PHYS460, Test 1, Fall 2016

You must show work to get credit. There are integrals at the back of the book that might be useful.

(1) (5 pts) Estimate the vibrational energies of the N_2 molecule in Joule and Kelvin. Clearly give the reasoning for your choice of parameters. I want numerical values.

(2) (5 pts) You have an electron in an infinite square well with length of 1.0 nm. The wave function at $t = 0$ is $\Psi(x,0) = A[3e^{i\alpha_1}\psi_1(x) + 5e^{i\alpha_2}\psi_2(x) + 2e^{i\alpha_3}\psi_3(x)]$ where $\alpha_n = n\pi/10$. Compute the average energy in J; give a numerical value to 0.1%.

(3) (5 pts) Find all of the allowed energies and normalized eigenstates for the potential $V(x) = (1/2)m\omega^2 x^2$ for $x > 0$ and $V(x) = \infty$ for $x < 0$. (This represents a spring that can be stretched but not compressed.) Hint: this requires careful thought but very little actual computation.

(4) (5 pts) At $t = 0$, a particle in a harmonic potential has the wave function: $\Psi(x,0) = A[2\psi_6(x)+i\psi_7(x)+2\psi_8(x)]$. Compute the expectation value of both the a_+ and a_- operators at $t = 0$.

(5) (10 pts) A particle of mass M experiences a potential where $V(x) = \infty$ for $x < 0$, $V(x) = -V_0$ for $0 < x < a$ and $V(x) = 0$ for $a < x$. (6 pts) Find the transcendental equation that will give the bound state energies. (4 pts) There are combinations of V_0 and a that do *not* give any bound states. Determine the condition on V_0 and a that means there will be at least one bound state.

(6) (10 pts) You have a mass M in a potential which is $V(x) = \infty$ for $x < 0$ and $V(x) = Fx$ for $x > 0$ and $F > 0$. At $t = 0$, the wave function is $\Psi(x,0) = Ax\exp(-x/L)$ where A and L are positive constants. Compute the expectation value of the energy.

(7) (10 pts) A particle is in the infinite square well. At $t = 0$, the wave function is $\Psi(x,0) = A[\psi_1(x) + (2-i)\psi_3(x) + (1+i)\psi_5(x)]$. (a) Compute A. (b) What is the smallest T where $\Psi(x,T) = \exp(i\alpha)\Psi(x,0)$? (c) What is the value of α? (d) Does it matter what the value of α is? Explain why you think it does/doesn't matter.

(8) (0 pts) I couldn't think up a new "funny" question for this test. Sorry! When I started with the stupid question thing, I didn't think ahead that I'd have to do it every time. I mean, really!, I didn't ask for this kind of pressure. What do you want from me? Blood? No! Don't answer that.

every class

1) The vibrational energies are going to be well approximated by $E_n = \hbar\omega n + E_0$. So the job is to estimate ω (or f). There are many OK ways to do this. I did

$V = \frac{1}{2} m\omega^2 x^2 = \frac{1}{2} k x^2$

I estimate that V increases by $\sim 1\,eV$ when x goes from 0 to $10^{-10}\,m$ $\Rightarrow$ $k \sim 2 \frac{1.6\times10^{-19}\,J}{(10^{-10}\,m)^2} = \text{few}\times10\,\frac{J}{m^2}$

$\omega = \sqrt{\frac{k}{m}} = \left(\text{few}\times10\,\frac{J}{m^2} / [14\cdot1.7\times10^{-27}\,kg]\right)^{1/2}$

$\sim \left(\text{few}\times10\,\frac{J}{m^2} / \text{few}\times10^{-26}\,kg\right)^{1/2} \sim \text{few}\times10^{13}\,\frac{rad}{s}$

$\left.\begin{array}{l}\hbar\omega \sim 10^{-34}\,Js\ \ \text{few}\times10^{13}\,\frac{rad}{s} \sim \text{few}\times10^{-21}\,J \\ \sim \text{couple } 100\,K\end{array}\right\}$ about a factor 10 too small

