1) **Position Matrix Elements of the Harmonic Oscillator**

Focus first on I_1, i.e.:

$$I_1 = \int_{-\infty}^{\infty} dx \left\{ \frac{1}{\sqrt{2}} \left[\frac{m\omega}{\pi\hbar} \right]^{1/4} \cdot 2\sqrt{\frac{m\omega}{\hbar}} x \cdot \exp(-m\omega x^2 / 2\hbar) \right\} x \left\{ \left[\frac{m\omega}{\pi\hbar} \right]^{1/4} \exp(-m\omega x^2 / 2\hbar) \right\}$$

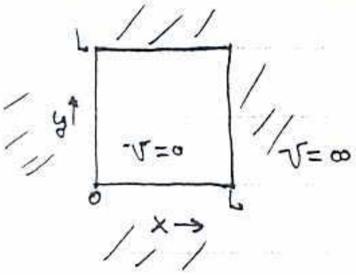
$$= \sqrt{\frac{2m\omega}{\hbar}} \cdot \left[\frac{m\omega}{\pi\hbar} \right]^{1/2} \int_{-\infty}^{\infty} dx \exp(-m\omega x^2 / \hbar) x^2$$

$$= \sqrt{\frac{2m\omega}{\hbar}} \cdot \frac{\hbar}{2m\omega} = \sqrt{\frac{\hbar}{2m\omega}}$$

[Note: to go from 2nd to 3rd lines, use the given Gaussian integral identity with $\sigma^2 = \dfrac{\hbar}{2m\omega}$.]

For I_0 the polynomial factor x^2 in integral above (for I_1) is replaced by x (to within an overall scale factor). Hence the integrand is odd and $I_0 = 0$. Similarly, in I_2 there is a polynomial factor of the form $Ax^3 + Bx$, where A, B are constants. Hence the integrand is odd and $I_2 = 0$.

(2) Particle in a 2D Box



An acceptable energy eigenfnctn. must (i) satisfy the Schrödinger Eq.

Inside the box, this reads:

$$-\frac{\hbar^2}{2m}\left[\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right]\psi(x,y) = E\,\psi(x,y)$$

(ii) satisfy appropriate boundary conditions. Here, we insist that $\psi(x,y)=0$ along all edges of the box.

Thus the appropriate energy eigenfunctions are: $\psi_{n_x,n_y}(x,y) = \underbrace{\left(\frac{2}{L}\right)}_{\text{normalization factor}} \sin\left(\frac{n_x\pi}{L}\right)\sin\left(\frac{n_y\pi}{L}\right)$; $n_x = 1,2,3,\ldots$ $n_y = 1,2,3,\ldots$

Corresponding energy eigenvalues: $E_{n_x,n_y} = \frac{h^2}{8mL^2}(n_x^2+n_y^2)$

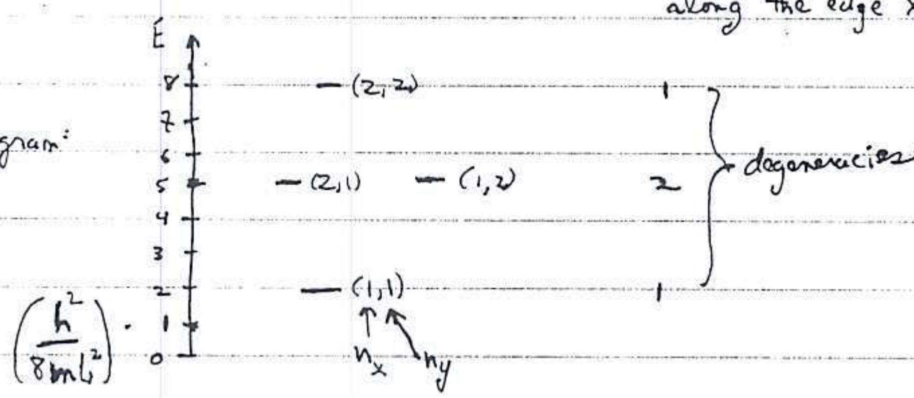
So, ...

