Quantum Mechanics M.T. 2000

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Problem Set No. 3

1. Orthogonality

   For the particle in the infinitely deep square well potential ($V = 0$ for $0 < x < a$, $V = \infty$ for $x \leq 0, x \geq a$) pick two energy eigenfunctions and check that they are orthogonal, first qualitatively by means of a sketch, then analytically by doing the integral.

2. Superposition of eigenfunctions

   Again, for a particle in the infinitely deep square well potential, suppose the state is described at a given time by the wavefunction

   $$\phi(x) = \frac{1}{\sqrt{a}}\left(\sin\left(\frac{\pi x}{a}\right) + \sin\left(\frac{2\pi x}{a}\right)\right).$$

   i) Show that this is not an energy eigenfunction. What are the possible results of a measurement of the energy of the particle and what are their relative probabilities? What do you expect the expectation value of the energy to be?

   ii) Show that ϕ is correctly normalized.

   iii) Calculate $\langle -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\rangle$. What physical quantity is this? How is the result related to your answer in part i)?

3. Momentum probability distribution

   Consider the following two normalised wavefunctions

   $$\phi_1(x) = \frac{1}{\sqrt{a}}\exp(-|x|/a), \quad \phi_2(x) = e^{ikx}\frac{1}{\sqrt{a}}\exp(-|x|/a).$$

   Calculate $\langle x\rangle$ and $\langle p\rangle$ for both of these wavefunctions.

   Sketch $|\phi_1|^2$ and $|\phi_2|^2$ versus x for fixed a.

   The momentum probability amplitude corresponding to a position probability amplitude $\phi(x)$ is

   $$\tilde{\phi}(p) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} e^{-ipx/\hbar}\phi(x)dx$$

   where the factor $1/\sqrt{2\pi\hbar}$ ensures that

   $$\int_{-\infty}^{\infty}|\tilde{\phi}(p)|^2 dp = 1$$

if $\phi(x)$ is normalised. (You can use the Dirac delta function covered in the Mathematical Physics lectures to check this).

Evaluate $\tilde{\phi}_1(p)$ and $\tilde{\phi}_2(p)$ and sketch both as a function of p, for fixed a.

Give an informal (qualitative) definition of the "spreads" of $|\phi_1(x)|^2$ in x and of $|\tilde{\phi}_1(p)|^2$ in p. Show that their product is of order $\hbar$.

4. Changes of state following a measurement

A particle in the infinite-sided box has the wavefunction of Set 2 Q 4. At a certain instant, its energy is measured and found to have the value $h^2/2ma^2$. What is the probability of finding the particle in the region $0 \leq x \leq a/2$ (i) before the energy measurement? (ii) after it? Explain the answers qualitatively, with the aid of a sketch.

Equations of motion for expectation values; conservation laws

5. (i) For any operators $\hat{A}, \hat{B}$, verify that

$$[\hat{A}, \hat{B}^2] = [\hat{A}, \hat{B}]\hat{B} + \hat{B}[\hat{A}, \hat{B}].$$

(ii) Let $\hat{H}$ be the energy operator $\hat{H} = \frac{\hat{p}^2}{2m} + V(x)$, in 1-D. Verify that $[x, \hat{H}] = i\hbar\hat{p}/m$. [You can do this by using (i), or using $\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)$].

With the same $\hat{H}$, show that $[\hat{p}, \hat{H}] = -i\hbar\frac{dV}{dx}$.

Combining this result with that of Set 2 Q 6 show that

$$i\hbar\frac{d}{dt}\langle\hat{p}\rangle = \langle[\hat{p}, \hat{H}]\rangle$$

for any wavefunction ψ.

Show also that

$$i\hbar\frac{d}{dt}\langle x\rangle = \langle[x, \hat{H}]\rangle.$$

(iii) State and prove a general result about

$$\frac{d}{dt}\langle\hat{A}\rangle$$

where $\hat{A}$ is any operator (not explicitly depending on t) representing an observable dynamical quantity.

(iv) What is the corresponding result if the operator $\hat{A}$ does depend explicitly on t?

6. Let $\hat{H}$ be the 1-D S.H.O. energy operator,

$$H = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2 x^2.$$

Show that $\frac{d\langle\hat{p}\rangle}{dt} = -m\omega^2\langle x\rangle$ and that $\frac{d\langle x\rangle}{dt} = \frac{1}{m}\langle\hat{p}\rangle$. Hence obtain the general solution for the variation of $\langle x\rangle$ with time.

7. The Hamiltonian for two particles of mass m in one dimension interacting via their mutual potential energy $V(x_1 - x_2)$ is given by

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_1^2} - \frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_2^2} + V(x_1 - x_2)$$

where x_1 and x_2 are the coordinates of the two particles. Show that the total momentum of the two particles is conserved. [Hint: the total momentum operator $\hat{P}$ is $\hat{P} = \hat{p}_1 + \hat{p}_2$ where $\hat{p}_1 = -i\hbar\frac{\partial}{\partial x_1}$ and similarly for $\hat{p}_2$.]

