PHYSICS 829

Home Work Assignment # 2 4/8/2011

Due: Fri., Apr. 15, 2011.

1. *Hellmann-Feynman theorem:*
(a) Consider a Hamiltonian $H(\lambda)$ that depends on a parameter λ. Let $E_n(\lambda)$ be the eigenvalues and $|\psi_n(\lambda)\rangle$ be the corresponding *normalized* eigenvectors. Prove that

$$\frac{dE_n(\lambda)}{d\lambda} = \langle\psi_n(\lambda)|\frac{\partial H}{\partial\lambda}|\psi_n(\lambda)\rangle$$

Hint: be sure to exploit the normalization!
This elementary theorem is very useful in many different contexts.
(b) Apply this theorem to the one-dimensional harmonic oscillator using (i) $\lambda = \omega$, (ii) $\lambda = \hbar$, and (iii) $\lambda = m$. Compare your results with those you obtained earlier using the virial theorem.
(c) Apply this theorem to the Hydrogen atom by choosing $\lambda = e$ and find $\langle 1/r\rangle$ (which was needed in the fine structure calculation). Compare with the virial theorem (p. 359 of Shankar).
(You can also find $\langle 1/r^2\rangle$ using Hellmann-Feynman if you choose $\lambda = \ell$, treating ℓ as a continuous variable, but then you need to be careful about the fact that the principal quantum number n is now a function of ℓ).

2. The probability density in quantum mechanics is given by the absolute square of the wavefunction, $\rho = |\Psi(\mathbf{r}, t)|^2$, and probability current by $\mathbf{J} = \hbar\,\mathrm{Im}\,(\Psi^*\nabla\Psi)\,/m$. Show that the time-dependent Schrödinger equation implies the continuity equation $\nabla\cdot\mathbf{J} + \partial\rho/\partial t = 0$ which describes the local conservation of probability.

3. The asymptotic form of the wavefunction in a scattering experiment is

$$\psi \sim Ae^{ikz} + Af(\theta,\varphi)e^{ikr}/r \quad (\text{for } r\to\infty)$$

(a) Calculate the incident and scattered fluxes using probability currents.
(b) Then show that the scattering cross section $\sigma(\theta,\varphi) = |f(\theta,\varphi)|^2$.
(c) What are the 1D and 2D analogs of the asymptotic ψ in the 3D case given above? In other words, what is $\psi(x)$ for $|x|\to\infty$ in 1D? and $\psi(r,\phi)$ for $r\to\infty$ in 2D?

4. Three-dimensional delta function: Shankar Ex. 12.6.4 (p. 342).

5. Green's function used in scattering theory: Show that

$$\left(\nabla^2 + k^2\right) \frac{e^{\pm ikr}}{r} = -4\pi\delta^{(3)}(\mathbf{r})$$

6. Shankar Ex. 19.3.1 (p. 533)

7. Shankar Ex. 19.3.2 (p. 533)

8. We will need the following important identity in our study of scattering:

$$e^{ikz} = e^{ikr\cos\theta} = \sum_{\ell=0}^{\infty} i^\ell (2\ell+1) j_\ell(kr) P_\ell(\cos\theta).$$

Shankar starts with the proof on p. 350, but gives up at some point saying "it can be shown that ...". We will start at the beginning and take it to the end.
(a) Show that any solution of the free-particle Schrödinger equation $\left(\nabla^2 + k^2\right)\psi = 0$ with energy $E = \hbar^2 k^2/2m$, can be written as

$$\psi(r,\theta,\varphi) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{+\ell} \left[A_{\ell,m} j_\ell(kr) + B_{\ell,m} n_\ell(kr)\right] P_\ell^m(\theta) e^{im\varphi}$$

where j_ℓ and n_ℓ are spherical Bessel and Neumann functions.
(b) For the plane wave e^{ikz}, show that
(i) we need to keep only $m = 0$ terms in the expansion, and
(ii) all B coefficients are identically zero.
(c) Determine the coefficients A_ℓ ($\equiv A_{\ell,0}$) using the orthogonality of the Legendre polynomials $P_\ell(\cos\theta)$ for different ℓ's. Hence show that $A_\ell j_\ell(kr)$ is proportional to the integral $I_\ell(kr) = \int_{-1}^{+1} dt e^{ikrt} P_\ell(t)$.
(d) It suffices to evaluate $I_\ell(kr)$ for $kr \gg 1$. Use integration by parts to write it as an expansion in *inverse* powers of kr and obtain $I_\ell(kr) \sim 2i^\ell \sin\left(kr - \ell\pi/2\right)/kr$ as $kr \to \infty$.
(e) Matching this to the (well known) large kr expansion of $j_\ell(kr)$, show that $A_\ell = i^\ell(2\ell+1)$, thus completing the proof.