To get the lowest energies ~~use~~ $\underline{E_0 + n\hbar\omega = E_n}$

Probs 2.5, 2.13, 2.37, 2.41

2) The average energy $\langle H\rangle = E_1|c_1|^2 + E_2|c_2|^2 + E_3|c_3|^2$

and $|c_1|^2 + |c_2|^2 + |c_3|^2 = (9 + 25 + 4)A^2 = 1$

$A^2 = 1/38$

$\langle H\rangle = \frac{1}{38}(9E_1 + 25E_2 + 4E_3) = \frac{1}{38}\frac{\pi^2\hbar^2}{2ma^2}(9\cdot1^2 + 25\cdot2^2 + 4\cdot3^2)$

$= \frac{145}{38}\frac{\pi^2\,(1.0546\times10^{-34}\,Js)^2}{2\ \ 9.109\times10^{-31}\,kg\,(10^{-9}\,m)^2}$

$= 2.299\times10^{-19}\,J = 1.435\,eV$

Prob 2.42

3) The ∞ wall at $x=0$ means $\psi(0)=0$. All of the n = odd harmonic oscillator functions satisfy this condition. If we number the new states $n_h = 0, 1, 2, \ldots$, then the old quantum numbers are $n = 1, 3, 5, \ldots = 2n_h + 1$

$E_{n_h} = (2n_h + 1 + \frac{1}{2})\hbar\omega = (n_h + \frac{3}{4})\,2\hbar\omega$

To find the normalized eigenstates, use Eq 2.85 <u>but</u> multiply by $\sqrt{2}$ because the integrals are only 0 to ∞

$\psi_{n_h}(x) = \sqrt{2}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\frac{1}{\sqrt{2^{2n_h+1}(2n_h+1)!}}\,H_{2n_h+1}\!\left(\sqrt{\frac{m\omega}{\hbar}}\,x\right)e^{-m\omega x^2/2\hbar}$

4) Find A $\int_{-\infty}^{\infty} \Psi^* \Psi \, dx = A^2 \left(|2|^2 + |i|^2 + |2|^2 \right) = A^2 \cdot 9$

Prob 2.13

$A = 1/3$

$\langle a_+ \rangle = \int_{-\infty}^{\infty} \Psi^* a_+ \Psi \, dx = \frac{1}{9} \int_{-\infty}^{\infty} (2\psi_6 - i\psi_7 + 2\psi_8) \, a_+ (2\psi_6 + i\psi_7 + 2\psi_8) \, dx$

$= \frac{1}{9} \int_{-\infty}^{\infty} (2\psi_6 - i\psi_7 + 2\psi_8)(2\sqrt{7}\psi_7 + i\sqrt{8}\psi_8 + 2\sqrt{9}\psi_9) \, dx$

$= \frac{1}{9} \left(-i2\sqrt{7} + i2\sqrt{8} \right) = \frac{2i(\sqrt{8} - \sqrt{7})}{9}$

$\langle a_- \rangle = \frac{1}{9} \int_{-\infty}^{\infty} (2\psi_6 - i\psi_7 + 2\psi_8)(2\sqrt{6}\psi_5 + i\sqrt{7}\psi_6 + 2\sqrt{8}\psi_7) \, dx$

$= \frac{1}{9} \left(2i\sqrt{7} - 2i\sqrt{8} \right) = -\frac{2i(\sqrt{8} - \sqrt{7})}{9}$

In the integrals I used $a_+ \psi_n = \sqrt{n+1}\,\psi_n$, $a_- \psi_n = \sqrt{n}\,\psi_{n-1}$, and ortho normality

5) Define two regions (1) $0 < x < a$ and (2) $a < x$

Oral Hwk 5

$\psi_1 = A \sin(lx)$ where $\frac{\hbar^2 l^2}{2m} - V_0 = E$

$\psi_2 = B e^{-kx}$ where $\frac{-\hbar^2 k^2}{2m} = E$

For bound states $-V_0 < E < 0$. ψ_1 has to be $\sin(\cdot)$ because must go to 0 at $x=0$. ψ_2 must be e^{-kx} and not e^{kx} because $\psi(x \to \infty) \to 0$

