Solution 7

1. See Section 4.3.1 of the notes.

2. (a) $\hat{\mathcal{H}} = \sum_i \hat{\mathcal{H}}_i$ and we can define raising (creation), $\hat{a}_i^\dagger$ and lowering (annihilation), $\hat{a}_i$ operators for each oscillator and the result follows trivially.

   (b) The partition function can be wriiten $Z = Z_1\, Z_2$ where

   $$Z_i = e^{-\beta\hbar\omega_i/2}/(1 - e^{-\beta\hbar\omega_i}) \quad ,$$

   (see Section 4.3.1. of the notes). $F = -k_B T \ln Z$ from which all other thermodynamic quantities follow.

   (c) $Z = \prod_{i=1}^{N} Z_i$ and $F = -k_B T \sum_{i=1}^{N} \ln Z_i$.

3. **

   (a) Neutrons, protons and electrons are all fermions, so Helium-3 has an odd number, and is itself a fermion, and hence its wave functions are antisymmetric. The formula from section of lecture notes on "Spin and Statistics", (with $N = 2$, $n_2 = n_3 = 1$) gives

   $$\psi_A = \frac{1}{\sqrt{2}} \left[\phi_2(\mathbf{q}_1, s_1)\phi_3(\mathbf{q}_2, s_2) - \phi_2(\mathbf{q}_2, s_2)\phi_3(\mathbf{q}_1, s_1)\right]$$

   If both particles are in state 2, there is complete cancellation, as expected - fermions cannot occupy the same state.

   (b) Helium-4 contains an even number of fermions, and is thus a boson, with a symmetric wave-function. We have $N = 2$, $n_2 = n_3 = 1$) and hence

   $$\psi_S = \frac{1}{\sqrt{2}} \left[\phi_2(\mathbf{q}_1, s_1)\phi_3(\mathbf{q}_2, s_2) + \phi_2(\mathbf{q}_2, s_2)\phi_3(\mathbf{q}_1, s_1)\right]$$

   If both particles are in state 2, the terms are equal, leading to a different normalisation (that follows from $N = n_2 = 2$)

   $$\psi_S = \frac{1}{2} \left[\phi_2(\mathbf{q}_1, s_1)\phi_2(\mathbf{q}_2, s_2) + \phi_2(\mathbf{q}_2, s_2)\phi_2(\mathbf{q}_1, s_1)\right] = \phi_2(\mathbf{q}_1, s_1)\phi_2(\mathbf{q}_2, s_2)$$

   (c) We have $N = 4, n_2 = n_3 = 2$, and write $\phi_j(1)$ for $\phi_j(\mathbf{q}_1, s_1)$ etc. The normalisation according to the formula is $(N! \prod n_j!)^{-1/2} = 96^{-1/2}$ but the terms group in fours, leading to

   $$\begin{aligned}\psi_S \;=\; & \frac{1}{\sqrt{6}} [\phi_2(1)\phi_2(2)\phi_3(3)\phi_3(4) + \phi_2(1)\phi_2(3)\phi_3(2)\phi_3(4) \\ & +\phi_2(1)\phi_2(4)\phi_3(2)\phi_3(3) + \phi_2(2)\phi_2(3)\phi_3(1)\phi_3(4) \\ & +\phi_2(2)\phi_2(4)\phi_3(1)\phi_3(3) + \phi_2(3)\phi_2(4)\phi_3(1)\phi_3(2)]\end{aligned}$$

4. See Q3 of Homework 4.

5. Linearity:

$$\hat{P}(\alpha\psi) = \phi\langle\phi|\alpha\psi\rangle = \alpha\phi\langle\phi|\psi\rangle = \alpha\hat{P}\psi$$

$$\hat{P}(\psi_1 + \psi_2) = \phi\langle\phi|\psi_1 + \psi_2\rangle = \phi\langle\phi|\psi_1\rangle + \phi\langle\phi|\psi_2\rangle = \hat{P}\psi_1 + \hat{P}\psi_2$$

Hermitian property:

$$\langle\psi_1|\hat{P}\psi_2\rangle = \langle\psi_1|\phi\rangle\langle\phi|\psi_2\rangle = \langle\psi_2|\phi\rangle^*\langle\phi|\psi_1\rangle^* = \langle\psi_2|\hat{P}\psi_1\rangle^* = \langle\hat{P}\psi_1|\psi_2\rangle$$

