University of California at San Diego – Department of Physics – Prof. John McGreevy

Physics 212C QM Spring 2023
Assignment 2 – Solutions

Due 12:30pm Tuesday, April 18, 2023

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1. **Brain-warmer: oscillator algebra.** Convince yourself that an operator $\mathcal{O}$ made of creation and annihilation operators $\mathbf{a}_k$ and $\mathbf{a}_k^\dagger$ for various k commutes with the number operator $\sum_k \mathbf{N}_k$ if and only if it has the same number of $\mathbf{a}$s as $\mathbf{a}^\dagger$s.

2. **Brain-warmer: Heisenberg time evolution of the harmonic chain.** Recall the expression for $\mathbf{q}_n$ in terms of creation and annihilation operators given in the lecture notes. Check that the expression for $\mathbf{p}_n$ in terms of creation and annihilation operators is consistent with the Heisenberg equations of motion

$$\mathbf{p}_n = m\dot{\mathbf{q}}_n = \frac{\mathbf{i}m}{\hbar}[\mathbf{H}, \mathbf{q}_n].$$

(That is, evaluate the right hand side of this expression using the algebra of $\mathbf{a}_k$ and $\mathbf{a}_k^\dagger$.

We have

$$\mathbf{q}_n = \sqrt{\frac{\hbar}{2Nm}} \sum_k \frac{1}{\sqrt{\omega_k}} \left(e^{\mathbf{i}kx}\mathbf{a}_k + e^{-\mathbf{i}kx}\mathbf{a}_k^\dagger \right) + \frac{1}{\sqrt{N}}\mathbf{q}_0$$

and

$$\mathbf{H}_0 = \sum_k \hbar\omega_k \left(\mathbf{a}_k^\dagger \mathbf{a}_k + \frac{1}{2} \right) + \frac{p_0^2}{2m}.$$

Therefore

$$\mathbf{p}_n = m\dot{\mathbf{q}}_n = \frac{\mathbf{i}m}{\hbar} \left(\sum_k \hbar\omega_k [\mathbf{a}_k^\dagger \mathbf{a}_k, \mathbf{q}_n] + [\frac{p_0^2}{2m}, \mathbf{q}_n] \right)$$

In the second term, only the $\mathbf{q}_0$ part contributes because modes of different k are orthogonal.

$$\mathbf{p}_n = \frac{\mathbf{i}m}{\hbar} \sum_k \sum_{k'} \hbar\omega_k \sqrt{\frac{\hbar}{2Nm\omega_{k'}}} \underbrace{[\mathbf{a}_k^\dagger \mathbf{a}_k, e^{\mathbf{i}k'x}\mathbf{a}_{k'} + e^{-\mathbf{i}k'x}\mathbf{a}_{k'}^\dagger]}_{=\left(-\mathbf{a}_k e^{\mathbf{i}kx} + \mathbf{a}_k^\dagger e^{-\mathbf{i}kx}\right)\delta_{k,k'}} + \frac{\mathbf{i}m}{\hbar\sqrt{N}} \underbrace{[\frac{p_0^2}{2m}, q_0]}_{=-\mathbf{i}p_0/m} \quad (1)$$

This indeed gives

$$\mathbf{p}_n = \frac{1}{\mathbf{i}} \sqrt{\frac{\hbar m}{2N}} \sum_k \sqrt{\omega_k} \left(e^{\mathbf{i}kx}\mathbf{a}_k - e^{-\mathbf{i}kx}\mathbf{a}_k^\dagger \right) + \frac{1}{\sqrt{N}}\mathbf{p}_0.$$

3. **Entropy and thermodynamics.** Consider a quantum system with hamiltonian $\mathbf{H}$ and Hilbert space $\mathcal{H}$. Its behavior in thermal equilibrium at temperature T can be described using the *thermal density matrix*

$$\boldsymbol{\rho}_\beta \equiv \frac{1}{Z} e^{-\beta \mathbf{H}}$$

where $\beta \equiv \frac{1}{T}$ specifies the temperature and Z is a normalization factor. (We can think about this as the density matrix resulting from coupling the system to a heat bath and tracing out the Hilbert space of the heat bath.) Expectation values are computed by $\langle \mathcal{O} \rangle \equiv \mathrm{tr} \boldsymbol{\rho}_\beta \mathcal{O}$.

