

$$F = \sum_{\mathbf{k}} F_{\mathbf{k}} = -k_B T \sum_{\mathbf{k}} \ln\left[1 + e^{-\beta\epsilon_{\mathbf{k}}} + e^{-2\beta\epsilon_{\mathbf{k}}} + e^{-\beta(3\epsilon_{\mathbf{k}}+U)}\right]$$

(c) The occupancy of the $\mathbf{k}$ state is

$$n_{\mathbf{k}} = \langle n_{\mathbf{k}}\rangle = -\frac{\partial F_{\mathbf{k}}}{\partial \mu} = \frac{e^{-\beta\epsilon_{\mathbf{k}}} + 2e^{-2\beta\epsilon_{\mathbf{k}}} + 3e^{-\beta(3\epsilon_{\mathbf{k}}+U)}}{1 + e^{-\beta\epsilon_{\mathbf{k}}} + e^{-2\beta\epsilon_{\mathbf{k}}} + e^{-\beta(3\epsilon_{\mathbf{k}}+U)}}$$

(d) Let us plot $n_{\mathbf{k}}$ at low temperatures. There are three regions to consider:

- $\epsilon_{\mathbf{k}} > 0$, $n_{\mathbf{k}} = 0$.
- $\epsilon_{\mathbf{k}} < 0$, but $\epsilon_{\mathbf{k}} + U > 0$, $n_{\mathbf{k}} = 2$.
- $\epsilon_{\mathbf{k}} + U < 0$ and $n_{\mathbf{k}} = 3$. so that there are two "Fermi surfaces" (see Fig. 1).

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In[61]:= num[x_, U_, β_] := (Exp[-β x] + 2. Exp[-2 β x] + 3 Exp[-β ((3. x) + U)] + 4 Exp[-β ((4 x) + 4 U)]) /
          (1 + Exp[-β x] + Exp[-2 β x] + Exp[-β ((3 x) + U)] + Exp[-β ((4 x) + 4 U)]);
         β = 80.;
         Plot[num[x, 1., β], {x, -3, 1.}, PlotRange → All, AxesLabel → {ϵ, n[ϵ]}]
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Out[61]=

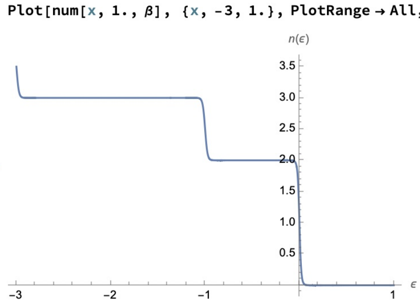

Figure 1: The occupancy versus $\epsilon_{\mathbf{k}}$, showing two Fermi surfaces.

2. (a) We may estimate the Bose Einstein transition temperature from

$$T_{BE} = \frac{3.31}{k_B}\left(\frac{\hbar^2 n^{2/3}}{m}\right) = \frac{3.31}{1.38\times 10^{-23}}\left(\frac{\hbar^2(10^{21}m^{-3})^{2/3}}{23m_p}\right) \approx 6.9\mu K.$$

These tiny temperatures are attained by "evaporative cooling" . Sodium atoms are held in a "magneto-optic" trap. Radio waves are used to "evaporate" the most energetic atoms in the trap, leaving behind the cold ones.

(b) In Helium-4, we may estimate the Bose Einstein transition temperature as

$$T_{BE} = \frac{3.31}{k_B}\left(\frac{\hbar^2 n^{2/3}}{m_{He}}\right) = \frac{3.31}{1.38\times 10^{-23}}\left(\frac{\hbar^2((122/(4m_p)))^{2/3}}{4m_p}\right) \approx 2.76K.$$

The actual condensation temperature is 2.21K. The difference in condensation temperatures is due to the repulsive interaction between atoms.