Projection property:

$$\hat{P}^2\psi = \phi\langle\phi|(\phi\langle\phi|\psi\rangle)\rangle = \phi\langle\phi|\phi\rangle\langle\phi|\psi\rangle = \phi\langle\phi|\psi\rangle = \hat{P}\psi$$

The density operator $\hat{\rho}$ was given in lectures as the following sum of projection operators:

$$\hat{\rho} = \sum_k \rho_k |\psi_k\rangle\langle\psi_k|$$

Since the sum of Hermitian operators is hermitian, the density operator is also Hermitian.

6. (a) From the definitions of $\tilde{p}(\mathbf{k}), \tilde{u}(\mathbf{k})$ since $u(\mathbf{r}), p(\mathbf{r})$ are real then the complex conjugates

$$\begin{aligned} \tilde{u}(\mathbf{k})^* &= \tilde{u}(-\mathbf{k}) \\ \tilde{p}(\mathbf{k})^* &= \tilde{p}(-\mathbf{k}) \end{aligned}$$

From the definitions of $\tilde{p}(\mathbf{k}), \tilde{u}(\mathbf{k})$, we can rewrite the Hamiltonian

$$H = V^{-1}\int d^3r \sum_{\mathbf{k},\mathbf{k}'} e^{i(\mathbf{k}+\mathbf{k}')\cdot\mathbf{r}} \left\{ \frac{\tilde{p}(\mathbf{k})\tilde{p}(\mathbf{k}')}{2m} - (\mathbf{k}\cdot\mathbf{k}')\frac{B}{2}\tilde{u}(\mathbf{k})\tilde{u}(\mathbf{k}') \right\}$$

Then using the fact that $\int d^3r e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}} = V\delta_{\mathbf{k}\mathbf{k}'}$ we can rewrite the Hamiltonian

$$H = \sum_{\mathbf{k}} \left\{ \frac{\tilde{p}(\mathbf{k})\tilde{p}(-\mathbf{k})}{2m} + \frac{Bk^2}{2}\tilde{u}(\mathbf{k})\tilde{u}(-\mathbf{k}) \right\} \quad ,$$

from which the result follows.

(b) The Hamiltonian can be written as a sum of simple harmonic oscillators with frequencies $\omega(\mathbf{k}) = \sqrt{Bk^2/m} = vk \quad :$

$$H = \sum_{\mathbf{k}} \left\{ \frac{|\tilde{p}(\mathbf{k})|^2}{2m} + \frac{m\omega^2(\mathbf{k})}{2}|\tilde{u}(\mathbf{k})|^2 \right\} \quad ,$$

Quantising the oscillators $\tilde{p}(\mathbf{k}) \to \hat{p}(\mathbf{k}), \tilde{u}(\mathbf{k}) \to \hat{u}(\mathbf{k})$, the Hamiltonian operator can be written as

$$\hat{H} = \sum_{\mathbf{k}} \hbar\omega(\mathbf{k})\left(\hat{a}^\dagger(\mathbf{k})\hat{a}(\mathbf{k}) + \frac{1}{2}\right) \equiv \sum_{\mathbf{k}} \hat{H}_{\mathbf{k}} \quad , \quad \hat{H}_{\mathbf{k}} = \hbar\omega(\mathbf{k})\left(\hat{a}^\dagger(\mathbf{k})\hat{a}(\mathbf{k}) + \frac{1}{2}\right) \quad ,$$

where

$$\begin{aligned} \hat{a}(\mathbf{k}) &= \sqrt{\frac{m\omega(\mathbf{k})}{2\hbar}}\left(\hat{u}(\mathbf{k}) + \frac{i}{m\omega(\mathbf{k})}\hat{p}(\mathbf{k})\right) \\ \hat{a}^\dagger(\mathbf{k}) &= \sqrt{\frac{m\omega(\mathbf{k})}{2\hbar}}\left(\hat{u}(\mathbf{k})^* - \frac{i}{m\omega(\mathbf{k})}\hat{p}(\mathbf{k})^*\right) . \end{aligned}$$