(a) Find a formal expression for Z by demanding that $\boldsymbol{\rho}_\beta$ is normalized appropriately. This is called the *partition function*.

$$tr(\boldsymbol{\rho}_\beta) = 1$$
$$\frac{1}{Z}\mathrm{tr}(e^{-\beta H}) = 1$$
$$Z = tr(e^{-\beta H}) = \sum_{E_m} e^{-\beta E_m}$$

(b) Recall that the von Neumann entropy of a density matrix is defined as

$$S[\rho] = -\mathrm{tr} \rho \log \rho.$$

Show that the von Neumann entropy of $\boldsymbol{\rho}_\beta$ can be written as

$$S_\beta = E/T + \log Z$$

where $E \equiv \langle \mathbf{H} \rangle$ is the expectation value for the energy. Convince yourself that this is same as the thermal entropy.

$$S = -tr(\boldsymbol{\rho}_\beta \log(\boldsymbol{\rho}_\beta))$$
$$S = -tr(\frac{1}{Z}e^{-\beta H} \log(\frac{e^{-\beta H}}{z}))$$
$$S = tr(\frac{1}{Z}e^{-\beta H}\beta H + \frac{1}{Z}e^{-\beta H} \log Z)$$
$$S = \beta tr(\frac{1}{Z}e^{-\beta H} H) + \frac{tr(e^{-\beta H} \log(Z))}{tr(e^{-\beta H})}$$
$$S = \beta \langle H \rangle + \log Z$$
$$S = E/T + \log Z$$

(c) Evaluate Z and E and the heat capacity $C = \partial_T E$ for the case where the system is a simple harmonic oscillator

$$\mathcal{H} = \text{span}\{|n\rangle, n = 0, 1, 2...\}, \quad \mathbf{H} = \hbar\omega\left(\mathbf{n} + \frac{1}{2}\right)$$

with $\mathbf{n}|n\rangle = n|n\rangle$.

The matrix elements of H are

$$H_{n'n} = \langle n'| H |n\rangle = \hbar\omega(\langle n'| \mathbf{n} |n\rangle + \frac{1}{2}\langle n'| n\rangle)$$

$$H_{n'n} = \hbar\omega(n + \frac{1}{2})\delta_{n'n}$$

$$Z = \text{tr}(e^{-\beta H})$$

$$Z = \sum_n \langle n| e^{-\beta H} |n\rangle$$

$$Z = \sum_n e^{-\beta H_{nn}} = e^{+\beta\hbar\omega\frac{1}{2}} \sum_{n=0}^{\infty} e^{-\beta\hbar\omega n}$$

Letting $x \equiv e^{-\beta\hbar\omega}$, we have a geometric series:

$$Z = x^{-\frac{1}{2}} \sum_{n=0}^{\infty} x^n = x^{1/2}\frac{1}{1-x}.$$

Next we find E

$$E = \langle H\rangle = tr(\boldsymbol{\rho} H)$$

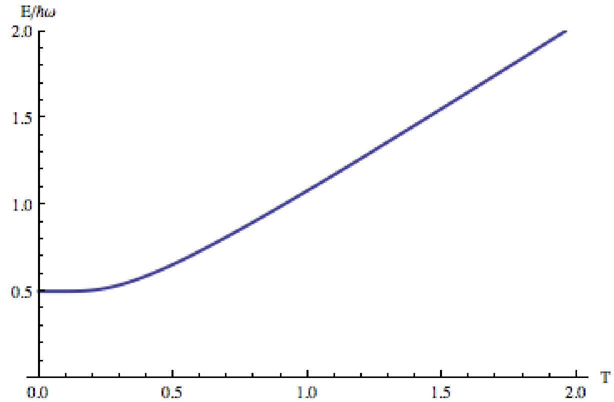
$$E = \text{tr}(\frac{1}{Z}e^{-\beta H}H)$$

