DIYU Seminar QM Homework 1

Blake Stacey

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Problem 1.1: *Commutator Relations*

To get anything done in quantum theory, we have to be comfortable with commutators. By well-nigh ubiquitous convention,

$$[A, B] \equiv AB - BA. \tag{1}$$

(a) Evaluate $[A, BC]$ in terms of $[A, B]$ and $[A, C]$. (*Hint*: add something which equals zero to $ABC - BCA$.)

(b) Evaluate $[AB, CD]$. You should get a sum of four terms, each involving a commutator of two operators.

Problem 1.2: *Canonical Commutator*

In lecture, we used the canonical relation

$$[x, p] = i\hbar, \tag{2}$$

and we proved that

$$\left[x, p^2\right] = 2i\hbar p. \tag{3}$$

By induction, prove that

$$[x, p^n] = i\hbar n p^{n-1}. \tag{4}$$

Problem 1.3: *Wavefunctions and Fourier transforms*

As derived in lecture and discussed in the reading (`http://www.sunclipse.org/?p=122`), in position space a momentum eigenstate of eigenvalue p has the following form:

$$\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}} \exp\left(\frac{ipx}{\hbar}\right). \tag{5}$$

Because the position eigenvectors $\langle x|$ form a complete basis, we can recover the eigenket $|p\rangle$ by summing over them:

$$|p\rangle = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} dx\, \exp\left(\frac{ipx}{\hbar}\right) |x\rangle\,. \tag{6}$$

By projecting a general state $|\psi\rangle$ into the $|x\rangle$ basis, we define the position-space wavefunction,

$$\psi(x) = \langle x|\psi\rangle\,, \tag{7}$$

but we can do the same thing just as well with the momentum basis:

$$\tilde{\psi}(p) = \langle p|\psi\rangle\,. \tag{8}$$

What does Eq. (6) imply about the Fourier transforms of $\psi(x)$ and $\tilde{\psi}(p)$?

Problem 1.4: *Thermodynamics of Oscillators*

This problem is derived from Shankar's Exercise 7.5.4. Recall from Eric's lectures on statistical mechanics that in the canonical ensemble, the probability of finding a system in a state j of energy E_j is

$$P(j) = \frac{\exp\left(-\frac{E_j}{k_B T}\right)}{Z}, \tag{9}$$

where the partition function Z involves a sum over all the states,

$$Z = \sum_j \exp\left(-\frac{E_j}{k_B T}\right). \tag{10}$$

The average thermal energy of the systems in the ensemble is

$$\langle E \rangle = \sum_j E_j P(j) = -\partial_\beta \log Z, \tag{11}$$

where for convenience we have defined $\beta = (k_B T)^{-1}$.

(a) The classical harmonic oscillator Hamiltonian is

$$H = \frac{p^2}{2m} + \frac{m\omega^2 x^2}{2}. \tag{12}$$

By integrating over x and p, show that the classical partition function is

$$Z_{\text{cl}} = \left(\frac{2\pi}{\beta m \omega^2}\right)^{1/2} \left(\frac{2\pi m}{\beta}\right)^{1/2} = \frac{2\pi}{\omega\beta}, \tag{13}$$

and therefore that

$$\langle E \rangle_{\text{cl}} = \frac{1}{\beta} = k_B T. \tag{14}$$

(b) Now imagine an ensemble of *quantum* harmonic oscillators in equilibrium at a fixed temperature T. Here, the Hamiltonian is

$$H = \hbar\omega\left(a^\dagger a + \frac{1}{2}\right), \tag{15}$$

and the energy of eigenstate $|n\rangle$ is

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right). \tag{16}$$

Calculate the partition function

$$Z = \sum_n e^{-\beta E_n}, \tag{17}$$

and find the average energy over all the oscillators in the ensemble, $\langle E \rangle_{\text{qm}}$.

(c) What happens to $\langle E \rangle_{\text{qm}}$ when T becomes much larger than $\hbar\omega/k_B$?

(d) Next, consider a system of $3N$ decoupled oscillators. (This is equivalent to a crystal of N atoms in three dimensions, if the oscillations are small.) Show that if the oscillators are treated classically, the specific heat per atom

$$C_{\text{cl}}(T) = \frac{\partial_T \langle E \rangle_{\text{cl}}}{N}, \tag{18}$$

is just $3k_B$. Note that this is independent of temperature and of the crystal's individual character. This agrees with experiment for large T but not as $T \to 0$. Assuming (following Einstein) that the oscillators all have the same frequency ω, show that

$$C_{\text{qm}}(T) = 3k_B \left(\frac{\theta_E}{T}\right)^2 \frac{e^{\theta_E/T}}{(e^{\theta_E/T} - 1)^2}, \tag{19}$$

where $\theta_E = \hbar\omega/k_B$ is the *Einstein temperature.* Show that for $T \gg \theta_E$, C_{qm} agrees with C_{cl}, while for small T,

$$C_{\text{qm}}(T) = 3k_B \left(\frac{\theta_E}{T}\right)^2 e^{-\theta_E/T}. \tag{20}$$

Einstein's model was improved by Debye, who calculated what happens when (as in a real crystal of coupled atoms) the normal modes do not all have the same frequency.

