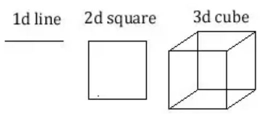
**PHYS 313: Quantum Mechanics I**

***Problem set #8 v.2*** (due November 29)

All problems are mandatory, unless marked otherwise. Each problem is 10 points.

**Townsend, Ch. 9**: 9.9, 9.11 (use information in Table 9.1 to find HCl moment of inertia), 9.19, 9.20(a,b) (this is a superposition problem, use the known expressions for $Y_{l,m}$ from (9.152a).

**Q1: multidimentional quantum wells** You are abducted by (very friendly) aliens who have access to words of different dimensions. You need to impress them with your knowledge of quantum mechanics by predicting the absorption spectrum of an infinite rectangular quantum well in 1D, 2D and 3D of size $a$.
(a) Find first 10 lowest eigen-energies of a free particle inside an infinite square well
$V(x) = \begin{cases} 0 & 0 < x_i \leq a \\ +\infty & otherwise \end{cases}$,
where $x_i$ represent coordinates in one, two or three dimensions. *I suggest you use some technology to make sure you don't miss any states, even MS Excell will be up to that task.*




(b) If you alien friends reveal they are in fact 11-dimensional beings, how many quantum numbers will you need to characterize a quantum state of an alien electron in an infinite 11D square well? What is the ground state and the first excited state energies of such system?

**Q2** In this problem we explore the concept of degeneracy: the situation in more than one quantum state corresponds to the same eigenvalue of an operator. For example, consider a three-dimentional space, in which a certain set of orthonormal kets - $|1\rangle$, $|2\rangle$ and $|3\rangle$ - are used as the base kets. In this basis the two operators $\hat{A}$ and $\hat{B}$ can be expressed as (with $a$ and $b$ both real):
$\hat{A} = \begin{pmatrix} a & 0 & 0 \\ 0 & -a & 0 \\ 0 & 0 & -a \end{pmatrix}$, $\hat{B} = \begin{pmatrix} b & 0 & 0 \\ 0 & 0 & -ib \\ 0 & ib & 0 \end{pmatrix}$
.
(a) It is easy to see that $\hat{A}$ has a degenerate spectrum, since $\hat{A}|1\rangle = a|1\rangle$, but $\hat{A}|2\rangle = -a|2\rangle$ and $\hat{A}|3\rangle = -a|3\rangle$, i.e., the states 2 and 3 yield the same eigenvalue. Does $\hat{B}$ also exhibits a degenerate spectrum?
(b) Show that $\hat{A}$ and $\hat{B}$ commute (and thus must have a set of common eigenstates).
(c) Find a new set of *orthonormal* kets which are simultaneously eigenkets of both $\hat{A}$ and $\hat{B}$. Specify the eigenvalues of $\hat{A}$ and $\hat{B}$ in each of the three eigenkets. Does your specification of the eigenvalues completely characterize each eigenket, or you have some freedom to choose how you define them?

**Q3** Someone mentioned in class that Morse potential gives a more accurate representation of the molecular energy spectrum that SHO (which is true). So let's investigate a little more!
The Morse potential is given by
$V(r) = D_e \left(e^{-2a(r-r_e)} - 2e^{-a(r-r_e)}\right)$
(a) Sketch this potential (it is convenient to use dimensionless units $x = ar$) and explain physical meaning of $D_e$ and $r_e$.
(b) The Shrodinger equation for such molecular potential can be written as follow (we neglect the molecular rotation): $-\frac{\hbar^2}{2\mu}\frac{d^2\psi(r)}{dr^2} + V(r)\psi(r) = E_n\psi(r)$.
By expanding the potential to the Tailor series around its minimum, and comparing it to the equation for the simple harmonic oscillator, find the oscillator frequency $\omega_0$ in terms of given parameters.
(c) It may surprise you, but one can solve the Schrodinger equation above analytically, and show that its energy spectrum is
$E_n^{Morse} = \hbar\omega_0(n+\frac{1}{2}) - \frac{\left[\hbar\omega_0(n+\frac{1}{2})\right]^2}{4D_e}$.
Sketch both spectra (exact $E_n^{Morse}$ and the approximate one obtained in previous question $E_n^{SHO}$) and calculate the difference $E_n^{Morse} - E_n^{SHO}$. Can you explain why we may expect to find this value negative?
(d) For an ideal SHO all transitions between the neighboring states occur at the same frequency: $E_{n+1}^{SHO} - E_n^{SHO} = \hbar\omega_0$. It is not hard to notice that for the Morse potential it is no longer true, and each frequency is a little different from each other. Find the expression for the frequencies for the transitions between $n$ and $n+1$ states $\hbar\omega_n = E_{n+1}^{Morse} - E_n^{Morse}$. Sketch expected absorption spectra for both SHO and Morse potentials if a laser frequency is scanned around the main resonant frequency $\omega_0$.