Physics 502 - Solutions for assignment 2

(Dated: October 23, 2023)

1. Ground state of weakly interacting bosons

a. First, we calculate the commutator of the α_k operators by writing each in terms of a_k and $a_k^\dagger$ and using the canonical commutation relations $[a_k, a_k'] = \left[a_k^\dagger, a_{k'}^\dagger\right] = 0$ and $\left[a_k, a_{k'}^\dagger\right] = \delta_{kk'}$. We immediately get $[\alpha_k, \alpha_{k'}] = \left[\alpha_k^\dagger, \alpha_{k'}^\dagger\right] = 0$ as must be true for Bosonic particles. Next, we demand

$$\begin{aligned} \left[\alpha_k, \alpha_{k'}^\dagger\right] &= \delta_{kk'} \\ \left(u_k^2 - v_k^2\right)\delta_{kk'} &= \delta_{kk'} \end{aligned}$$

so that $u_k^2 - v_k^2 = 1$.

The definition of a symplectic matrix U_k is

$$U_k^T \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} U_k = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}.$$

By subbing in the given matrix U_k for the definition of the α_k operators, one can easily confirm that U_k is symplectic given that $u_k^2 - v_k^2 = 1$.

Similarly, it can easily be shown that $U_k^\dagger U_k \neq \mathbb{I}$ and, hence, U_k is not unitary.

b. Using $a_k = u_k\alpha_k + v_k\alpha_{-k}^\dagger$ and $a_k^\dagger = u_k\alpha_k^\dagger + v_k\alpha_{-k}$ and substituting into the Hamiltonian $H = \frac{1}{2}N^2V_0 + \sum_k' \left(\hbar\Omega_k a_k^\dagger a_k + \frac{1}{2}\eta_k(a_k a_{-k} + a_k^\dagger a_{-k}^\dagger)\right)$, we find that in order for terms such as $\alpha_k\alpha_{-k}$ and $\alpha_k^\dagger\alpha_{-k}^\dagger$ to cancel we must set $2\Omega_k u_k v_k + \eta_k(u_k^2 + v_k^2) = 0$ or equivalently

$$\tanh 2\theta_k = -\frac{\eta_k}{\Omega_k} = -\frac{N_0 V_k}{\epsilon_k + N_0 V_k}$$

using that $2\sinh\theta\cosh\theta = \sinh 2\theta$ and $\sinh^2\theta + \cosh^2\theta = \cosh 2\theta$.

c. α_k is the annihilation operator for quasi-particle excitations, hence, in the ground state where no such quasi-particles should be excited, $\alpha_k|\Phi_0\rangle = 0$. Substituting for a_k and $a_k^\dagger$,

$$\langle n_k\rangle_0 = \langle\Phi_0|(u_k\alpha_k^\dagger + v_k\alpha_{-k})(u_k\alpha_k + v_k\alpha_{-k}^\dagger)|\Phi_0\rangle$$

$$= \langle\Phi_0|v_k^2\alpha_{-k}\alpha_{-k}^\dagger|\Phi_0\rangle$$

using $\alpha_k|\Phi_0\rangle = 0$ and $\langle\Phi_0|\alpha_k^\dagger\alpha_{-k}^\dagger|\Phi_0\rangle = 0$. Finally, noting that $\alpha_{-k}\alpha_{-k}^\dagger = 1 + \alpha_{-k}^\dagger\alpha_{-k}$ we find

$$\langle n_k\rangle_0 = \langle\Phi_0|v_k^2|\Phi_0\rangle = v_k^2$$

Solving for v_k^2 in terms of $\tanh 2\theta$, we have

$$v_k^2 = \sinh^2\theta_k = \frac{1}{2}(\cosh 2\theta_k - 1) = \frac{1}{2}\left(\frac{\Omega_k}{\omega_k} - 1\right)$$