3. (a) If the interaction has the form

$$V(r) = \begin{cases} U, & (r < R), \\ 0, & (r > R), \end{cases} \tag{2}$$

then in second-quantized form, the interaction Hamiltonian is

$$V = \frac{U}{2}\sum_{\sigma,\sigma'}\int d^3x \int_{|\vec{x}'-\vec{x}|<R} d^3x'[\psi^\dagger{}_\sigma(x)\psi^\dagger{}_{\sigma'}(x')\psi_{\sigma'}(x')\psi_\sigma(x)]. \tag{3}$$

(ii) Inverting the Fourier transform, we have $c_{\vec{k}\sigma} = \int d^3x\psi_\sigma(\vec{x})e^{-i\vec{k}\cdot\vec{x}}$, so that

$$\begin{aligned}
[c_{\vec{k}\sigma},\ c^\dagger{}_{\vec{k}'\sigma'}]_\pm &= \int d^3xd^3x'[\psi_\sigma(x),\ \psi^\dagger{}_{\sigma'}(x')]_\pm e^{-i(\vec{k}\cdot\vec{x}-\vec{k}'\cdot\vec{x}')} \\
&= \delta_{\sigma\ \sigma'}\int d^3xe^{-i(\vec{k}-\vec{k}')\cdot\vec{x}} \\
&= \delta_{\sigma\ \sigma'}(2\pi)^3\delta^{(3)}(\vec{k}-\vec{k}').
\end{aligned} \tag{4}$$

(iii) In momentum space, we may write

$$V = \frac{1}{2}\int\frac{d^3kd^3k'd^3q}{(2\pi)^9}V(q)\left[c^\dagger{}_{\vec{k}+\vec{q}\sigma}c^\dagger{}_{\vec{k}'-\vec{q}\sigma'}c_{\vec{k}'\sigma'}c^\dagger{}_{\vec{k}\sigma}\right], \tag{5}$$

where

$$V(\vec{q}) = \int d^3xV(\vec{x})e^{i\vec{q}\cdot\vec{x}} = \frac{4\pi U}{q}\int_0^R drr\sin(qr) = \left(\frac{4\pi R^3U}{3}\right)F(qR) \tag{6}$$

and

$$F(x) = \frac{3}{x^2}\left[\frac{\sin x}{x} - \cos x\right]. \tag{7}$$

The form of the interaction in momentum space is sketched above. The hard core in real space is manifested as a long-range oscillatory component in momentum space.

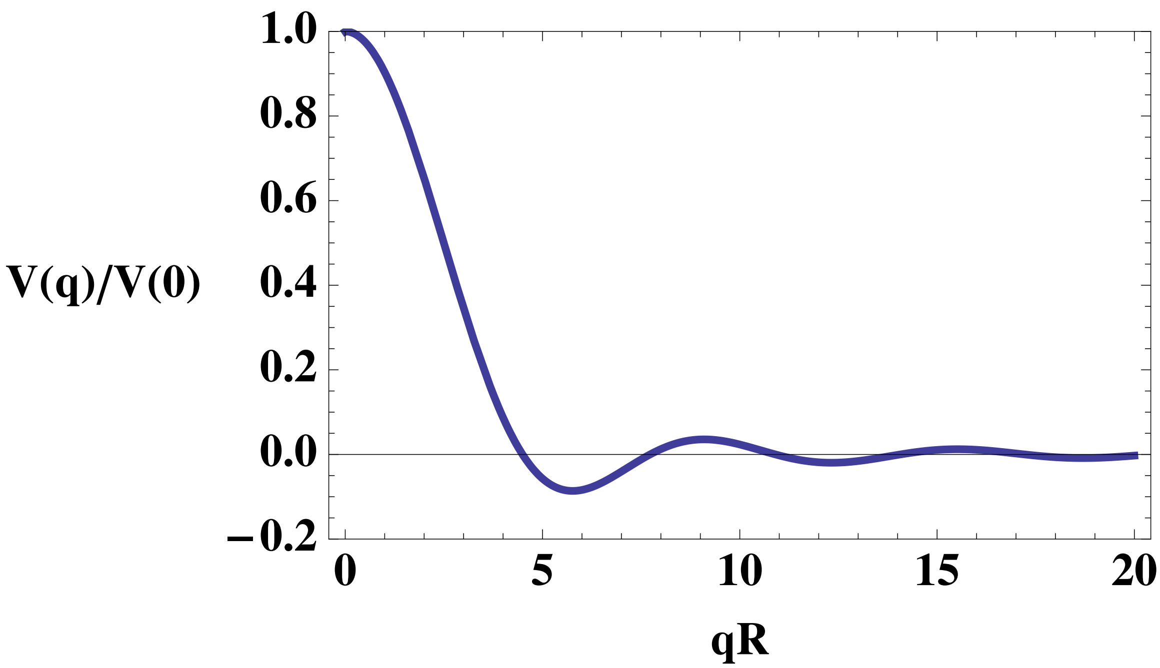

Figure 2: Fourier transformed potential $V(q)$ for "hard sphere" potential.