(c) The energy is given by

$$\begin{aligned}
E &= \langle H\rangle = \frac{1}{Z}\mathrm{Tr}\left(\hat{H}e^{-\beta\hat{H}}\right) \quad , \quad Z = \mathrm{Tr}\left(e^{-\beta\hat{H}}\right) \\
&= \sum_{\mathbf{k}}\langle H_{\mathbf{k}}\rangle = \sum_{\mathbf{k}}\frac{1}{Z_{\mathbf{k}}}\mathrm{Tr}\left(\hat{H}_{\mathbf{k}}e^{-\beta\hat{H}_{\mathbf{k}}}\right) = -\sum_{\mathbf{k}}\frac{\partial\ln Z_{\mathbf{k}}}{\partial\beta} \quad ,
\end{aligned}$$

where the trace over the energy eigenstates of each of the oscillators can be done independently

$$\begin{aligned}
Z_{\mathbf{k}} &= \sum_{n=0}^{\infty} e^{-\beta\hbar\omega(\mathbf{k})(n+1/2)} = \frac{e^{-\beta\hbar\omega(\mathbf{k})/2}}{1-e^{-\beta\hbar\omega(\mathbf{k})}} \\
\ln Z_{\mathbf{k}} &= -\frac{\beta\hbar\omega(\mathbf{k})}{2} - \ln\left(1-e^{-\beta\hbar\omega(\mathbf{k})}\right) \quad .
\end{aligned}$$

So the energy can be written as

$$E = E_0 + \sum_{\mathbf{k}}\frac{\hbar\omega(\mathbf{k})e^{-\beta\hbar\omega(\mathbf{k})}}{1-e^{-\beta\hbar\omega(\mathbf{k})}} \quad ; \quad E_0 = \sum_{\mathbf{k}}\frac{\hbar\omega(\mathbf{k})}{2} \quad ,$$

from which the result follows.

(d) Taking the integral limit of the sum over $\mathbf{k}$ (and noting that since $\omega(\mathbf{k})$ is a function of $k = |\mathbf{k}|$ only, we can use the spherical symmetry of the integrand in spherical polar coordinates,

$$\int d^3k f(k) = \int_0^{2\pi} d\phi \int_0^{\pi}\sin\theta d\theta\int_0^{\infty} k^2 dk f(k) \to \int_0^{\infty} 4\pi k^2 dk f(k) \quad :$$

The expression for the energy is

$$E = E_0 + \frac{V}{(2\pi)^3}\int d^3k\frac{\hbar vk}{e^{\beta\hbar vk}-1} = E_0 + \frac{V}{(2\pi)^3}\int_0^{\infty} 4\pi k^2 dk\frac{\hbar vk}{e^{\beta\hbar vk}-1}$$

Changing variable to $x = \beta\hbar vk$, this can be rewritten as

$$E = E_0 + \frac{V\left(k_BT\right)^4}{2\pi^2\left(\hbar v\right)^3}\int_0^{\infty}\frac{x^3dx}{e^x-1}$$

from which an expression for $A = \dfrac{V\pi^2k_B^4}{30\left(\hbar v\right)^3}$ follows.

(e) The specific heat then behaves like $C_V \propto T^3$ and hence the 3rd law is satisfied by this system.

7. (a) From the definitions (Fermi-Dirac statistics) in the notes, the average occupation numbers for the positive and negative energy states are respectively,

$$\begin{aligned}
\langle n(\mathbf{k})\rangle_+ &= \frac{1}{z^{-1}e^{\beta\hbar ck}+1} \\
\langle n(\mathbf{k})\rangle_- &= \frac{1}{z^{-1}e^{-\beta\hbar ck}+1}
\end{aligned}$$

where $z = \exp\left(\beta\mu\right)$.

(b) Similarly (see lecture notes) , the probability that a +ve/-ve energy state of wavenumber $\mathbf{k}$ has $n_{\mathbf{k}}$ particles is

$$\begin{aligned} p_+(n_{\mathbf{k}}) &= \frac{e^{-\beta(\hbar ck-\mu)n_{\mathbf{k}}}}{1+ze^{-\beta\hbar ck}} \\ p_-(n_{\mathbf{k}}) &= \frac{e^{\beta(\hbar ck+\mu)n_{\mathbf{k}}}}{1+ze^{\beta\hbar ck}} \quad , \end{aligned}$$

where $n_{\mathbf{k}} = 0, 1$ as they are fermions. An occupied state has $n = 1$ while an unoccupied state has $n = 0$. Therefore

$$p_+(1) = \langle n(\mathbf{k})\rangle_+ \,, p_+(0) = 1 - p_+(1) \quad \text{and} \quad p_-(1) = \langle n(\mathbf{k})\rangle_- \,, p_-(0) = 1 - p_-(1)$$