As $k \to 0$ we see that v_k^2 diverges. As $k \to \infty$, $\frac{\Omega_k}{\omega_k} \to 1$ so that $v_k^2 \to 0$.

d. Assuming the form $\hat{O} = \prod_k \exp(z_k a_k^\dagger a_{-k}^\dagger)$ and considering the relation $a_k|\Phi_0\rangle = \frac{v_k}{u_k} a_{-k}^\dagger|\Phi_0\rangle$ gives

$$a_k \prod_{k'=-\infty}^{\infty} \exp(z_{k'} a_{k'}^\dagger a_{-k'}^\dagger)|0\rangle = \frac{v_k}{u_k} a_{-k}^\dagger \prod_{k'=-\infty}^{\infty} \exp(z_{k'} a_{k'}^\dagger a_{-k'}^\dagger)|0\rangle. \tag{1}$$

To compute the left hand side explicitly, we first compute the following commutator

$$\begin{aligned}
&\left[a_k, \exp\left(z_{k'} a_{k'}^\dagger a_{-k'}^\dagger\right)\right] \\
&= \sum_{n=0}^{\infty} \frac{1}{n!} z_{k'}^n \left[a_k, {a_{k'}^\dagger}^n {a_{-k'}^\dagger}^n\right] \\
&= \sum_{n=0}^{\infty} \frac{1}{n!} z_{k'}^n \left\{{a_{k'}^\dagger}^n \left[a_k, {a_{-k'}^\dagger}^n\right] + \left[a_k, {a_{k'}^\dagger}^n\right] {a_{-k'}^\dagger}^n\right\} \\
&= \sum_{n=0}^{\infty} \frac{1}{n!} z_{k'}^{n+1} \left({a_{k'}^\dagger}^{n+1} {a_{-k'}^\dagger}^n \delta_{k,-k'} + {a_{k'}^\dagger}^n {a_{-k'}^\dagger}^{n+1} \delta_{kk'}\right)
\end{aligned}$$

where, in the last equality, we have used the commutator in the hint and shifted the summation variable $n \to n+1$. Pulling out a factor of $a_{-k}^\dagger$ we finally obtain

$$\left[a_k, \exp\left(z_{k'} a_{k'}^\dagger a_{-k'}^\dagger\right)\right] = a_{-k}^\dagger \left(\delta_{k,-k'} z_{-k} + \delta_{kk'} z_k\right) \exp\left(z_{k'} a_{k'}^\dagger a_{-k'}^\dagger\right).$$

We can now use this to compute the left hand side of eq. (1) by commuting the a_k operator through the product of exponentials until it annihilates the vacuum:

$$\begin{aligned}
&a_k \prod_{k'=-\infty}^{\infty} \exp\left(z_{k'} a_{k'}^\dagger a_{-k'}^\dagger\right)|0\rangle \\
&= \prod_{k'<-k} \exp\left(z_{k'} a_{k'}^\dagger a_{-k'}^\dagger\right) \left[a_{-k}^\dagger z_{-k} \exp\left(z_k a_k^\dagger a_{-k}^\dagger\right) + \exp\left(z_k a_k^\dagger a_{-k}^\dagger\right) a_k\right] \prod_{k'>-k} \exp\left(z_{k'} a_{k'}^\dagger a_{-k'}^\dagger\right)|0\rangle \\
&= z_{-k} a_{-k}^\dagger \prod_{k'=-\infty}^{\infty} \exp\left(z_{k'} a_{k'}^\dagger a_{-k'}^\dagger\right)|0\rangle \\
&\quad + \prod_{k'<k} \exp\left(z_{k'} a_{k'}^\dagger a_{-k'}^\dagger\right) \left[a_{-k}^\dagger z_k \exp\left(z_k a_k^\dagger a_{-k}^\dagger\right) + \exp\left(z_k a_k^\dagger a_{-k}^\dagger\right) a_k\right] \prod_{k'>k} \exp\left(z_{k'} a_{k'}^\dagger a_{-k'}^\dagger\right)|0\rangle \\
&= \left(z_{-k} + z_k\right) a_{-k}^\dagger \prod_{k'=-\infty}^{\infty} \exp\left(z_{k'} a_{k'}^\dagger a_{-k'}^\dagger\right)|0\rangle.
\end{aligned}$$