<u>Compatibility</u>

8. Show that it is possible to have quantum states for a particle (in 1-D, for simplicity) in which the momentum and the kinetic energy both have well-defined values, but that this is possible for the momentum and the total energy only if the potential energy is a constant.

9. Find a wavefunction (not normalised) such that $\hat{p}_x = -i\hbar\frac{\partial}{dx}, \hat{p}_y = -i\hbar\frac{\partial}{\partial y}$ and $\hat{p}_z = -i\hbar\frac{\partial}{\partial z}$ all have well-defined values, say $\hbar k_x, \hbar k_y$, and $\hbar k_z$ (i.e. you are looking for a wavefunction for a particle with definite momentum (vector) $\hbar\mathbf{k}$). Why can all three components of momentum have well-defined values?

<u>Uncertainty relations</u>

10. As a simple example of a time-independent wavepacket, consider the function

$$\phi(x) = \frac{1}{2\Delta k}\int_{k_0-\Delta k}^{k_0+\Delta k} e^{ikx}dk$$

which may be regarded as a superposition of (complex) waves e^{ikx} with different k's, lying within Δk on either side of a central value k_0. Evaluate this integral and show that

$$|\phi(x)|^2 = \frac{\sin^2(\Delta k.x)}{(\Delta k.x)^2} \quad .$$

Sketch $|\phi(x)|^2$ versus x, for a "small" value of Δk and for a "large" value of Δk (recall that Δk is the spread in the wavenumbers of the packet). $|\phi(x)|^2$ is mostly concentrated in the region bounded by its first zeros on either side of the origin; if the size of this region is denoted by "Δx", show that "Δx" $\Delta k = 2\pi$. Connect this to the uncertainty relation $\Delta x \Delta p \geq \frac{1}{2}\hbar$.

[The reason we used quotes in "Δx" is that there is a mathematically precise definition of Δx (without quotes), namely $\Delta x = [\langle (x - \langle x \rangle)^2 \rangle]^{\frac{1}{2}}$; see Q 11].

11. From Set 2 Q 9 (i) we know that $e^{-x^2/2a^2}$ is an eigenfunction of the 1-D S.H.O. with eigenvalue $\frac{1}{2}\hbar\omega$, where $a^2 = \hbar/m\omega$ and the potential energy is $\frac{1}{2}m\omega^2 x^2$. Find the expectation values of x, x^2, p and p^2 for a particle described by this wavefunction. You may need

$$\int_{-\infty}^{\infty} e^{-\alpha x^2} dx = \sqrt{\frac{\pi}{\alpha}}; \qquad \int_{-\infty}^{\infty} x^2 e^{-\alpha x^2} dx = \frac{1}{2\alpha}\sqrt{\frac{\pi}{\alpha}}.$$

Define $\Delta x = [\langle (x - \langle x \rangle)^2 \rangle]^{\frac{1}{2}}, \Delta p = [\langle (\hat{p} - \langle \hat{p} \rangle)^2 \rangle]^{1/2}$ where $\langle \ldots \rangle$ denotes expectation value in a definite state. Show that in this case $\Delta x \Delta p = \frac{1}{2}\hbar$.

[Hint: for $\langle \hat{p}^2 \rangle$ use $\hat{p}^2/2m + \frac{1}{2}m\omega^2 x^2 = E$].

[Extra problems]

12. [Superposition versus mixture]

Note: the concept of a "mixture" is not in the syllabus for A3

(i) Calculate the average value of x for the particle in the infinite-sided box, having the wavefunction at $t = 0$

$$\phi(x) = \frac{1}{\sqrt{a}}\left(\sin\frac{\pi x}{a} + \sin\frac{2\pi x}{a}\right) \qquad \text{("superposition")}$$

$$\left[\int_0^a x \sin^2\frac{\pi x}{a} dx = \int_0^a x \sin^2\frac{2\pi x}{a} dx = \frac{a^2}{4}, \int_0^a x \sin\frac{\pi x}{a} \sin\frac{2\pi x}{a} dx = -\frac{8a^2}{9\pi^2}.\right]$$

Explain the result by reference to a sketch of $|\phi(x)|^2$ (c.f. Set 2 Q 4).

(ii) Suppose we *don't know* the precise wavefunction for another particle in this box, but we know that there is a 50 % chance that it has wavefunction $\phi_1(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{\pi}{a}\right)$ and a 50 % chance that it has wavefunction $\phi_2(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{2\pi x}{a}\right)$.

This is called a "mixture" of ϕ_1 and ϕ_2, not a superposition. What is the average value of x?

Compare this with the answer of part (i).

(iii) Consider yet another particle with wavefunction

$$\phi_\delta = \frac{1}{\sqrt{a}}\left(\sin\frac{\pi x}{a} + e^{i\delta}\sin\frac{2\pi x}{a}\right).$$

What are the possible results of an energy measurement, and what are their relative probabilities?