$$E = \frac{1}{Z}\sum_n \langle n| (e^{-\beta H}H) |n\rangle$$

$$E = \frac{1}{Z}\sum_n E_n e^{-\beta H_{nn}} = \frac{1}{Z}\hbar\omega\sum_{n=0}^{\infty}(n + 1/2)\, x^{n+1/2} = \frac{1}{Z}\hbar\omega x\partial_x\left(\sum_{n=0}^{\infty} x^n\right)$$

where $x \equiv e^{-\beta\omega}$.

$$E = \hbar\omega\frac{1}{Z}x\partial_x Z = \hbar\omega\frac{1}{2}\frac{1+x}{(1-x)^2} = \hbar\omega\frac{1}{2}\frac{1+x}{1-x}.$$

It looks like this: 

(d) Now evaluate the low-temperature equilibrium heat capacity for a harmonic mattress (the d-dimensional version of the harmonic chain). That is, find the heat capacity for a collection of harmonic oscillators labelled by wavenumber $\vec{k}$ in d dimensions,

$$\mathbf{H} = \sum_k \hbar\omega_k \left(a_k^\dagger a_k + \frac{1}{2} \right)$$

with dispersion relation $\omega_k = v_s|k|$.

In terms of the normal modes, this is just a collection of oscillators labelled by k, with frequency ω_k. The partition function is $Z = \prod_k Z_k$ so $\log Z = \sum_k \log Z_k$ and the expected energy is

$$\langle H \rangle = -\partial_\beta \log Z = \sum_k E_k, \tag{2}$$

with $E_k = \hbar\omega_k \frac{1}{2} \frac{1+e^{-\beta\omega_k}}{1-e^{-\beta\omega_k}}$. The heat capacity is similarly a sum over k.

In the thermodynamic limit, the sum over k becomes an integral $\sum_k \rightsquigarrow L^d \int đ^d k$. If we are just interested in temperatures small compared to the energy scales associated with the lattice (*i.e.* the bandwidth), we can approximate the dispersion as linear. This is because a mode doesn't contribute to the heat capacity if its frequency is much bigger than the temperature.

Then the heat capacity is

$$C_V = \sum_k \left(\frac{\omega_k}{T}\right)^2 \frac{e^{-\omega_k/T}}{\left(1-e^{-\omega_k/T}\right)^2} \tag{3}$$

$$= \left(\frac{1}{T}\right)^2 L^d \underbrace{\int đ^d k}_{=(2\pi)^{-d}\int d^{d-1}\Omega k^{d-1}dk} \omega_k^2 \frac{e^{-\omega_k/T}}{\left(1-e^{-\omega_k/T}\right)^2} \tag{4}$$

$$= \left(\frac{1}{T}\right)^2 L^d K_{d-1} v_s^d \int d\omega \omega^{d+1} f(\omega/T) \tag{5}$$

$$= v_s^d T^d L^d K_{d-1} \underbrace{\int dx x^{d+1} f(x)}_{=\zeta(d)d!} . \tag{6}$$

Here $K_d \equiv \frac{\Omega_d}{(2\pi)^d}$ where Ω_d is the volume of the unit d-sphere. In the last step we extracted the temperature dependence of the integral by scaling, *i.e.* just be redefining the integration variable to leave behind an numerical integral independent of everything except the dimension of space. The important conclusion is that the specific heat $c_V = C_V/L^d \propto T^d$.

