Problem Set PS02

ISSUED: 1/13/99 **Due: 1/20/00**

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Instructions. Complete all questions before class on the due date. You are encouraged to work together. Be sure to struggle with the problem before seeking help. Many of the exercises are very similar to problems in the book. Understanding the solution to these problems will be helpful in completing the assigned exercises.

Mathematical Exercises

1. See if you can show that

$$\int_0^{2\pi} \left(\lim_{\epsilon \to 0} e^{i\epsilon x} \right) dx = \lim_{\epsilon \to 0} \left(\int_0^{2\pi} e^{i\epsilon x} dx \right) = 2\pi.$$

You will have to use l'Hopitals rule (see your calculus book). This can be used to help you with problem 4.

Exercises

2. Evaluate $\langle \phi \rangle$ and $\langle \cos\phi \rangle$ for a particle on ring in the m^{th} quantum state.

3. Benzene absorbs light at about 280nm. Where would we predict benzene to absorb if we treated the π-electrons as particles on a ring (radius 1.3Å)? What is the %error? (Hint: look at your conjugated systems lab from last semester.)

4. Show that the wavefunctions for a particle on a ring are orthonormal. That is, show

$$\int_0^{2\pi} \psi_{m'}^* \psi_m d\phi = \begin{cases} 1 & m' = m \\ 0 & m' \neq m \end{cases}.$$

5. The Hamiltonian which governs the quantum behavior of a *particle on a sphere* is exactly the same as the Hamiltonian for general rotations (Eq. (11.85) of the notes).

   (a) Draw an energy level diagram for a particle on a sphere. Verify that the degeneracy of the energy levels is given by $g = 2l + 1$.

   (b) Draw the spectrum for a particle on a sphere.

   (c) Comment on how the spectrum changes with changing mass and the radius of a the sphere

   (d) Draw the wavefunctions for $l = 2$, $m = 0$ and for $l = 3$, $m = 0$ on the wooden balls I provide. Draw the nodes in regular pencil and then color in red the regions where the wavefunction is positive and color in blue the regions where the wavefunction is negative. (Hints: 1; it helps to plot the wavefunctions on a piece of paper first and then identify where the nodes are and 2; both these wavefunctions have no ϕ dependence so all of your nodes should be latitude lines and none should be longitude lines.)

6. Let $\Psi = C\left(\psi_m + \psi_{-m}\right)$, where ψ_m and ψ_{-m} are the eigenfunctions for the particle on a ring. Find C such that Ψ is normalized.

Conceptual Problems

7. We saw the spherical harmonic functions last semester when we solved for the hydrogen atom, now we see them coming in with rotation and the particle on a sphere. How is the particle in a sphere related to the hydrogen atom?

8. Fill in the following table as it pertains to n particles on a sphere (don't forget Hund's rule, p177 of the notes)

# of particles $n =$	1	2	3	4	5	6	7	8	9	10
ground state term symbol										

9. Give the ground state term symbols for hydrogen through neon (don't forget Hund's rule). How do these compare with your table in the previous problem.

10. Cut two strips of paper (11" by 1"). For the first strip tape the two ends together to form a simple loop. For the second strip put one 180° twist in the paper before taping the ends together—you have made what is called a Möbius strip. Put your pencil in the middle of the first strip and draw a continuous line (don't pick up your pencil) until you reach the point where you started. Repeat for the Möbius strip. How many times did you rotate your strips of paper before you got back to the point where you started? What is the "spin" of the simple loop and of the Möbius strip?

11. I claim that the particle on a ring model violates the uncertainty principle. We note that the $m = 0$ level corresponds to zero energy—this model has no zero point energy. If the energy is zero then the momentum is exactly zero. On the other hand we know that the particle is located on the ring ($0 \leq \phi < 2\pi$). We thus know its position to some extent and know it momentum exactly therefore the uncertainty principle is violated. Do you agree with my claim? If not, why not?