Problem 1.5: *The Harmonic Oscillator in the Heisenberg Picture*

In the Schrödinger picture of quantum mechanics, time evolution is governed by the Schrödinger Equation,

$$i\hbar\partial_t \left|\psi(t)\right\rangle = H \left|\psi(t)\right\rangle. \tag{21}$$

We noted two lectures ago that by looking at the (possibly time-dependent) expectation value for a general observable A,

$$\langle A\rangle (t) = \left\langle \psi(0) \middle| e^{\frac{iHt}{\hbar}} A e^{-\frac{iHt}{\hbar}} \middle| \psi(0) \right\rangle, \tag{22}$$

we could move to a new representation of the physics, which we called the Heisenberg picture. In the Heisenberg picture, the time dependence lies in the operators, not the states. From Eq. (22) we see that

$$A(t) = e^{iHt/\hbar} A e^{-iHt/\hbar}. \tag{23}$$

The time evolution of $A(t)$ is governed by Heisenberg's equation of motion,

$$\partial_t A(t) = \frac{i}{\hbar}\left[H, A(t)\right]. \tag{24}$$

(a) Calculate the commutators $[H, x]$ and $[H, p]$, given that the Schrödinger operators x and p satisfy $[x, p] = i\hbar$ and H has the harmonic-oscillator form.

(b) Using the results of part (a) and Heisenberg's equation of motion, show that the Heisenberg operators $x(t)$ and $p(t)$ satisfy

$$\partial_t x(t) = \frac{p(t)}{m}, \tag{25}$$

$$\partial_t p(t) = -m\omega^2 x(t). \tag{26}$$

(c) Apply the initial conditions $x(0) = x$ and $x'(0) = p/m$ (which you should be able to justify from Eq. (23)) to show that

$$x(t) = x\cos\omega t + \frac{p}{m\omega}\sin\omega t, \tag{27}$$

$$p(t) = p\cos\omega t - m\omega x\sin\omega t. \tag{28}$$

(d) Recall the translation operator we defined in lecture,

$$T(\lambda) = \exp\left(-\frac{i\lambda p}{\hbar}\right), \tag{29}$$

which effected a translation by λ of the states it acts upon. We showed that

$$xT(\lambda)|x\rangle = (x+\lambda)T(\lambda)|x\rangle, \tag{30}$$

or in other words that

$$T(\lambda)|x\rangle = |x+\lambda\rangle. \tag{31}$$

Now, we want to translate an *energy eigenstate of the harmonic oscillator.* Take the ground state $|0\rangle$ and translate by x_0 to obtain a new state, which we'll call $|x_0\rangle$:

$$|x_0\rangle = T(x_0)|0\rangle. \tag{32}$$

Show that

$$\langle x_0|x|x_0\rangle = x_0, \tag{33}$$

$$\langle x_0|p|x_0\rangle = 0. \tag{34}$$

It is useful to remember that $[T(\lambda), p] = 0$. With these results, show that

$$\langle x(t)\rangle = \langle x_0|x(t)|x_0\rangle = x_0 \cos\omega t, \tag{35}$$

$$\langle p(t)\rangle = \langle x_0|p(t)|x_0\rangle = -m\omega x_0 \sin\omega t. \tag{36}$$

The *expectation values* for position and momentum in this state satisfy the *classical* harmonic oscillator's equations of motion.

Problem 1.6: *Two-State Systems and Time Evolution*

This problem is based on Sakurai 2.9, as modified by R. L. Jaffe. Consider a system with *two* permissible states. We take a box with a particle in it and place a partition down the middle. The state in which the particle is on the left side with total certainty we label $|L\rangle$, and the state in which the particle is on the right we label $|R\rangle$. Because of quantum tunneling, the particle can slip through the barrier, and so the time evolution operator must include terms which take $|L\rangle$ to $|R\rangle$ and vice versa. Our Hamiltonian will be the following:

$$H = \begin{pmatrix} 0 & \Delta \\ \Delta & 0 \end{pmatrix}, \tag{37}$$

in the basis where

$$|L\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \; |R\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \tag{38}$$

We can also write H in the equivalent form

$$H = \Delta(|L\rangle\langle R| + |R\rangle\langle L|). \tag{39}$$

Here, Δ is a real number with units of energy which parameterizes the strength of the tunneling effect.

(a) Find the normalized eigenstates of H and their eigenvalues.

(b) Suppose that at time $t = 0$, the system's state is given by

$$|\psi(0)\rangle = c_L|L\rangle + c_R|R\rangle. \tag{40}$$

Find $|\psi(t)\rangle$ by applying the time-evolution operator. (*Hint*: rewrite $|L\rangle$ and $|R\rangle$ in terms of the energy eigenstates.)

(c) Let's say that at $t = 0$, the particle is definitely on the left-hand side:

$$|\psi(0)\rangle = |L\rangle \,. \tag{41}$$

As a function of time, what is the probability that the particle will be on the *right*-hand side?

(d) Suppose that I had goofed and, not respecting the symmetry of the problem, had written the Hamiltonian

$$H' = \Delta \, |L\rangle \langle R| \,. \tag{42}$$

Solve the general time evolution with H' and show that probability is not conserved.