4. **Gaussian identity.** Show that for a gaussian quantum system

$$\left\langle e^{\mathbf{i}K\mathbf{q}}\right\rangle = e^{-A(K)\left\langle \mathbf{q}^2\right\rangle}$$

and determine $A(K)$. Here $\langle ...\rangle \equiv \langle 0| ... |0\rangle$. Here by 'gaussian' I mean that $\mathbf{H}$ contains only quadratic and linear terms in both $\mathbf{q}$ and its conjugate variable $\mathbf{p}$ (but for the formula to be exactly correct as stated you must assume $\mathbf{H}$ contains only terms quadratic in $\mathbf{q}$ and $\mathbf{p}$; for further entertainment fix the formula for the case with linear terms in $\mathbf{H}$).

Versions of this problem appear in Peskin problem 11.1a) and in Green-Schwarz-Witten volume 1 page 429.

One can do it by algebra (as in GSW), using Campbell-Baker-Hausdorff to put the annihilation operators on the right and the creation operators on the left:

$$e^{\alpha(\mathbf{a}+\mathbf{a}^\dagger)} = e^{\alpha^2/2} e^{\alpha\mathbf{a}^\dagger} e^{\alpha\mathbf{a}} .$$

The vacuum expectation value of the RHS is $e^{\alpha^2/2}$.

But it is, I think, more illuminating to do it by path integral. (In the case when there are indices, $Kq = K_\alpha q_\alpha = K \cdot q$, this technique is worth the effort. And this method makes it manifest that it is $K_\alpha \langle q_\alpha q_\beta\rangle K_\beta$ that appears in the exponent on the RHS.) The path integral representation is

$$\left\langle e^{\mathbf{i}K\mathbf{q}}\right\rangle = \frac{1}{Z}\int \prod_i dq_i \; e^{-q_i D_{ij} q_j} e^{\mathbf{i}K q_0} \tag{7}$$

with $Z = \int \prod_i dq_i \ e^{-q_i D_{ij} q_j}$. Here i, j are discrete time labels, and D_{ij} is the matrix which discretizes the action. Repeated indices are summed. A word about where this formula comes from: the vacuum can be prepared by starting in an arbitrary state and acting with e^{-TH} for some large T, and then normalizing (as usual when discussing path integrals, it's best to not worry about the normalization and only ask questions which don't depend on it),

$$|0\rangle = \mathcal{N} e^{-\mathbf{H}T} |\text{any}\rangle .$$

To see this, just expand in the energy eigenbasis. This 'imaginary time evolution operator' $e^{-\mathbf{H}T}$ has a path integral representation just like the real time operator, by nearly the same calculation

$$e^{-\mathbf{H}T} = \int [Dq] e^{-\int_{-T}^{0} d\tau L(q(\tau), \dot{q}(\tau))}.$$

Doing the same thing to prepare $\langle 0|$, making a sandwich of $e^{q(0)\cdot k} = e^{\int d\tau q(\tau)\cdot k\delta(\tau)}$, and taking $T \to \infty$ we can forget about the arbitrary states at the end, and we arrive at (7).

Once we arrive at this path integral representation, it can be evaluated in two steps: First, we can absorb the insertion into the action:

$$e^{-\frac{1}{2}q_i D_{ij} q_j} e^{\mathbf{i}Kq_0} = e^{-\frac{1}{2}q_i D_{ij} q_j + \mathbf{i}Kq_0} = e^{-\frac{1}{2}\tilde{q}_i D_{ij}\tilde{q}_j} e^{\frac{1}{2}J_i D_{ij}^{-1} J_j}$$

with $J_j = -\mathbf{i}K\delta_{j,0}$, and D^{-1} is the inverse of the kinetic matrix, i.e. the propagator:

$$\langle q_i q_j \rangle = D_{ij}^{-1}.$$

So, plugging in the value of J, we arrive at the answer:

$$\left\langle e^{\mathbf{i}K\mathbf{q}} \right\rangle = e^{-\frac{1}{2}K^2 D_{00}^{-1}} = e^{-\frac{1}{2}K^2 \langle q_0 q_0 \rangle} = e^{-\frac{1}{2}K^2 \left\langle \mathbf{q}^2 \right\rangle}.$$