Modern Physics and Quantum Mechanics
Fall 2001 Proficiency and Diagnostic

1. Cosmic ray photons from space are bombarding your laboratory and smashing massive objects to pieces. Your detectors indicate that two fragments, each of mass m_0, depart such a collision moving at a speed of $0.6c$ at angles of $60°$ relative to the photon's original direction of motion.

a. In terms of m_0 and c, what is the energy of the cosmic ray photon?

The components of the fragment's momenta in the direction perpendicular to the original photon's direction of motion will cancel, and the components along that direction will reinforce. Conservation of three momentum tells us that

$$p_i = 2\,p_f \cos(60^o).$$

Using the relativistic definition of momentum, $\mathbf{p}_f = m\gamma(v_f)\mathbf{v_f}$, where $\gamma(v_f) = 1/\sqrt{1 - v_f^2/c^2} = 1.25$,

$$p_\gamma = p_i = 2\,p_f \cos(60^o) = \frac{2\,m_0 v\,\cos(60^o)}{\sqrt{1 - v^2/c^2}}.$$

Now since for a photon $E_\gamma = p_\gamma c$, then

$$E_\gamma = 2\,m_0 \cdot 0.6c^2 \cos(60^o) \cdot 1.25 = \frac{3}{4}\,m_0 c^2.$$

b. In terms of m_0, what is the mass M of the particle being struck (assumed to be initially stationary)?

Use conservation of relativistic energy, and the fact that the total relativistic energy (including rest energy) of the final fragments is

$$E_f = m_0 \gamma(v_f) c^2 = 1.25\,m_0 c^2$$

so that

$$E_i = E_\gamma + Mc^2 = 2E_f,$$

and we have that

$$M = \frac{2E_f - E_\gamma}{c^2} = \frac{2.5\,m_0 c^2 - 0.75\,m_0 c^2}{c^2} = 1.75\,m_0.$$

2. The Pauli spin operators for a particle of spin 1/2 are given by the matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

a. Write the normalized eigenvectors of σ_z, $|+\rangle$ and $|-\rangle$ which are defined such that $\sigma_z|+\rangle = |+\rangle$ and $\sigma_z|-\rangle = -|-\rangle$, as column vectors in the same basis as the Pauli matrices given above. (You can assume, without loss of generality, that these vectors are real.)

Assume that $|+\rangle = \begin{pmatrix} x \\ y \end{pmatrix}$. Then since $\sigma_z|+\rangle = |+\rangle$, we have that

$$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} x \\ y \end{pmatrix},$$

or that $x = x$ and $-y = y$. This means that $y = 0$, and to normalize the eigenvector we need $x = 1$, so that $|+\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$. Similarly, the eigenvalue equation for $|-\rangle$ gives $x = -x$ and $-y = -y$ and so $|-\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$.

b. Consider a wave vector $|\psi\rangle = a|+\rangle + b|-\rangle$. Assuming that a is a real number, $0 \le a \le 1$, show that $b = e^{i\phi}\sqrt{1-a^2}$, where $\phi \in [0, 2\pi\rangle$ is an arbitrary angle.

This wave vector must be normalized, so

$$1 = \langle\psi|\psi\rangle = [a^*\langle+| + b^*\langle-|]\,[a|+\rangle + b|-\rangle] = |a|^2 + |b|^2 = a^2 + |b^2|,$$

so we have

$$|b^2| = 1 - a^2,$$

and so $b = e^{i\phi}\sqrt{1-a^2}$.

c. Find the expectation values of σ_x, σ_y, and σ_z in the state $|\psi\rangle$ in terms of a and ϕ.