4. (a) We begin by noting that the matrix elements for the tight-binding Hamiltonian are

$$\langle i|H|j\rangle = \begin{cases} \epsilon & (i=j) \\ -t & \text{(i, j, nearest neighbors)} \\ 0 & \text{(otherwise)} \end{cases} \tag{8}$$

where ϵ is the energy of an isolated orbital and $-t$ is the hopping matrix element. Now the orbital at site A, position $\mathbf{r}_j$ is connected to orbitals at sites B which are located in the unit cells at positions $\mathbf{r}_j$, $\mathbf{r}_j - \mathbf{b}$ and $\mathbf{r}_j - \mathbf{a}$. (Note the minus signs). Consequently, the tight-binding Hamiltonian takes the form

$$H = \overbrace{-t \sum_j \left\{ \left[{\psi^\dagger}_B(\mathbf{r}_i) + {\psi^\dagger}_B(\mathbf{r}_i - \mathbf{a}) + {\psi^\dagger}_B(\mathbf{r}_i - \mathbf{b}) \right] \psi_A(\mathbf{r}_i) + \text{H.c} \right\}}^{\text{hopping between nearest neighbors}} + (\epsilon - \mu) \sum_i (n_A(i) + n_B(i)). \tag{9}$$

Here ${\psi^\dagger}_{A,B}(\mathbf{r}_j)$ creates an electron at site A or B respectively in the unit cell located at position $\mathbf{r}_j$.

(b) If we Fourier transform, writing

$$ {\psi^\dagger}_\lambda(\mathbf{r}_j) = \frac{1}{\sqrt{N_s}} \sum_{\mathbf{k}} {c^\dagger}_{\mathbf{k}\lambda} e^{-i\mathbf{k}\cdot\mathbf{r}_j} \qquad (\lambda = A, B) \tag{10}$$

then substituting into the Hamiltonian, we obtain

$$\begin{aligned} H &= -\frac{t}{N_s}\sum_{j,\mathbf{k},\mathbf{k}'}\left[c^{\dagger}{}_{\mathbf{k}B}(1+e^{i\mathbf{k}\cdot\mathbf{a}}+e^{i\mathbf{k}\cdot\mathbf{b}})c_{\mathbf{k}A}\overbrace{e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}_j}}^{\to N_s\delta_{\mathbf{k},\mathbf{k}'}}+\text{H.c}\right]+(\epsilon-\mu)\sum_{\mathbf{k}\lambda}c^{\dagger}{}_{\mathbf{k}\lambda}c_{\mathbf{k}\lambda} \\ &= \sum_{\mathbf{k}}\left(c^{\dagger}{}_{\mathbf{k}B},c^{\dagger}{}_{\mathbf{k}A}\right)\begin{pmatrix}\epsilon-\mu & \Delta(\mathbf{k})\\ \Delta^*(\mathbf{k}) & \epsilon-\mu\end{pmatrix}\begin{pmatrix}c_{\mathbf{k}B}\\ c_{\mathbf{k}A}\end{pmatrix} \qquad (11)\end{aligned}$$

where

$$\Delta(\mathbf{k}) = -t(1+e^{i\mathbf{k}\cdot\mathbf{a}}+e^{i\mathbf{k}\cdot\mathbf{b}})$$

The eigenvalues of the matrix

$$\begin{bmatrix}\epsilon-\mu & \Delta^*(\mathbf{k})\\ \Delta(\mathbf{k}) & \epsilon-\mu\end{bmatrix}$$

are

$$\begin{aligned}\epsilon_{\mathbf{k}\pm} &= \pm|\Delta(\mathbf{k})|+(\epsilon-\mu)\\ &= \pm t\sqrt{(3+2\cos(\mathbf{k}.\mathbf{a})+2\cos(\mathbf{k}.\mathbf{b})+2\cos(\mathbf{k}.(\mathbf{a}-\mathbf{b})))}+(\epsilon-\mu) \qquad (12)\end{aligned}$$