Comparing this with eq. (1) we conclude that $z_k = v_k/(2u_k)$ and, hence, that the ground state is

$$|\Phi_0\rangle = \prod_{k=-\infty}^{\infty} \exp\left(\frac{1}{2}\tanh\left(\theta_k\right) a_k^\dagger a_{-k}^\dagger\right)|0\rangle. \tag{2}$$

2. Liquid ^{4}He

Following the hints provided in the question we calculate the temperature dependence of the uncondensed fraction

$$n'(T) = \frac{1}{\Omega}\sum_k \langle a_k^\dagger a_k\rangle.$$

Using $a_k = \cosh\theta_k \alpha_k + \sinh\theta_k \alpha_{-k}^\dagger$ and $a_k^\dagger = \cosh\theta_k \alpha_k^\dagger + \sinh\theta_k \alpha_{-k}$, we obtain

$$a_k^\dagger a_k = \cosh^2\theta_k \alpha_k^\dagger \alpha_k + \sinh^2\theta_k \alpha_{-k}\alpha_{-k}^\dagger + \cosh\theta_k \sinh\theta_k(\alpha_k^\dagger \alpha_{-k}^\dagger + \alpha_{-k}\alpha_k).$$

Assuming no temperature dependence of θ_k we need to calculate $\langle \alpha_k^\dagger \alpha_k\rangle$, $\langle \alpha_{-k}\alpha_{-k}^\dagger\rangle$, $\langle \alpha_{-k}\alpha_k\rangle$ and $\langle \alpha_k^\dagger \alpha_{-k}^\dagger\rangle$. The last two terms will vanish in this average since the Hamiltonian is diagonal in the α_k's. From the Bose-Einstein distribution with $\mu = 0$ we have

$$\langle \alpha_k^\dagger \alpha_k\rangle = \frac{1}{e^{\beta\hbar\omega_k} - 1}$$

and

$$\langle \alpha_{-k}\alpha_{-k}^\dagger\rangle = 1 + \frac{1}{e^{\beta\hbar\omega_{-k}} - 1}.$$

Summing over the momentum k and replacing $k \to -k$ in the second term we get

$$n'(T) = \frac{1}{\Omega}\sum_k [\frac{\cosh^2\theta_k + \sinh^2\theta_k}{e^{\beta\hbar\omega_k} - 1} + \sinh^2\theta_k].$$

We can now replace the sum by an integral and linearize the spectrum for small k, taking $\cosh^2\theta_k + \sinh^2\theta_k = \cosh(2\theta_k) = \frac{\Omega_k}{\omega_k} = \frac{\epsilon_k + N_0 V_k}{\sqrt{\epsilon_k(\epsilon_k + 2N_0V_k)}}$. For short range interactions this is $\approx \frac{\sqrt{V_0 N_0 m}}{\hbar k}$

$$n'(T) \approx \int \frac{k^2 dk}{2\pi^2}\frac{\sqrt{V_0 N_0 m}}{\hbar k}\frac{1}{e^{\beta\hbar c k} - 1}.$$