We need to find $\langle\psi|\sigma_x|\psi\rangle$, $\langle\psi|\sigma_y|\psi\rangle$ and $\langle\psi|\sigma_z|\psi\rangle$. This is a problem in matrix algebra,

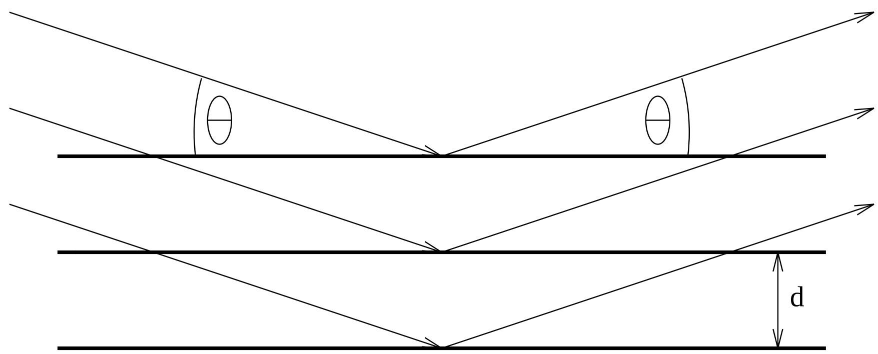
$$\begin{aligned} \langle\psi|\sigma_x|\psi\rangle &= [a^*(1,0) + b^*(0,1)] \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \left[a \begin{pmatrix} 1 \\ 0 \end{pmatrix} + b \begin{pmatrix} 0 \\ 1 \end{pmatrix} \right] \\ &= [a^*(1,0) + b^*(0,1)] \left[a \begin{pmatrix} 0 \\ 1 \end{pmatrix} + b \begin{pmatrix} 1 \\ 0 \end{pmatrix} \right] \\ &= b^*a + a^*b = a(b^* + b) = 2a\sqrt{1-a^2}\cos(\phi), \end{aligned}$$

and similarly

$$\begin{aligned} \langle\psi|\sigma_y|\psi\rangle &= [a^*(1,0) + b^*(0,1)] \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \left[a \begin{pmatrix} 1 \\ 0 \end{pmatrix} + b \begin{pmatrix} 0 \\ 1 \end{pmatrix} \right] \\ &= [a^*(1,0) + b^*(0,1)] \left[a \begin{pmatrix} 0 \\ i \end{pmatrix} + b \begin{pmatrix} -i \\ 0 \end{pmatrix} \right] \\ &= ia(b^* - b) = 2a\sqrt{1-a^2}\sin(\phi), \end{aligned}$$

and finally

$$\begin{aligned} \langle\psi|\sigma_z|\psi\rangle &= [a^*(1,0) + b^*(0,1)] \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \left[a \begin{pmatrix} 1 \\ 0 \end{pmatrix} + b \begin{pmatrix} 0 \\ 1 \end{pmatrix} \right] \\ &= [a^*(1,0) + b^*(0,1)] \left[a \begin{pmatrix} 1 \\ 0 \end{pmatrix} + b \begin{pmatrix} 0 \\ -1 \end{pmatrix} \right] \\ &= a^2 - b^*b = a^2 - (1-a^2) = 2a^2 - 1. \end{aligned}$$



3. Neutron scattering is often done by cooling fast neutrons, which are among the fission products from a nuclear reactor, by thermalizing them in a moderator such as solid deuterium oxide (D_2O ice) held at some constant cryogenic temperature T. The average kinetic energy of neutrons from such a source is,

$$E = \frac{1}{2}m\langle v^2\rangle = \frac{3}{2}kT \ ,$$

where m is the neutron mass, $\langle v^2\rangle$ is the mean-square velocity, and k is Boltzmann's constant. The neutron mass is $m_{\rm n} = 1.68 \times 10^{-27}$ kg.

(a) What is the de Broglie wave length λ_n, for neutrons, in terms of their energy, mass, and Planck's constant?

The de Broglie wave length is $\lambda = h/p = h/(mv)$, and since $E = mv^2/2$ (note we are assuming $v << c$ so we can use a nonrelativistic approximation here) then $v = \sqrt{2E/m}$ and so

$$\lambda = \frac{h}{mv} = \frac{h}{m\sqrt{2E/m}} = \frac{h}{\sqrt{2mE}}.$$

(b) What is the de Broglie wave length for neutrons with the average kinetic energy in terms of the temperature of the source?