(see Fig. 3)

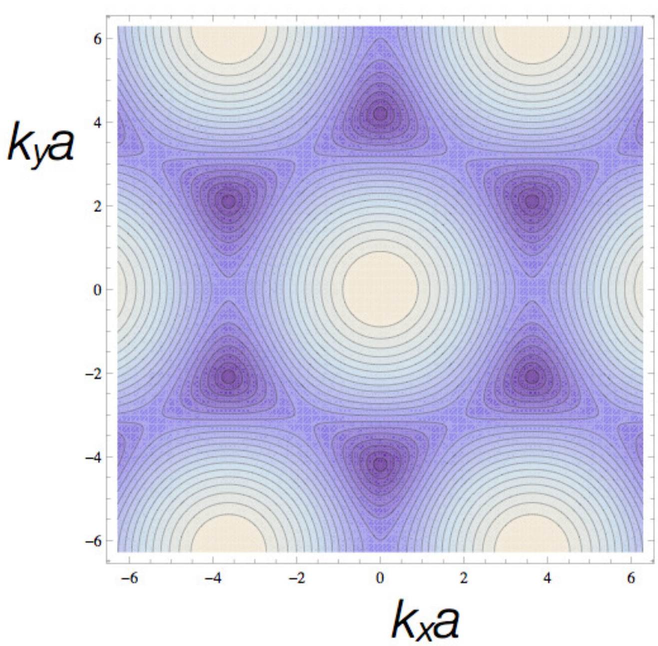

Figure 3: Contour plot of quasiparticle dispersion $\epsilon_{\mathbf{k}}$.

(c) If $e^{i\mathbf{K}\cdot\mathbf{a}} = e^{i\frac{2\pi}{3}}$, $e^{i\mathbf{K}\cdot\mathbf{b}} = e^{-i\frac{2\pi}{3}}$, then clearly,

$$\Delta(\mathbf{K}) \propto (1+e^{i\mathbf{K}\cdot\mathbf{a}}+e^{i\mathbf{K}\cdot\mathbf{b}}) = (1+e^{i\frac{2\pi}{3}}+e^{-i\frac{2\pi}{3}}) = 0$$

To satisfy the conditions

$$\begin{aligned}\mathbf{K}.\mathbf{a} &= \frac{\sqrt{3}}{2}(K_x a) + \frac{1}{2}K_y a = \frac{2\pi}{3} \\ \mathbf{K}.\mathbf{b} &= \frac{\sqrt{3}}{2}(K_x a) - \frac{1}{2}K_y a = -\frac{2\pi}{3}\end{aligned} \tag{13}$$

we require $K_x = 0$, $K_y = \frac{4\pi}{3a}$, or $\mathbf{K} = \frac{4\pi}{3a}\mathbf{j}$. When $\mathbf{k} = \pm\mathbf{K}$, $\Delta(\mathbf{k}) = \Delta(\pm\mathbf{K}) = 0$.

(d) If we expand $\Delta(\mathbf{p}+\mathbf{K})$ for small $\mathbf{p}$, we obtain

$$\begin{aligned}\Delta(\mathbf{k}) &= -t\big[1 + e^{i\frac{2\pi}{3}}(1 + i\mathbf{p}\cdot\mathbf{a}) + e^{-i\frac{2\pi}{3}}(1 + i\mathbf{p}\cdot\mathbf{b})\big] \\ &= -it\big[e^{i\frac{2\pi}{3}}\mathbf{p}\cdot\mathbf{a} + e^{-i\frac{2\pi}{3}}\mathbf{p}\cdot\mathbf{b}\big] \\ &= -it\big[(-\frac{1}{2} + i\frac{\sqrt{3}}{2})\mathbf{p}\cdot\mathbf{a} + (-\frac{1}{2} - i\frac{\sqrt{3}}{2})\mathbf{p}\cdot\mathbf{b}\big] \\ &= it\left[\frac{\sqrt{3}}{2}p_x a - i\frac{\sqrt{3}}{2}p_y a\right] = \overbrace{\left(\frac{\sqrt{3}ta}{2}\right)}^{\tilde{c}}[p_y + ip_x]\end{aligned} \tag{14}$$