To get eigenstates solve continuity equations

$\psi_1(a) = \psi_2(a)$ and $\psi_1'(a) = \psi_2'(a)$

$A \sin(la) = B e^{-ka}$ and $A l \cos(la) = -kBe^{-ka}$

The equation for bound states $\boxed{l \cot(la) = -k}$ (take ratio)

For there to be a bound state ψ_1 must be decreasing at some x

$\Rightarrow l \cdot a > \pi/2$ or equally $\frac{\sqrt{2mV_0}}{\hbar} a > \pi/2$ or $V_0 > \frac{\hbar^2 \pi^2}{8ma^2}$

6) First find A from normalization $A^2 \int_0^\infty x^2 e^{-2x/L} dx = A^2\, 2! \left(\frac{L}{2}\right)^3$

Probs 2.7, 2.9

$A = 2/L^{3/2}$

$\langle PE \rangle = A^2 \int_0^\infty F\, x^3 e^{-2x/L}\, dx = \frac{4}{L^3} F\, 3! \left(\frac{L}{2}\right)^4 = \frac{3}{2} \cdot F \cdot L$

To compute $\langle KE \rangle$ you need $\psi''(x)$

$$\frac{d\psi}{dx} = A\left(1 - x/L\right) e^{-x/L}$$

$$\frac{d^2\psi}{dx^2} = A\left(-\frac{2}{L} + \frac{x}{L^2}\right) e^{-x/L}$$

$$\langle KE \rangle = A^2 \left(\frac{-\hbar^2}{2m}\right) \int_0^\infty \left(-\frac{2x}{L} + x^2/L^2\right) e^{-2x/L}\, dx$$

$$= \frac{4}{L^3}\left(\frac{-\hbar^2}{2m}\right)\left(-\frac{2}{L} 1! \left(\frac{L}{2}\right)^2 + \frac{1}{L^2} 2! \left(\frac{L}{2}\right)^3\right)$$

$$= \frac{4}{L^3}\left(\frac{-\hbar^2}{2m}\right)\left(-\frac{L}{2} + \frac{L}{4}\right) = -\frac{4}{L^3}\frac{\hbar^2}{2m}\left(-\frac{L}{4}\right) = \frac{\hbar^2}{2mL^2}$$

$$\boxed{\langle H \rangle = \frac{\hbar^2}{2mL^2} + \frac{3}{2} FL}$$

7) To find A use normalization

Probs 2.5, 2.6, 2.39

$A^2\left(|1|^2 + |2-i|^2 + |1+i|^2\right) = A^2\left(1 + (2+i)(2-i) + (1+i)(1-i)\right)$

$= A^2(1+5+2) = 1 \implies \boxed{A = 1/\sqrt{8}}$

For the rest the exact coefficients don't matter

$$\Psi(x,t) = C_1 e^{-iE_1 t/\hbar} \psi_1 + C_3 e^{-iE_3 t/\hbar} \psi_3 + C_5 e^{-iE_5 t/\hbar} \psi_5$$

$$= e^{-iE_1 t/\hbar}\left(C_1\psi_1 + C_3 e^{-i(E_3-E_1)t/\hbar} + C_5 e^{-i(E_5-E_1)t/\hbar}\psi_5\right)$$

For this to equal $e^{i\alpha}\Psi(x,0)$, then $\frac{(E_3-E_1)T}{\hbar} = n\,2\pi$ and

$(E_5 - E_1)T/\hbar = m\,2\pi$ with m and n integers

$\frac{E_3 - E_1}{\hbar} T = \frac{\hbar\pi^2}{2ma^2} 8T = n\,2\pi \qquad \frac{(E_5 - E_1)}{\hbar} T = \frac{\hbar\pi^2}{2ma^2} 24T = m\,2\pi$

If $n=1$ then $m=3$ ✓ $\boxed{T = \frac{ma^2}{2\hbar\pi}}$

$\alpha = -E_1 T/\hbar = -\frac{\hbar^2\pi^2}{2ma^2}\frac{ma^2}{2\hbar^2\pi} = \boxed{-\pi/4}$

Since α is an overall phase, it does not contribute to any expectation value