(a) (i) $\sin(\pi x/L)\sin(3\pi y/L)$ is an (unnormalized) energy eigenfnctn. corresponding to $n_x=1$, $n_y=3$, so $\boxed{E_{1,3} = \left(\frac{h^2}{8mL^2}\right)\cdot 10}$

(ii) $\sin(\pi x/L)\cdot\sin(3\pi y/2L)$ is not an energy eigenfnctn; it doesn't vanish everywhere along the edge $y=L$

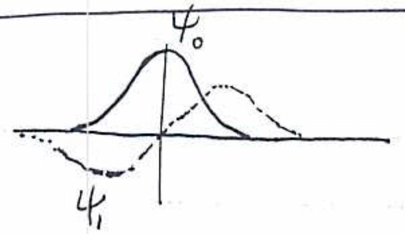
(iii) $\cos(\pi x/L)\sin(4\pi y/L)$ is not an energy eigenfnctn; it doesn't vanish anywhere along the edge $x=0$

(b) Energy diagram:



(3) 1D Harmonic Oscillator and Basic Quantum Measurement Principles

(a) $\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} e^{-m\omega x^2/2\hbar}$



; $E_0 = \frac{1}{2}\hbar\omega$, $E_1 = \frac{3}{2}\hbar\omega$ } corresponding energy eigenvalues

(b) $\psi_1(x) = \frac{1}{\sqrt{2}}\left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} H_1\left(\sqrt{\frac{m\omega}{\hbar}}\, x\right) e^{-m\omega x^2/2\hbar}$, w/ $H_1(y) \equiv 2y$ = Hermite polynomial "H_1"

(c) (i) $P_0 \equiv$ Probability that a measurement of energy yields $E_0 = (.949)^2 = \boxed{0.9}$

$P_1 = (.316)^2 = \boxed{0.1}$; $P_2 = \boxed{0}$

(ii) $\langle E \rangle = P_0 E_0 + P_1 E_1 = .9\left(\frac{1}{2}\hbar\omega\right) + .1\left(\frac{3}{2}\hbar\omega\right) = \boxed{0.6\hbar\omega}$

P 7.1) [redacted]) The force constant for a $H^{19}F$ molecule is 966 N m^{-1}.
a) Calculate the zero point vibrational energy for this molecule for a harmonic potential.
b) Calculate the light frequency needed to excite this molecule from the ground state to the first excited state.

a)

$$E_1 = h\sqrt{\frac{k}{\mu}}\left(1+\frac{1}{2}\right) = \frac{3}{2}\times 1.055\times 10^{-34}\,\mathrm{J\,s}\times\sqrt{\frac{966\ \mathrm{N\,m^{-1}}}{\frac{1.0078\times 18.9984}{1.0078+18.9984}\times 1.66\times 10^{-27}\,\mathrm{kg\,amu^{-1}}}}$$

$$E_1 = 1.23\times 10^{-19}\,\mathrm{J}$$

$$E_0 = \hbar\sqrt{\frac{k}{\mu}}\left(\frac{1}{2}\right) = \frac{1}{3}E_1 = 4.10\times 10^{-20}\,\mathrm{J}$$

b) $$\nu = \frac{E_1 - E_0}{h} = \frac{1.23\times 10^{-19}\,\mathrm{J} - 4.10\times 10^{-20}\,\mathrm{J}}{6.626\times 10^{-34}\,\mathrm{J\,s}} = 1.24\times 10^{14}\,\mathrm{s}^{-1}$$

P7.2 [redacted]) By substituting in the Schrödinger equation for the harmonic oscillator, show that the ground-state vibrational wave function is an eigenfunction of the total energy operator. Determine the energy eigenvalue.

