Quantum Mechanics M.T. 2000

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Problem Set No. 2

1. Probability current density

   Derive the continuity equation relating the rate of change of probability density $\psi^*\psi$ to the gradient of a probability current density j, and find the expression for j. Find j for the plane wave solution $\psi(x,t) = A\, e^{ikx-i\omega t}$ and express your answer in terms of the particle velocity p/m. [Note: A is in general complex].

2. 1-D barrier

   Particles of mass m and energy E are incident from the region $x < 0$ on the "finite step" potential $V(x) = 0$ for $x \leq 0$, $V(x) = V_0$ for $x > 0$, with $V_0 > E$.
   (i) Explain why the solution of the time independent Schrodinger equation in the region $x \leq 0$ may be taken to have the form $\phi_1(x) = e^{ikx} + re^{-ikx}$ where $k = (2mE/\hbar^2)^{\frac{1}{2}}$, and why the solution in the region $x > 0$ has the form $\phi_2(x) = ae^{-Kx}$ where $K = [2m(V_0 - E)/\hbar^2]^{\frac{1}{2}}$.
   (ii) By imposing suitable boundary conditions at $x = 0$ show that

   $$r = \frac{k - iK}{k + iK}, \quad a = \frac{2k}{k + iK}.$$

   (iii) Is your solution for the wavefunction an energy eigenstate? Is it a momentum eigenstate?
   (iv) Compute the probability current density in the two regions. Discuss your result.
   Also, show that r can be written as $e^{-2i\alpha}$ where $\alpha = \tan^{-1}(K/k)$, and hence show that

   $$|\phi_1(x)|^2 = 4\cos^2(kx + \alpha).$$

   Make two separate sketches, for the special cases $E = V_0/2$ and $E = V_0$, of $|\phi_1|^2$, and of $|\phi_2|^2$, showing how they match at $x = 0$.
   (v) Estimate the penetration distance into the region $x > 0$ for an electron with $V_0 - E = 1eV$.

3. Necessary integrals

   You will need certain integrals repeatedly over the next few weeks. They are given here; make sure that you can do them and then keep this piece of paper handy.

   $$\int_0^a \sin\left(\frac{n\pi x}{a}\right) \sin\left(\frac{m\pi x}{a}\right) = \begin{cases} \frac{a}{2}, & \text{if } n = m; \\ 0, & \text{otherwise.} \end{cases} \qquad (1)$$

$$\int_0^a \sin\left(\frac{n\pi x}{a}\right)\cos\left(\frac{m\pi x}{a}\right) = \begin{cases} \frac{2an}{\pi(n^2-m^2)}, & \text{if } n+m \text{ is odd;} \\ 0, & \text{otherwise.} \end{cases} \tag{2}$$

4. Non-stationary state, time dependent expectation value

(i) Verify that, for a particle of mass m confined to the region $0 \le x \le a$ by infinitely high walls, the wavefunction

$$\psi(x,t) = \frac{1}{\sqrt{2}}\left\{\sqrt{\frac{2}{a}}\sin\left(\frac{\pi x}{a}\right)e^{-iE_1t/\hbar} + \sqrt{\frac{2}{a}}\sin\left(\frac{2\pi x}{a}\right)e^{-iE_2t/\hbar}\right\}$$

is a normalised solution of the appropriate time-dependent Schrodinger equation, provided that

$$E_1 = \hbar^2\pi^2/2ma^2, \quad E_2 = 4\hbar^2\pi^2/2ma^2.$$

(ii) Does this particle have a definite energy? If the energy of this particle were to be measured, what possible values would be obtained? What is the probability of getting each of these possible results?
(iii) Show that

$$|\psi(x,t)|^2 = \frac{1}{a}\left\{\sin^2\left(\frac{\pi x}{a}\right) + \sin^2\left(\frac{2\pi x}{a}\right) + 2\sin\left(\frac{\pi x}{a}\right)\sin\left(\frac{2\pi x}{a}\right)\cos\omega t\right\}$$

where $\omega = (E_2 - E_1)/\hbar = 3E_1/\hbar$. Make rough sketches of $|\psi|^2$ for $t = 0$, $t = h/12E_1$, $t = h/6E_1$, $t = h/4E_1$.
(iv) Given that

$$\int_0^a x\sin\left(\frac{\pi x}{a}\right)\sin\left(\frac{2\pi x}{a}\right)dx = -\frac{8a^2}{9\pi^2},$$

show that a particle with this wavefunction has $\langle x\rangle = a/2$ - $(16a/9\pi^2)\cos\omega t$. Discuss the connection between this result and the sketches of $|\psi|^2$.
(v) What is the value of ω for an electron confined to a distance comparable to the size of an atom (say 10^{-10} m)? What is the wavelength of radiation having this (circular) frequency?

5. Expectation values, classical equations of motion

For a system in a state described by a general wavefunction $\psi(x,t)$, how is the quantum mechanical expectation value of the momentum, $\langle p\rangle$, calculated?