Scaling the k variable by $\beta\hbar c$ where $c = \sqrt{\frac{V_0 N_0}{m}}$ will give

$$n'(T) \propto T^2 \int \frac{x dx}{e^x - 1}.$$

Restoring all the constants we have

$$n_0(T) = n_0(0) - \frac{m}{12\hbar^3 c}(k_B T)^2.$$

For long range interactions, $\frac{\Omega_k}{\omega_k} \approx \frac{\sqrt{N_0 m e^2}}{\hbar k^2}$, $\hbar\omega_k = \sqrt{\frac{\hbar^2 k^2}{2m}\left(\frac{\hbar^2 k^2}{2m} + 2N_0 V_k\right)} \approx \hbar e\sqrt{\frac{N_0}{m}}\left(1 + \frac{\hbar^2 k^4}{8mN_0 e^2}\right)$ and

$$n'(T) \approx \int \frac{k^2 dk}{2\pi^2}\frac{\sqrt{N_0 m e^2}}{\hbar k^2}\frac{1}{e^{C + Ak^4} - 1} \approx \frac{\sqrt{N_0 m e^2}}{\hbar 2\pi^2} e^{-C} A^{-\frac{1}{4}} \int_0^\infty dx e^{-x^4}$$

with $C = \beta\hbar e\sqrt{N_0/m}$ and $A = \beta\hbar^3/(8m^{\frac{3}{2}}\sqrt{N_0}e)$ so that in low T limit,

$$n_0(T) - n_0(0) \sim T^{1/4}\exp(-\hbar e\sqrt{N_0/m}/(k_B T)).$$

3. Phonons in a cubic lattice

a. The Hamiltonian can be written as

$$\mathcal{H} = \sum_{n,i}\left[\frac{p_{l,i}^2}{2m} + \frac{1}{2}K\sum_{\delta}(u_{l,i} - u_{l+\delta,i})^2\right] = \sum_{n,i}\left[\frac{p_{l,i}^2}{2m} + K\sum_{\delta}(u_{l,i}^2 - u_{l,i}u_{l+\delta,i})\right],$$

where $l = na$ goes over the lattice sites and $i = x, y, z$ (direction of displacement, i.e, polarization) and δ is a vector that runs over the nearest neighbours. Note that in lower dimensions (1,2) we still have to take into account motion in all three directions (the direction of the vector q is restricted but it's polarization is in three dimensions). As before we can define the dynamical matrix, which is already diagonal in x, y, z:

$$V^{i,j}(l, l') = \begin{cases} 2K\delta_{ij} & l = l' \\ -K\delta_{ij} & l = l' \pm a \end{cases}$$

This leads to the dispersion

$$\omega_{q\mu} = \sqrt{\frac{V_{q\mu}}{M}} = 2\sqrt{\frac{K}{M}}\left[\sum_{i=1}^{d}\sin^2(aq_i/2)\right]^{\frac{1}{2}},$$

independent of polarization direction. For small $|q|$ this can be approximated by $\omega_q = cq$ with $c = \sqrt{\frac{K}{M}}a$

b. The density of states is defined by:

$$D(\omega) = \frac{1}{V}\sum_{q,\mu}\delta(\omega - \omega_{q,\mu})$$

In the limit of long wavelengths we can approximate this as

$$D(\omega) = \frac{1}{V}\sum_{q,\mu}\delta(\omega - cq) = 3\int\frac{d^dq}{(2\pi)^d}\delta(\omega - cq) = \frac{3}{(2\pi)^d}\Phi(d)\int dq q^{d-1}\delta(\omega - cq)$$

$$= \frac{3}{(2\pi)^d}\Phi(d)\frac{\omega^{d-1}}{c^d} = \frac{3}{2^{d-1}\pi^{d/2}\Gamma(d/2)}\frac{\omega^{d-1}}{c^d}$$

where the function $\Phi(d)$ is just the angular integral, i.e, the surface of a unit sphere in d dimensions. The specific heat due to phonons is given by

$$c_v = \frac{d\langle E\rangle}{dT} = \frac{d}{dT}\sum_{q,\mu}\hbar\omega_{q,\mu}\left(\langle n_{q,\mu}\rangle + \frac{1}{2}\right)$$

$$= \frac{d}{dT}\sum_{q,\mu}\hbar\omega_{q,\mu}\frac{1}{e^{\beta\hbar\omega_{q,\mu}}-1} = \frac{1}{k_BT^2}\int d\omega D(\omega)\frac{(\hbar\omega)^2e^{\beta\hbar\omega}}{(e^{\beta\hbar\omega}-1)^2}.$$