(c) Follows directly from (b) above

(d) If at zero temperature all negative energy Dirac states are occupied and all positive energy ones are empty, this means that $\mu(T = 0) = 0$.
The mean total particle number is given by

$$N = \sum_{\mathbf{k}} \{\langle n(\mathbf{k})\rangle_+ + \langle n(\mathbf{k})\rangle_-\} = \sum_{\mathbf{k}} \{\langle n(\mathcal{E}_+(\mathbf{k}))\rangle_+ + \langle n(-\mathcal{E}_+(\mathbf{k}))\rangle_-\} \quad ,$$

where $\mathcal{E}_+(\mathbf{k}) = \hbar ck$.
At $T = 0$ this gives $N(T = 0) = \sum_{\mathbf{k}} 1$ and if the mean total number of particles is fixed this must be true for all T.
This implies that

$$\sum_{\mathbf{k}} \{\langle n(\mathcal{E}_+(\mathbf{k}))\rangle_+ + \langle n(-\mathcal{E}_+(\mathbf{k}))\rangle_-\} = \sum_{\mathbf{k}} 1 \quad , \qquad \text{for all } T. \tag{1}$$

Now from (c) above

$$\sum_{\mathbf{k}} \{\langle n(\mathcal{E}_+(\mathbf{k}) + \mu)\rangle_+ + \langle n(\mu - \mathcal{E}_+(\mathbf{k}))\rangle_-\} = \sum_{\mathbf{k}} 1 \tag{2}$$

Equating equations (1) and (2) implies that $\mu(T) = 0$ for all T.
This means that every unoccupied -ve energy state leads to an occupied +ve energy state. As T increases from 0, 'particles' leave -ve energy states and begin to populate the +ve energy states.

(e) The mean excitation energy is then given by

$$\begin{aligned} E &= \gamma \sum_{\mathbf{k}} \{\mathcal{E}_+(\mathbf{k})\langle n(\mathbf{k}, z = 1)\rangle_+ - \mathcal{E}_+(\mathbf{k})\langle n(\mathbf{k}, z = 1)\rangle_-\} \\ &= E_0 + \gamma \sum_{\mathbf{k}} 2\mathcal{E}_+(\mathbf{k})\langle n(\mathbf{k}, z = 1)\rangle_+ \,, \text{ where } E_0 = \gamma \sum_{\mathbf{k}} \mathcal{E}_-(\mathbf{k}) = -\gamma \sum_{\mathbf{k}} \mathcal{E}_+(\mathbf{k}) \,, \end{aligned}$$

using the results of (c) and (d) above. Taking the integral limit of the sum over $\mathbf{k}$ (and noting that since $\mathcal{E}_+(\mathbf{k})$ is a function of $k = |\mathbf{k}|$ only, we can use the circular symmetry of the integrand in plane polar coordinates,

$$\int d^2k f(k) = \int_0^{2\pi} d\phi \int_0^{\infty} kdk f(k) \to \int_0^{\infty} 2\pi kdk f(k) \quad :$$

$\Rightarrow$ the expression for the energy is

$$E = E_0 + \frac{4A}{(2\pi)^2} \int d^2k \frac{\mathcal{E}_+(k)}{e^{\beta\mathcal{E}_+(k)} + 1} = E_0 + \frac{4A}{(2\pi)^2} \int_0^{\infty} 2\pi kdk \frac{\hbar ck}{e^{\beta\hbar ck} + 1}$$

(f) Hence the energy is given by

$$E(T) - E(0) = \frac{3\zeta(3)A(k_BT)^3}{\pi(\hbar c)^2}$$

(g) The heat capacity is

$$C_V = \left(\frac{\partial E}{\partial T}\right)_V = \frac{9\zeta(3)Ak_B(k_BT)^2}{\pi(\hbar c)^2}$$

(h) From (f) it is clear that the 3rd law is satisfied for Graphene.