For a particle described by the same wavefunction $\psi(x,t)$ as in Q.4,

(i) show that $\langle p\rangle = (8\hbar/3a)\sin\omega t$ where $\omega = 3E_1/\hbar$;
(ii) deduce, using the result of question 4 for $\langle x\rangle$, that

$$m\frac{d}{dt}\langle x\rangle = \langle p\rangle.$$

6. The wavefunction $\psi(x,t)$ satisfies the Schrodinger equation

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x)\psi.$$

Consider

$$\frac{d}{dt}\langle p\rangle = \frac{d}{dt}\left\{\int \psi^*(x,t)\left[-i\hbar\frac{\partial}{\partial x}\right]\psi(x,t)dx\right\}$$

$$= -i\hbar\left\{\int\left[\frac{\partial\psi^*}{\partial t}\frac{\partial\psi}{dx} + \psi^*\frac{\partial}{\partial x}\frac{\partial\psi}{\partial t}\right]dx\right\}.$$

Substitute for $\partial\psi/\partial t$ and for $\partial\psi^*/\partial t$ and do some integrations by parts (assuming that ψ and $\partial\psi/\partial x \to 0$ as $x \to \pm\infty$) to show that

$$\frac{d}{dt}\langle p\rangle = -\langle\frac{dV}{dx}\rangle.$$

[This shows that expectation, or average, values obey the classical equations of motion.]

7. <u>Momentum operator</u>

Verify that if the momentum operator $\hat{p}$ is represented by $-i\hbar(\partial/\partial x)$ (in one dimension) acting on wavefunctions, then

$$[x,\hat{p}]\phi(x) = i\ \hbar\ \phi(x)$$

for any differentiable wavefunction $\phi(x)$, where $[\hat{A},\hat{B}]$ means $\hat{A}\hat{B}-\hat{B}\hat{A}$ for any two operators $\hat{A}$, $\hat{B}$.

8. <u>Hermitian conjugate</u>

The Hermitian conjugate $\hat{A}^\dagger$ of a differential operator $\hat{A}$ is defined via its matrix elements between arbitrary wavefunctions ϕ_1 and ϕ_2:

$$\int_{-\infty}^{\infty}\phi_1^*(x)\hat{A}^\dagger\phi_2(x)dx \overset{def}{=} \int_{-\infty}^{\infty}\left(\hat{A}\phi_1(x)\right)^*\phi_2(x)dx$$

provided ϕ_1 and ϕ_2 vanish at $x = \pm\ \infty$. Show that

(i)

$$\left(\frac{\partial}{\partial x}\right)^\dagger = -\frac{\partial}{\partial x}.$$

(You will need to do an integration by parts - see Rae p67,68)

(ii)

$$\left(\frac{\partial^2}{\partial x^2}\right)^\dagger = \frac{\partial^2}{\partial x^2}$$

Deduce from (i) that the momentum operator is Hermitian. Why are dynamical quantities (energy, momentum ...) represented by Hermitian operators in quantum mechanics?

9. Eigenfunctions, eigenvalues

(i) Show that $u(y) = e^{-\frac{1}{2}y^2}$ is an eigenfunction of the operator $-(\partial^2/\partial y^2) + y^2$ and find the eigenvalue. Use your result to find one energy eigenvalue E and associated eigenfunction ϕ, of the equation

$$\left(\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega^2 x^2\right)\phi = E\phi$$

(which is the Schrodinger equation for the one-dimensional simple harmonic oscillator).
(ii) Is $\mathrm{e}^{-|x|/a}$ an eigenfunction of momentum? (Careful: a sketch and some thought is the best approach).
(iii) Find a in terms of $\hbar$, m, e and ε_0 such that the function $\exp(-r/a)$ is an eigenfunction of the operator

$$-\frac{\hbar^2}{2m}\frac{1}{r^2}\left[\frac{d}{dr}\left(r^2\frac{d}{dr}\right)\right] - \frac{e^2}{4\pi\varepsilon_o r}$$

which is the energy operator for spherically symmetrical states of a particle of mass m and charge $-e$ in the potential due to a heavy charge $+e$ at the origin. Evaluate the associated eigenvalue, in eV, for an electron.

10. [An extra problem]

The disk in McMurry's book has a programme called "Wave Packets" which forms such superpositions, both for the infinite square well case and for the 1-D S.H.O. case. You can run Q.4 on it; here is another one to try.

Suppose that $t = 0$ the wavefunction for the system is $\psi(x,0) = \delta^{-\frac{1}{2}}$ for $0 < x < \delta$ and zero for $\delta < x < a$ (so $|\psi|^2$ is normalised). Let $\psi(x,0) = \sum_n a_n\sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)$. Evaluate the coefficients a_n (it's first year Fourier series theory). Plug these into McMurry's programme (n=1 to 13, a=1, δ=0.5 say) and see what happens.]