Since $E = 3kT/2$ we have

$$\lambda = \frac{h}{m\sqrt{2E/m}} = \frac{h}{\sqrt{3mkT}}.$$

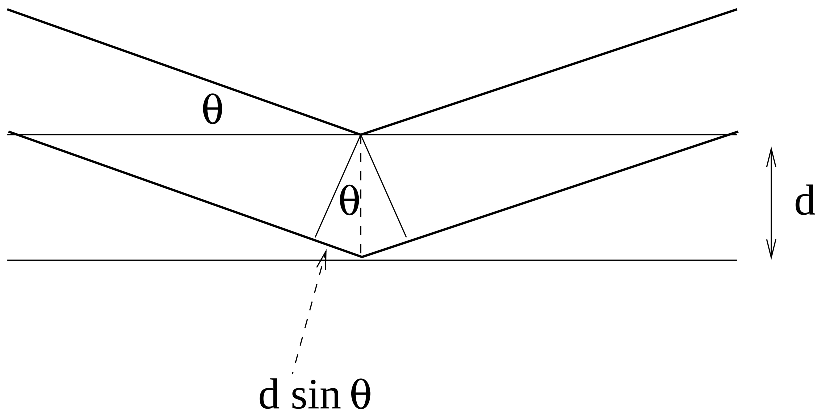
(c) Hydrogen freezes at 20.25 K and can be used to keep the D_2O moderator at a fixed temperature. What is the de Broglie wave length λ_n (in Å) for neutrons with the average energy corresponding to that temperature? What is the average neutron energy E (in eV)?

Substitute into the answer from (b),

$$\lambda = \frac{6.6 \times 10^{-34}\ \text{Js}}{\sqrt{3 \cdot 1.68 \times 10^{-27}\ \text{kg} \cdot 1.38 \times 10^{-23}\ \text{J/K} \cdot 20.25\ \text{K}}} = 5.57 \times 10^{-10}\ \text{m} = 5.57\ \text{Å}.$$

Also,

$$E = \frac{3}{2}\frac{1.38 \times 10^{-23}\ \text{J/K} \cdot 20.25\ \text{K}}{1.6 \times 10^{-19}\ \text{J/eV}} = 0.0026\ \text{eV}.$$



(d) The neutrons are monochromatized at the 20.25 K thermal intensity maximum λ_n and diffracted off a crystalline target with lattice spacing $d = 4.21$ Å. What is the scattering angle θ that would give Bragg diffraction of the neutrons from this crystal? Use the convention for diffraction shown in the figure.

Referring to the diagram, we see that the path difference for neutrons which scatter off *adjacent* planes in the crystal is just $2d\sin(\theta)$, so that we get constructive interference when this is an integral number of de Broglie wavelengths, i.e.

$$n\lambda = 2d\sin(\theta),$$

and so we have

$$\sin(\theta) = \frac{n\lambda}{2d} = n\frac{5.57\text{Å}}{8.42\text{Å}} = 0.661\, n,$$

and we see that $n = 1$ is the *only* possibility and there $\theta = \sin^{-1}(0.661) = 41.4^{\text{o}}$.

4. The time-independent wave function for a particle of mass m which moves in a one-dimensional potential $V(x)$ has the form $\psi(x) = A\exp\left[-a^2x^2\right]$, where $a = \sqrt{m\omega/2\hbar}$ and A is a normalization constant.

a. Using the time-independent Schrödinger equation, find $V(x)$ and the energy eigenvalue for $\psi(x)$.