Show that

$$\mid \phi_\delta(x) \mid^2 = \frac{1}{a}\left(\sin^2\frac{\pi x}{a} + \sin^2\frac{2\pi x}{a} + 2\cos\delta\sin\frac{\pi x}{a}\sin\frac{2\pi x}{a}\right)$$

and hence show that

$$\langle x\rangle_\delta = \int x|\phi_\delta|^2 dx = \frac{a}{2} - \frac{16a\cos\delta}{9\pi^2}.$$

Suppose now that δ is actually varying randomly, outside our control. We have to take an average over δ before comparing our "predictions" with "experiment". Perform the average of $\langle x\rangle_\delta$ over δ assuming that δ is uniformly distributed over the interval $(-\pi, \pi)$. Discuss the result with reference to parts (i) and (ii).

13. [Parity]

Note : The parity operator may not be required for paper A3, but "parity" is mentioned in the QM syllabus. It is also in the "Sub-Atomic Physics" syllabus for A5.

The definition of the parity operator $\hat{P}$ is (in 1-D):
(a) on wavefunctions, $\hat{P}\psi(x) = \psi(-x)$
(b) on the Hamiltonian, $\hat{P}\hat{H}(x)\hat{P}^{-1} = \hat{H}(-x)$.

(i) Show that $\frac{d}{dt}\int \psi^*\hat{P}\psi dx = 0$ if $[\hat{P}, \hat{H}] = 0$, and that if ψ is an eigenfunction of $\hat{P}$ with eigenvalue η then η is independent of time. What are the possible values of η?

(ii) Is it possible to have a quantum state for a particle in 1-D in which the energy, the momentum and the parity have well-defined values? What about *pairs* of these three observables?

14. Is the parity a good quantum number if the energy operator (in 1-D) is
   (i) $\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2 x^2$
   (ii) $\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2 x^2 + e\mathcal{E}x$?

   What physical problem might be represented by (ii)?

15. [Time dependent packets; dispersion]

Note : time-dependent packets are outside the A3 syllabus.

A simple example of a time-dependent wave packet is provided by a superposition of waves for which the *frequency is proportional to the wavenumber*: $\omega = ck$. Light, of course, is such a wave. Consider the packet

$$\phi(x,t) = \frac{1}{2\Delta k}\int_{k_o-\Delta k}^{k_o+\Delta k} e^{ik(x-ct)}dk$$

(Note that $\phi(x,0)$ is our packet in Q 10).

Evaluate the integral and show that

$$|\phi(x,t)|^2 = \frac{\sin^2[\Delta k(x-ct)]}{[\Delta k(x-ct)]^2}$$

(as in Q 10). For fixed t, at what x is $|\phi(x,t)|^2$ a maximum, and at what values of x do the first zeros of $|\phi(x,t)|^2$ away from the maximum occur? Sketch $|\phi(x,t)|^2$ for fixed t versus x.

Describe how the packet moves along in x as t varies. Does the *shape* of the function $|\phi(x,t)|^2$ change?

Consider now the packet for fixed x, as t varies. Where is the maximum as a function of t for fixed x, and where do the first minima on either side of it occur? If the spread in the packet in time, "Δt", is defined as the distance between the first minima on either side of the central maximum, show that $\Delta\omega$ "Δt" $= 2\pi$, where $\Delta\omega = c\Delta k$. Relate this to the uncertainty relation $\Delta E\ \Delta t\ \geq \frac{1}{2}\hbar$.

(ii) A time-dependent free-particle (plane wave) solution of the 1-D Schrödinger equation is $\psi(x,t) = N\exp(ikx - iEt/\hbar)$ where N is a normalization constant and $E = p^2/2m = \hbar^2k^2/2m = \hbar\omega$. It follows that for these waves the frequency ω is *not* proportional to k but to k^2: $\omega = \hbar k^2/2m$. This makes a dramatic difference to the way a packet of these waves evolves with time: the packet does *not* maintain its shape, but "flattens out", a phenomenon called *dispersion* (of the packet). Consider the packet

$$\psi(x,t) = \frac{1}{2\Delta k}\int_{k_0-\Delta k}^{k_0+\Delta k} e^{ikx - i\hbar k^2 t/2m}dk$$

(note that $\psi(x,0)$ is again our packet from Q 10). This time the integral can *not* be done in terms of elementary functions. However, if $k_0 \gg \Delta k$ and the t-term in the exponent is "not too big" we can expand "k^2" about the point $k = k_0$ by a Taylor series: $k^2 = k_0^2 + (k - k_0).2k_0$, and we are back to only a *linear* term in the exponent, which can be integrated exactly. Show that in this approximation

$$|\psi(x,t)|^2 = \frac{\sin^2[\Delta k(x - vt)]}{[\Delta k(x - vt)]^2}$$

where $v = \hbar k_0/m$, and describe how this packet moves as t varies.