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① $\int_0^{2\pi} \lim_{\varepsilon\to 0} e^{i\varepsilon x}\,dx = \int_0^{2\pi} dx = 2\pi$ ✓

$\lim_{\varepsilon\to 0}\int_0^{2\pi} e^{i\varepsilon x}dx = \lim_{\varepsilon\to 0}\frac{1}{i\varepsilon}e^{i\varepsilon x}\Big|_0^{2\pi} = \lim_{\varepsilon\to 0}\frac{1}{i\varepsilon}\left(e^{i2\pi\varepsilon}-1\right)$

$= \frac{0}{0}$ use l'hopitals rule

$\lim_{\varepsilon\to 0}\dfrac{\frac{d}{d\varepsilon}(e^{i2\pi\varepsilon}-1)}{\frac{d(i\varepsilon)}{d\varepsilon}} = \lim_{\varepsilon\to 0}\frac{2\pi i}{i} = \frac{2\pi \cancel{i}}{\cancel{i}} = 2\pi$ ✓

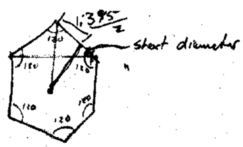
② $\langle\phi\rangle = \frac{1}{2\pi}\int_0^{2\pi} e^{-im\phi}\,\phi\, e^{im\phi}\,d\phi = \frac{1}{2\pi}\int_0^{2\pi}\phi\, d\phi = \frac{4\pi^2}{2\pi(2)} = \boxed{\pi}$

$\langle\cos\phi\rangle = \frac{1}{2\pi}\int_0^{2\pi} e^{-im\phi}\cos\phi\, e^{im\phi}d\phi = \frac{1}{2\pi}\int_0^{2\pi}\cos\phi = \frac{1}{2\pi}\left[\cancel{\sin(2\pi)-\sin 0}\right]^{0}$

$= \boxed{0}$

③ From CRC hand book $C=C = 1.395$ Å

so



④ $\frac{1}{2\pi}\int_0^{2\pi} e^{-im'\phi}e^{im\phi}d\phi = \frac{1}{2\pi}\int_0^{2\pi} e^{i(m-m')\phi}d\phi$

$= \frac{1}{2\pi}\frac{1}{i(m-m')}\left(e^{2\pi i(m-m')}-1\right)$

$m'=m$ then $\frac{1}{2\pi}\frac{0}{0}$ but just like problem 1 so

$\frac{1}{2\pi}2\pi = 1$ ✓

$m'\neq m$ then $m-m' = j$, $j = \pm1, \pm2, \pm3, \pm4 \ldots$

$= \frac{1}{2\pi}\frac{1}{ij}\left(\cancel{e^{i\pi j}-1}\right)^{0} = 0$ ✓

⑤ ⓐ $E_\ell = \frac{\ell(\ell+1)h^2}{8\pi^2 I}$ $\ell = 0, 1, 2 \ldots$

$\overline{m=2}\ \overline{m=1}\ \overline{m=0}\ \overline{m=-1}\ \overline{m=-2}$ $\ell=2$ $g=5=2\ell+1$

$\overline{m=1}\ \overline{m=0}\ \overline{m=-1}$ $\ell=1$ $g=3=2\ell+1$

$\overline{\quad}$ $\ell=0$ $g=1=2\ell+1$

5 cont

ⓑ $\Delta E = E_{\ell+1} - E_\ell = \frac{(\ell+1)(\ell+2)h^2}{8\pi^2 I} - \frac{\ell(\ell+1)h^2}{8\pi^2 I}$

$= (\cancel{\ell^2}+3\ell+2-\cancel{\ell^2}-\ell)\left(\frac{h^2}{8\pi^2 I}\right)$

$= (2\ell+2)\frac{h^2}{8\pi^2 I} = \frac{(\ell+1)h^2}{4\pi^2 I}$

| | | | | ....

ΔE increase with even spacing.

ⓒ $\uparrow m$ $\Delta E\downarrow$, $\uparrow R$ $\Delta E\downarrow$

ⓓ wooden balls

⑦ The wavefunctions for a particle on a sphere is equivalent to the angular wavefunctions for the hydrogen atom. In the hydrogen atom ℓ is confined to be less than $n-1$ when n is the principle quantum number.