As usual the temperature dependence can be found by substitution $x = \beta\hbar\omega$ and since $D(\omega) \propto \omega^{d-1}$ this leads to $c_v \propto T^d$.

c. The Debye model requires $\int_0^{\omega_D} D(\omega)d\omega = Nd$. With a linearized dispersion and the density of states that was found in (a) this gives:

$$\frac{3V}{2^{d-1}\pi^{d/2}\Gamma(d/2)}\frac{\omega_D^d}{dc^d} = Nd, \qquad \omega_D = 2\sqrt{\pi}\sqrt{\frac{K}{M}}\left(\frac{d^2N}{6V}\Gamma(\frac{d}{2})\right)^{1/d}$$

d. The average of the displacement is conveniently calculated when written in terms of creation and annihilation operators, $u_q^i = \sqrt{\frac{\hbar}{2M\omega_q}}(a^\dagger_{-q,\mu} + a_{q,\mu})$. The square leads to four terms of which only two average to a non-zero value ($\langle aa\rangle$ and $\langle a^\dagger a^\dagger\rangle$ average to zero). The non vanishing terms give the occupation number, which is given by the Bose-Einstein distribution function. This yields

$$\langle u^2\rangle = \frac{\hbar}{2MN}\sum_{q,\mu}\frac{1}{\omega_{q,\mu}}\left(\frac{2}{e^{\beta\hbar\omega_{q\mu}}-1}+1\right).$$

Replacing the sum by an integral and writing it in terms of $D(\omega)$ we find

$$\langle u^2\rangle = \frac{\hbar V}{2MN}\int_0^{\omega_D} d\omega\frac{D(\omega)}{\omega}\left(\frac{2}{e^{\beta\hbar\omega}-1}+1\right).$$

The first term represents thermal fluctuations while the second represents quantum fluctuations (zero-point motion) of the ions. We now substitute the long wavelength form $D(\omega) = A_d\omega^{d-1}/c^d$ found above and perform the integral. We find

$$\langle u^2\rangle = \frac{\hbar^{2-d}V}{2MNc^d}A_d\left[2b_d(k_BT)^{d-1} + \frac{(\hbar\omega_D)^{d-1}}{d-1}\right]$$

with

$$b_d = \int_0^\infty dx\frac{x^{d-2}}{e^x-1}.$$

Clearly this last integral is infrared divergent for $d \leq 2$, implying that lattices are unstable in lower dimensions: the melting temperature, which is inversely proportional to the above integral, is zero. In $d = 2$ the lattice is stable at $T = 0$. In $d = 1$ quantum fluctuation destroy the lattice even at $T = 0$. These results can be understood as consequences of general theorem due to Mermin and Wagner.

In $d = 3$ we can use the Lindemann criterion to determine T_M,

$$T_M = \left[c_L^2\frac{4M\hbar c^3}{k_B^2a} - \frac{3}{2\pi^2}\theta_D^2\right]^{1/2},$$

with $\theta_D = \hbar\omega_D/k_B$ the Debye temperature.

e) For the Polonium crystal we have $a = 3.34$Å, $T_M = 527$K and $M = 209 \times 1.67 \times 10^{-27}$kg. We first estimate c by neglecting θ_D in the above equation – we expect that $T_M \gg \theta_D$. This yields

$$c \simeq \left[(k_B T_M)^2 \frac{a}{4M\hbar c_L}\right]^{1/3} \simeq 1064\text{m/s}.$$

From c we now deduce the Debye temperature as

$$\theta_D = \frac{\hbar c}{k_B a} 2\sqrt{\pi}(2\sqrt{\pi}/3)^{1/3} \simeq 51\text{K}$$

which indeed is much smaller than T_M and our solution is self-consistent. The values of c and θ_D appear to be reasonable as they fall within the expected range for solids.