33-755 Homework 11

Nathaniel D. Hoffman

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Harmonic Oscillator in Thermal Equilibrium

The density operator for a harmonic oscillator in thermal equilibrium is

$$\hat{\rho} = \frac{1}{Z} e^{-\frac{\hat{\mathbf{H}}}{k_B T}},$$

where

$$\hat{\mathbf{H}} = \frac{\hat{\mathbf{P}}^2}{2m} + \frac{1}{2} m\omega^2 \hat{\mathbf{X}}^2 = \left(\hat{\mathbf{N}} + \frac{1}{2}\right)\hbar\omega$$

with $\hat{\mathbf{N}} = \hat{\mathbf{a}}^\dagger \hat{\mathbf{a}}$.

(a) Show that $e^{\frac{\hat{\mathbf{H}}}{k_B T}} a e^{-\frac{\hat{\mathbf{H}}}{k_B T}} = a e^{-\frac{\hbar\omega}{k_B T}}$, and hence $\left\langle \hat{\mathbf{a}}^\dagger \hat{\mathbf{a}} \right\rangle \equiv \mathrm{Tr}\left[\hat{\rho}\hat{\mathbf{N}}\right] = \left\langle \hat{\mathbf{a}}\hat{\mathbf{a}}^\dagger \right\rangle e^{-\frac{\hbar\omega}{k_B T}}$.

Using Baker-Campbell-Hausdorff, we know that

$$e^A B e^{-A} = B + [A, B] + \frac{1}{2}[A, [A, B]] + \cdots + \frac{1}{n!}\left[A, \overbrace{\cdots}^{n}\right]$$

so

$$e^{\frac{\hat{\mathbf{H}}}{k_B T}} \hat{\mathbf{a}} e^{-\frac{\hat{\mathbf{H}}}{k_B T}} = \hat{\mathbf{a}} + \frac{1}{k_B T}\left[\hat{\mathbf{H}}, \hat{\mathbf{a}}\right] + \ldots$$

The commutator of $\hat{\mathbf{H}}$ and $\hat{\mathbf{a}}$ is $-\hbar\omega\hat{\mathbf{a}}$, so each additional commutation just adds an extra power of $-\frac{\hbar\omega}{k_B T}$:

$$= \hat{\mathbf{a}} + -\frac{\hbar\omega}{k_B T}\hat{\mathbf{a}} + \frac{1}{2}(-\frac{\hbar\omega}{k_B T})^2 \hat{\mathbf{a}} + \cdots + \frac{1}{n!}(-\frac{\hbar\omega}{k_B T})^n \hat{\mathbf{a}}$$

We can factor out the operator $\hat{\mathbf{a}}$ and the rest is a series which sums to an exponential

$$= \hat{\mathbf{a}} \sum_n \frac{(-\frac{\hbar\omega}{k_B T})^n}{n!} = \hat{\mathbf{a}} e^{-\frac{\hbar\omega}{k_B T}}$$

(b) Use the commutation relation $\left[\hat{\mathbf{a}}, \hat{\mathbf{a}}^\dagger\right] = 1$ to show that $\left\langle \hat{\mathbf{N}} \right\rangle = \frac{1}{e^{\frac{\hbar\omega}{k_B T}} - 1}$.

$$\left\langle \hat{\mathbf{N}} \right\rangle = \mathrm{Tr}\left(\hat{\rho}\hat{\mathbf{N}}\right) = \sum_n \langle n| \hat{\rho}\hat{\mathbf{N}} |n\rangle = \sum_n n \langle n| \hat{\rho} |n\rangle = \sum_n \frac{n}{Z} e^{-\frac{\hbar\omega n}{k_B T}} = \frac{1}{Z}\left(\frac{1}{1 - e^{\frac{\hbar\omega}{k_B T}}}\right)$$
$$= \frac{1}{e^{\frac{\hbar\omega}{k_B T}} - 1}$$

Zero-Point Motion of a Harmonic Chain

(a) Show that the expectation values of kinetic and potential energy of the harmonic oscillator obey the virial relation for quadratic potentials, $\left\langle \hat{\mathbf{V}} \right\rangle = \left\langle \hat{\mathbf{K}} \right\rangle$ when in an energy eigenstate. Use this result to calculate the mean square displacement $\left\langle \hat{\mathbf{X}}^2 \right\rangle$ in the ground state. Show, further, that the time average expectation value $\overline{\left\langle \hat{\mathbf{V}} \right\rangle} = \overline{\left\langle \hat{\mathbf{K}} \right\rangle}$ regardless of the quantum state.

$$\left\langle \hat{\mathbf{K}} \right\rangle = \left\langle \frac{\hat{\mathbf{P}}^2}{2m} \right\rangle = \frac{1}{2m}\left(-\frac{\hbar m\omega}{2}\right)\left\langle (\hat{\mathbf{a}}^\dagger - \hat{\mathbf{a}})^2 \right\rangle$$