⑥ $1 = \int_0^{2\pi}\psi^*\psi\,d\phi = c^2\int_0^{2\pi}(\psi_m+\psi_{-m})^*(\psi_m+\psi_{-m})d\phi = c^2\Big[\int\psi^*_m\psi_m d\phi^{\,1} + \int\psi^*_m\psi_{-m}d\phi^{\,0} + \int\psi^*_{-m}\psi_m d\phi^{\,0} + \int\psi^*_{-m}\psi_{-m}d\phi^{\,1}\Big]$

$1 = c^2(2) \Rightarrow \boxed{c = \frac{1}{\sqrt{2}}}$

⑧ $g_s = 2S+1$

↑ ↑ — — — $\ell=2$

↑↓ ↑↓ ↑↓ $\ell=1$

↑↓ $\ell=0$

$n=1$ $M_{max}=0 \Rightarrow L=0$; $M_{S_{max}}=\frac{1}{2} \Rightarrow S=\frac{1}{2} \Rightarrow g_s=2$; Term symbol $\boxed{^2S}$

$n=2$ $M_{max}=0 \Rightarrow L=0$; $M_{S_{max}}=0 \Rightarrow S=0 \Rightarrow g_s=1$; Term symbol $\boxed{^1S}$

$n=3$ $M_{max}=1 \Rightarrow L=1$; $M_{S_{max}}=\frac{1}{2} \Rightarrow S=\frac{1}{2} \Rightarrow g_s=2$; Term symbol $\boxed{^2P}$

$n=4$ $M_{max}=2 \Rightarrow L=2$; $M_{S_{max}}=0 \Rightarrow S=0 \Rightarrow g_s=1$; Term symbol ^1D
$M_{max}=1 \Rightarrow L=1$; $M_{S_{max}}=1 \Rightarrow S=1$ $g_s=3$; Term symbol $\boxed{^3P}$ ← ground state by Hund's rule

$n=5$ $M_{max}=2 \Rightarrow L=2$; $M_{S_{max}}=\frac{1}{2} \Rightarrow S=\frac{1}{2}$ $g_s=2$; Termsymbol ^2D
$M_{max}=0 \Rightarrow L=0$; $M_{S_{max}}=\frac{3}{2} \Rightarrow S=\frac{3}{2}$ $g_s=4$; Term symbol $\boxed{^4S}$ ← ground state by Hund's rule

$n=6$ $M_{max}=1 \Rightarrow L=1$; $M_{S_{max}}=1 \Rightarrow S=1$ $g_s=3$; Termsymbol $\boxed{^3P}$ ← Note same as the $n=4$ case

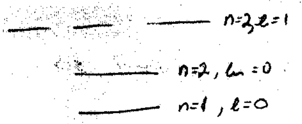
$n=7$ $M_{max}=1 \Rightarrow L=1$; $M_{S_{max}}=\frac{1}{2} \Rightarrow S=\frac{1}{2}$ $g_s=2$; Term symbol $\boxed{^2P}$ ← Note same as $n=3$ case

$n=8$ $M_{max}=0 \Rightarrow L=0$; $M_{S_{max}}=0 \Rightarrow S=0$; Term symbol $\boxed{^1S}$

$n=9$ $M_{max}=2 \Rightarrow L=2$; $M_{S_{max}}=\frac{1}{2} \Rightarrow S=\frac{1}{2}$ $g_s=2$; Term symbol $\boxed{^2D}$

$n=10$ $M_{max}=4 \Rightarrow L=4$; $M_{S_{max}}=0 \Rightarrow S=0$ $g_s=1$; Term symbol ^1G
$M_{max}=3 \Rightarrow L=3$; $M_{S_{max}}=1 \Rightarrow S=1$ $g_s=3$; Term symbol $\boxed{^3F}$ ground state by Hund's rule

(9) Similar to (7) but



see handout for term symbols

The Term symbols compare to (7) but off set by 2 places do to the extra non degenerate energy level for the atoms.

(10) paper strips

(11) You should disagree with my claim because for the particle on a ring "all space" is from 0 to 2π. Since we have know idea where our particle is in all its space, The uncertainty in position is infinite. This allows the momentum and hence the energy to be exactly zero with no uncertainty.