so that we can write

$$\begin{aligned}\begin{pmatrix}\epsilon-\mu & \Delta(\mathbf{p}+\mathbf{K}) \\ \Delta^*(\mathbf{p}+\mathbf{K}) & \epsilon-\mu\end{pmatrix} &\approx \begin{pmatrix}\epsilon-\mu & \tilde{c}(p_y+ip_x) \\ \tilde{c}(p_y-ip_x) & \epsilon-\mu\end{pmatrix} = (\epsilon-\mu)\underline{1} + \tilde{c}\ (p_y\sigma_x - p_x\sigma_y) \\ &= (\epsilon-\mu)\underline{1} + \tilde{c}\ (\vec{\sigma}\times\mathbf{p})\end{aligned} \tag{15}$$

In the vicinity of $\mathbf{k}\sim\mathbf{K}$, we thus have

$$\begin{aligned}&\sum_{\mathbf{p}\sim 0}\left(c^{\dagger}{}_{\mathbf{p}+\mathbf{K}B}, c^{\dagger}{}_{\mathbf{p}+\mathbf{K}A}\right)\begin{bmatrix}\epsilon-\mu & \Delta(\mathbf{p}+\mathbf{K}) \\ \Delta^*(\mathbf{p}+\mathbf{K}) & \epsilon-\mu\end{bmatrix}\begin{pmatrix}c_{\mathbf{p}+\mathbf{K}B} \\ c_{\mathbf{p}+\mathbf{K}A}\end{pmatrix} \\ &= \sum_{\mathbf{p}\sim 0}\psi^{\dagger}{}_{\mathbf{p}+}\left((\epsilon-\mu)\underline{1} + \tilde{c}\vec{\sigma}\times\mathbf{p}\right)\psi_{\mathbf{p}+}\end{aligned} \tag{16}$$

where

$$\psi_{\mathbf{p}+} = \begin{pmatrix}c_{\mathbf{p}+\mathbf{K}B} \\ c_{\mathbf{p}+\mathbf{K}A}\end{pmatrix}, \tag{17}$$

Similarly, for $\mathbf{k} = \mathbf{p}-\mathbf{K}$, where $\mathbf{p}$ is small, we have

$$\begin{bmatrix}\epsilon-\mu & \Delta(\mathbf{p}-\mathbf{K}) \\ \Delta^*(\mathbf{p}-\mathbf{K}) & \epsilon-\mu\end{bmatrix} \approx \begin{bmatrix}\epsilon-\mu & -\tilde{c}(p_y-ip_x) \\ -\tilde{c}(p_y+ip_x) & \epsilon-\mu\end{bmatrix} = (\epsilon-\mu)\underline{1} + \tilde{c}(\mathbf{p}\times\vec{\sigma}^T) \tag{18}$$

so that

$$\sum_{\mathbf{p}\sim 0}\left(c^{\dagger}{}_{\mathbf{p}-\mathbf{K}B}, c^{\dagger}{}_{\mathbf{p}-\mathbf{K}A}\right)\begin{bmatrix}\epsilon-\mu & \Delta(\mathbf{p}-\mathbf{K}) \\ \Delta^*(\mathbf{p}-\mathbf{K}) & \epsilon-\mu\end{bmatrix}\begin{pmatrix}c_{\mathbf{p}+\mathbf{K}B} \\ c_{\mathbf{p}-\mathbf{K}A}\end{pmatrix} = \sum_{\mathbf{p}\sim 0}\psi^{\dagger}{}_{\mathbf{p}-}\left((\epsilon-\mu)\underline{1} + \tilde{c}(\vec{\sigma}\times\mathbf{p})\right)\psi_{\mathbf{p}-} \tag{19}$$

where

$$\psi_{\mathbf{p}-} = \begin{pmatrix}c_{\mathbf{p}-\mathbf{K}A} \\ -c_{\mathbf{p}-\mathbf{K}B}\end{pmatrix}, \tag{20}$$

Combining the two contributions (18) and (21), the low energy Hamiltonian thus has the form

$$H = \sum_{\mathbf{p}\lambda} {\psi^\dagger}_{\mathbf{p}\lambda} (\tilde{c}\ (\vec{\sigma} \times \mathbf{p}) + (\epsilon - \mu)\underline{1}) \psi_{\mathbf{p}\lambda} \qquad (21)$$