If we expand the operators in the last statement, we get two squared terms which will have no expectation value, since the eigenstates of energy are orthonormal. However, the terms $\hat{\mathbf{a}}^\dagger\hat{\mathbf{a}} = \hat{\mathbf{N}}$ and $\hat{\mathbf{a}}\hat{\mathbf{a}}^\dagger = \hat{\mathbf{N}} + 1$ will have expectation values, so the stuff in the expectation brackets evaluates to $-2n$ (because of the minus sign between them in the square). Therefore

$$\left\langle \hat{\mathbf{K}} \right\rangle = \frac{\hbar\omega}{2} n$$

Similarly,

$$\left\langle \hat{\mathbf{V}} \right\rangle = \frac{m\omega^2}{2}\left\langle \hat{\mathbf{X}}^2 \right\rangle = \frac{m\omega^2}{2}\left(\frac{\hbar}{2m\omega}\right)\left\langle 2\hat{\mathbf{N}} \right\rangle = \frac{\hbar\omega}{2} n = \left\langle \hat{\mathbf{K}} \right\rangle$$

Next, we can evaluate the mean square displacement in the ground state by noting that $\left\langle \hat{\mathbf{X}}^2 \right\rangle = \frac{2}{m\omega}\left\langle \hat{\mathbf{V}} \right\rangle = \frac{\hbar}{m\omega} n$. In the ground state, $n = 0$, so $\left\langle \hat{\mathbf{X}}^2 \right\rangle_0 = 0$.
I'm not quite sure what the time average expectation value is, so I don't know what to do for the last part of the question.

(b) Consider the infinite periodic chain of coupled oscillators discussed by Cohen-Tannoudji (complement J_V). Express the position of the jth oscillator, $\hat{\mathbf{X}}_j$ in terms of the normal mode coordinates $\hat{\boldsymbol{\Xi}}(k)$, with $k \in (-\pi/l, \pi/l)$, where l is the period of the chain.

The conversion between $\hat{\mathbf{X}}$ and $\hat{\boldsymbol{\Xi}}$ is like a discrete Fourier transform in one direction and a continuous transform in the other direction. In the classical example, we wrote these transforms as

$$x_j(t) = \frac{l}{2\pi}\int_{-\frac{\pi}{l}}^{\frac{\pi}{l}} \xi(k,t) e^{\imath kjl}$$

so, following this logic, we should be able to just promote each side to a quantum operator:

$$\hat{\mathbf{X}}_q = \frac{l}{2\pi}\int_{-\frac{\pi}{l}}^{\frac{\pi}{l}} \hat{\boldsymbol{\Xi}}(k) e^{\imath qkl}$$

(c) Evaluate the expectation value $\left\langle \Xi(k)\Xi^\dagger(k') \right\rangle$ in the ground state.

First, we can define

$$\hat{\mathbf{\Xi}}(k) = \sqrt{\frac{\hbar}{2m\Omega(k)}}(\hat{\mathbf{a}}^\dagger(k) + \hat{\mathbf{a}}(k))$$

similar to the position operator in x-space. With this in mind, the expectation value should be similar to that of $\hat{\mathbf{X}}^2$:

$$\left\langle \hat{\mathbf{\Xi}}(k)\hat{\mathbf{\Xi}}^\dagger(k') \right\rangle = \frac{\hbar}{2m\sqrt{\Omega(k)\Omega(k')}} \left\langle \hat{\mathbf{a}}^\dagger(k)\hat{\mathbf{a}}(k') + \hat{\mathbf{a}}(k)\hat{\mathbf{a}}^\dagger(k') \right\rangle$$

In the ground state, I'm guessing $k = k' = 0$, so we just get two number operator equivalents which pull out k values from k energy states, so

$$\left\langle \hat{\mathbf{\Xi}}(k)\hat{\mathbf{\Xi}}^\dagger(k') \right\rangle_{k=k'=0} = \frac{\hbar}{m\Omega(0)} \left. k \right|_0 = 0$$

(d) Let the potential U vanish but keep V nonzero (i.e. $\omega = 0$ but $\omega_1 \neq 0$ in Cohen-Tannoudji's notation). Show that the mean square displacement $\left\langle \hat{\mathbf{X}}_j^2 \right\rangle$ of each mass j diverges in the ground state, but the mean square separation of neighboring masses $\left\langle (\hat{\mathbf{X}}_{j+1} - \hat{\mathbf{X}}_j)^2 \right\rangle$ remains finite.

Using the results from the previous two problems, we can see that

$$\left\langle \hat{\mathbf{X}}_j^2 \right\rangle = \frac{l^2}{4\pi^2} \int_{-\frac{\pi}{l}}^{\frac{\pi}{l}} \frac{\hbar^2}{m^2\Omega^2(k)} k^2 e^{2\imath jkl}$$

Here, $\Omega^2(k) = 4\omega_1^2 \sin^2\left(\frac{kl}{2}\right)$. This integral is best done with Mathematica, and it diverges. Next, we want to look at the separation:

$$(\hat{\mathbf{X}}_{j+1} - \hat{\mathbf{X}}_j)^2 = \left(\frac{l}{2\pi} \int_{-\frac{\pi}{l}}^{\frac{\pi}{l}} \hat{\mathbf{\Xi}}(k) \left(e^{\imath(j+1)kl} - e^{\imath jkl} \right) \right)^2$$

I couldn't figure out how to get Mathematica to perform this integral (the only difference is the exponential term, and it outputs a whole bunch of hypergeometric-type functions, so I'd assume that means the answer is finite).