$$-\frac{\hbar^2}{2\mu}\frac{d^2\psi_n(x)}{dx^2} + \frac{kx^2}{2}\psi_n(x) = E_n\psi_n(x)$$

$$-\frac{\hbar^2}{2\mu}\frac{d^2\left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\frac{1}{2}\alpha x^2}}{dx^2} + \frac{kx^2}{2}\left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\frac{1}{2}\alpha x^2} = \frac{\hbar^2}{2\mu}\frac{d\left\{\alpha x\left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\frac{1}{2}\alpha x^2}\right\}}{dx} + \frac{kx^2}{2}\left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\frac{1}{2}\alpha x^2}$$

$$= \frac{\hbar^2}{2\mu}\left\{\alpha\left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\frac{1}{2}\alpha x^2} - \alpha^2 x^2\left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\frac{1}{2}\alpha x^2}\right\} + \frac{kx^2}{2}\left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\frac{1}{2}\alpha x^2}$$

$$= \frac{\hbar^2}{2\mu}\left\{\alpha\left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\frac{1}{2}\alpha x^2} - \alpha^2 x^2\left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\frac{1}{2}\alpha x^2}\right\} + \frac{\hbar^2\alpha^2 x^2}{2\mu}\left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\frac{1}{2}\alpha x^2} = \frac{\hbar^2}{2\mu}\alpha\left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\frac{1}{2}\alpha x^2}$$

$$= \frac{\hbar^2}{2\mu}\sqrt{\frac{k\mu}{\hbar^2}}\left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\frac{1}{2}\alpha x^2} = \frac{\hbar}{2}\sqrt{\frac{k}{\mu}}\left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\frac{1}{2}\alpha x^2} = E_1\psi_1(x) \text{ with } E_1 = \frac{\hbar}{2}\sqrt{\frac{k}{\mu}}$$

P7.4) Evaluate the average kinetic and potential energies, $\langle E_{kinetic}\rangle$ and $\langle E_{potential}\rangle$, for the ground state ($n = 0$) of the harmonic oscillator by carrying out the appropriate integrations.

We use the standard integrals $\int_0^\infty x^{2n}e^{-ax^2}\,dx = \dfrac{1\cdot 3\cdot 5\cdots(2n-1)}{2^{n+1}a^n}\sqrt{\dfrac{\pi}{a}}$ and

$$\int_0^\infty e^{-ax^2}dx = \left(\frac{\pi}{4a}\right)^{1/2}$$

$$\langle E_{potential}\rangle = \int \psi_0^*(x)\left(\frac{1}{2}kx^2\right)\psi_0(x)\,dx$$

$$= \frac{1}{2}k\left(\frac{\alpha}{\pi}\right)^{1/2}\int_{-\infty}^{\infty} x^2e^{-\alpha x^2}dx = k\left(\frac{\alpha}{\pi}\right)^{1/2}\int_0^\infty x^2e^{-\alpha x^2}dx$$

$$= k\left(\frac{\alpha}{\pi}\right)^{1/2}\frac{1}{4\alpha}\sqrt{\frac{\pi}{\alpha}} = k\frac{1}{4\alpha} = \frac{\hbar}{4}\sqrt{\frac{k}{\mu}}$$

$$\langle E_{kinetic}\rangle = \int \psi_0^*(x)\left(-\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial x^2}\right)\psi_0(x)\,dx$$

$$= \int_{-\infty}^{\infty}\left(\frac{\alpha}{\pi}\right)^{1/4}e^{-\frac{1}{2}\alpha x^2}\left(-\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial x^2}\right)\left(\frac{\alpha}{\pi}\right)^{1/4}e^{-\frac{1}{2}\alpha x^2}dx$$

$$= -\frac{\hbar^2}{\mu}\left(\frac{\alpha}{\pi}\right)^{1/2}\int_0^\infty e^{-\alpha x^2}\left(\alpha x^2 - \alpha\right)dx$$

$$= -\frac{\hbar^2}{\mu}\left(\frac{\alpha}{\pi}\right)^{1/2}\left(\frac{\alpha}{4}\sqrt{\frac{\pi}{\alpha}} - \frac{\alpha}{2}\sqrt{\frac{\pi}{\alpha}}\right) = \frac{\hbar^2}{\mu}\frac{\alpha}{4}$$

$$= \frac{\hbar^2}{4\mu}\sqrt{\frac{k\mu}{\hbar^2}} = \frac{\hbar}{4}\sqrt{\frac{k}{\mu}}$$