We have that

$$H|\psi\rangle = \left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right]|\psi\rangle = E|\psi\rangle,$$

so we can substitute $|\psi\rangle$ into this to find $V(x)$ and E. One derivative gives us

$$\frac{d}{dx}|\psi\rangle = A(-2a^2x)\exp\left[-a^2x^2\right],$$

and a second gives us

$$\frac{d^2}{dx^2}|\psi\rangle = A\left[(-2a^2) + (-2a^2x)^2\right]\exp\left[-a^2x^2\right] = \left[-2a^2 + 4a^4x^2\right]|\psi\rangle,$$

so that

$$H|\psi\rangle = \left[-\frac{\hbar^2}{2m}\left[-2a^2 + 4a^4x^2\right] + V(x)\right]|\psi\rangle = E|\psi\rangle.$$

This equation can only be satisfied if

$$E = \frac{\hbar^2 a^2}{m}, \quad V(x) = \frac{2\hbar^2 a^4}{m}x^2.$$

b. Identify the system. Which one of its quantum states is described by $\psi(x)$?

This is a harmonic oscillator and the wave function describes its ground state.

5. The Hamiltonian for the hydrogen atom is given by

$$H = -\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin(\theta)}\frac{\partial}{\partial\theta}\left(\sin(\theta)\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2(\theta)}\frac{\partial^2}{\partial\phi^2}\right] - \frac{e^2}{r}\ ,$$

where r, θ and ϕ are spherical coordinates of the position of the electron relative to the nucleus, m is the reduced mass, and e is the charge of the proton.

(a) What are the quantum numbers characterizing the wave functions of the hydrogen atom?

The wavefunctions have orbital angular momentum $l = 0, 1, 2, ...$ and its projection along some (conventionally the z-) axis, $-l \leq m \leq +l$. There is also a radial quantum number $n = 0, 1, 2...$, which tells us the number of nodes in the radial wavefunction.

(b) Consider an s-wave state. Obtain the value of α for which the wave function

$$\psi(r) = C\exp(-\alpha r)$$

is a solution of Schrödinger's equation. Find the corresponding energy eigenvalue. Calculate the normalization constant C.

Since there is no angular dependence then we have

$$H\psi(r) = -\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d\psi(r)}{dr}\right)\right] - \frac{e^2}{r}\psi(r).$$

To find the action of H we need to evaluate

$$\frac{d}{dr}\left(r^2\frac{d\psi(r)}{dr}\right) = C\frac{d}{dr}\left[r^2(-\alpha)\exp(-\alpha r)\right] = -C\alpha\left[2r - \alpha r^2\right]\exp(-\alpha r) = [-2\alpha r + \alpha^2 r^2]\psi(r).$$

This means that

$$H\psi(r) = \left[-\frac{\hbar^2}{2m}\left(-\frac{2\alpha}{r} + \alpha^2\right) - \frac{e^2}{r}\right]\psi(r),$$

and this wave function can only be a solution of $H\psi = E\psi$ if

$$\alpha = \frac{me^2}{\hbar^2},$$

so that

$$E = -\frac{\hbar^2}{2m}\alpha^2 = -\frac{\hbar^2}{2m}\frac{m^2e^4}{\hbar^4} = -\frac{me^4}{2\hbar^2}.$$

To find C we need to integrate $\psi(r)$ over all space and set the result to unity,

$$\int |\psi(r)|^2 d^3r = 4\pi C^2 \int_0^\infty r^2 \exp(-2\alpha r)dr = 4\pi C^2 \frac{1}{4\alpha^3} = 1,$$

so that $C = \alpha^{3/2}/\sqrt{\pi}$.

(c) Obtain the expectation values of $\vec{p}^2$ and $1/r$ for the wave function in (b). Hint: the Hamiltonian above contains the expression for $\vec{p}^2$ in spherical coordinates.

We have almost done all of what is required to answer this question, because we have the Hamiltonian calculated *for this wave function* and split into the kinetic and potential energy terms,

$$H\psi(r) = \left[-\frac{\hbar^2}{2m}\left(-\frac{2\alpha}{r} + \alpha^2\right) - \frac{e^2}{r}\right]\psi(r),$$

and then we know that

$$\int d^3r\, \psi^*(r) H \psi(r) = \int d^3r \left[-\frac{\hbar^2}{2m}\left(-\frac{2\alpha}{r} + \alpha^2\right) - \frac{e^2}{r}\right]\psi^2(r),$$

First evaluate

$$\int d^3r\, \psi^2(r)\frac{1}{r} = \frac{\alpha^3}{\pi}4\pi \int r dr \exp(-2\alpha r) = \frac{\alpha^3}{\pi}4\pi\frac{1}{4\alpha^2} = \alpha,$$

and then we know that

$$\int d^3r\, \psi^*(r)\left(\frac{\mathbf{p}^2}{2m}\right)\psi(r) = \frac{\hbar^2\alpha^2}{2m} = -E,$$

and so it follows that

$$\int d^3r\, \psi^*(r)\mathbf{p}^2\psi(r) = \hbar^2\alpha^2.$$

(d) Verify that the expectation value of the kinetic energy is $-1/2$ times that of the potential energy (virial theorem).

Since above we saw that the kinetic energy was $-E$, then it must be true that the potential energy is $2E$ since they add to E.

6. Consider a quantum mechanical system with two states, $|\alpha\rangle$ and $|\beta\rangle$. In this orthonormal basis of states the Hamiltonian is given by the matrix

$$H = \begin{pmatrix} W & V \\ V & -W \end{pmatrix}.$$

(a) Obtain the exact energy eigenvalues.

We simply have to find the eigenvectors and eigenvalues of the Hamiltonian matrix. Assume the eigenvector has the form $|\psi\rangle = \begin{pmatrix} x \\ y \end{pmatrix}$, then we have

$$H|\psi\rangle = \begin{pmatrix} W & V \\ V & -W \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} Wx + Vy \\ Vx - Wy \end{pmatrix} = E \begin{pmatrix} x \\ y \end{pmatrix}.$$

This has a non-trivial solution (not $x = y = 0$) when the determinant $(W - E)(-E - W) - V^2$ is zero, so $E^2 - W^2 = V^2$, and $E = \pm\sqrt{W^2 + V^2}$ are the two energy eigenvalues.

(b) Consider the Hamiltonian as $H = H_W + H_V$,

$$H_W = \begin{pmatrix} W & 0 \\ 0 & -W \end{pmatrix}, \qquad H_V = \begin{pmatrix} 0 & V \\ V & 0 \end{pmatrix},$$

and assuming that $|V| \ll |W|$ obtain the energy eigenvalues to second order perturbation theory in V.

The eigenvalues of the unperturbed Hamiltonian are just W and $-W$, and of course the eigenvectors are just $|+\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ corresponding to $E = +W$ and $|-\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ corresponding to $E = -W$. Then the first order perturbation theory result is that

$$E_+ = E_+^0 + \langle +|H_V|+\rangle = +W + 0, \quad E_- = E_-^0 + \langle -|H_V|-\rangle = -W + 0,$$

and we see that because the perturbation has no diagonal elements there is no correction to first order in V. The second order correction is

$$E_+ = E_+^0 + \langle +|H_V|+\rangle + \frac{|\langle -|H_V|+\rangle|^2}{E_+^0 - E_0^-} = W + 0 + \frac{V^2}{2W} = W + \frac{V^2}{2W}$$

and similarly

$$E_- = E_-^0 + \langle -|H_V|-\rangle + \frac{|\langle +|H_V|-\rangle|^2}{E_-^0 - E_0^+} = -W + 0 + \frac{V^2}{-2W} = -\left(W + \frac{V^2}{2W}\right).$$

(c) Compare your results in (a) and (b) and verify that they agree to second order in V.

When $V << W$ we have that

$$\sqrt{W^2 + V^2} = W\sqrt{1 + V^2/W^2} = W[1 + V^2/(2W^2) + \mathrm{O}(V/W)^3] = W + V^2/(2W) + \mathrm{O}(V/W)^3,$$

and so the result follows.