

$$\Psi_n = \left(\frac{m\omega_0}{\pi\hbar}\right)^{\frac{1}{4}} \frac{1}{\sqrt{2^n n!}} e^{-\frac{m\omega_0}{2\hbar}x^2} H_n(x\sqrt{\frac{m\omega_0}{\hbar}}) \quad H_n(3) = (-1)^n e^{\frac{x^2}{2}} \frac{d^n e^{-\frac{x^2}{2}}}{dx^n}$$

$$n=1 \quad H_1(3) = -1 e^{\frac{x^2}{2}} (-2x) e^{-\frac{x^2}{2}} = 2x \Rightarrow \Psi_1 = \left(\frac{m\omega_0}{\pi\hbar}\right)^{\frac{1}{4}} \frac{1}{\sqrt{2}} e^{-\frac{m\omega_0}{2\hbar}x^2} \cdot 2x \sqrt{\frac{m\omega_0}{\hbar}} = \sqrt{\frac{m\omega_0}{\hbar}} \left(\frac{m\omega_0}{\pi\hbar}\right)^{\frac{1}{4}} x e^{-\frac{m\omega_0}{2\hbar}x^2} = A \sin \frac{\sqrt{\frac{m\omega_0}{\hbar}} x}{\sqrt{2}}$$

Structure of matter: Homework to exercise 8 $\langle p_x \rangle = \int_{-\infty}^{\infty} \psi^* \hat{p}_x \psi dx = i\hbar \frac{d}{dx} \int_{-\infty}^{\infty} x e^{-\frac{m\omega_0}{2\hbar}x^2} \frac{d}{dx} (x e^{-\frac{m\omega_0}{2\hbar}x^2}) dx$

MATRIX ELEMENTS/UNCERTAINTY RELATION

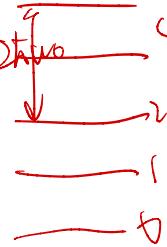
Due on November 28th 2023 at noon! $f_{nk} = -\frac{2}{\pi\hbar} \frac{|C_n(R_k)|^2}{E_n - E_k}$

Please indicate your name on the solution sheets and send it to your seminar leader!

$$\sum_k f_{nk} = \frac{2m}{\hbar} \sum_l |W_{nl}|^2 = 1 \quad n=0 \Rightarrow \sum_k f_{k0} = \frac{2m}{\hbar} \sum_l W_{0l} |x_{l0}|^2 = 1 = f_{00}$$

- Multiple-choice test: Please tick all box(es) with correct answer(s)!
(correctly ticked box: +1/2 point; wrongly ticked box: -1/2 point)

$$\begin{aligned} n=1 & \quad f_{11} + f_{01} = 1 \Rightarrow f_{11} = 2 \\ n=2 & \quad f_{21} + f_{12} \Rightarrow f_{21} = 3 \\ n=3 & \quad f_{43} + f_{32} \Rightarrow f_{43} = 4 \end{aligned}$$

 $2\frac{m\omega_0}{\hbar}$	<p>Consider an electric dipole transition between the two eigenstates $m = 2$ and $n = 4$ of a harmonic oscillator. The oscillator strength f_{nm} of this transition is f_{42}</p>	<table border="1"> <tr><td>2</td></tr> <tr><td>4</td></tr> <tr><td>-24</td></tr> <tr><td>42i</td></tr> </table>	2	4	-24	42i	
2							
4							
-24							
42i							
	<p>Consider the first excited state ($E_1 = \frac{3}{2}\hbar\omega_0$) of a one-dimensional harmonic oscillator. In this state, the expectation value of the momentum will be</p>	<table border="1"> <tr><td>$+\sqrt{3}\hbar\omega_0 m$</td></tr> <tr><td>$-\sqrt{3}\hbar\omega_0 m$</td></tr> <tr><td>0</td></tr> </table>	$+\sqrt{3}\hbar\omega_0 m$	$-\sqrt{3}\hbar\omega_0 m$	0	<input checked="" type="checkbox"/>	
$+\sqrt{3}\hbar\omega_0 m$							
$-\sqrt{3}\hbar\omega_0 m$							
0							

- True or wrong? Make your decision (tick the appropriate box):

(2 points): 1 point per correct decision, 0 points per wrong or no decision

Assertion	true	wrong
The oscillator strength is dimensionless.	<input checked="" type="checkbox"/>	
The oscillator strength cannot be negative.		<input checked="" type="checkbox"/>

- Assume a quantum state described by a wavefunction $\Psi(\mathbf{r}, t) = e^{-i\frac{E_n t}{\hbar}} \psi(\mathbf{r})$ with $\psi(\mathbf{r})$ - real. Show that in such a state, the expectation value of the momentum must be zero. (2 points)
- From Heisenberg's uncertainty relation, find an estimation for the minimum energy of the ground state of a harmonic oscillator! (4 Points)
- Assume an electron confined in a rectangular potential box of length $L = 1\text{ nm}$ with impermeable walls (one-dimensional case). Obtain the transition matrix element x_{jk} and the corresponding oscillator strength for $k = 1$ and $j = 2$. (6 points)
- By explicitly calculating the variances of coordinate x and momentum p_x , show that in any stationary state of the particle confined in a 1D box with impermeable walls, Heisenberg's uncertainty relation $\langle (\Delta x)^2 \rangle \langle (\Delta p_x)^2 \rangle \geq \frac{\hbar^2}{4}$ for the coordinate and the momentum p_x is fulfilled! (10 points)

$$\textcircled{3} \quad \langle p \rangle = \int_V (\varphi^*(r) - i\hbar \nabla \varphi(r)) dr \quad p(r) \text{-real} \Rightarrow \varphi = -i\hbar \int_V \varphi \nabla \varphi dr$$

$$\nabla \varphi^2 = 2\varphi \nabla \varphi \Rightarrow \langle p \rangle = -\frac{i\hbar}{2} \int_V \nabla \varphi^2 dr = -\frac{i\hbar}{2} [\varphi^2]_{-\infty}^{\infty} = 0$$

$$\textcircled{4} \quad \langle (\Delta x)^2 \rangle \leq \langle (\Delta p)^2 \rangle \geq \frac{\hbar^2}{4} \quad \sigma^2 = \langle (\Delta j)^2 \rangle = \langle j^2 \rangle - \langle j \rangle^2 \quad \langle p^2 \rangle = p^2 \quad \langle x^2 \rangle = x^2$$

$$\langle (\Delta x)^2 \rangle = \langle x^2 \rangle - \langle x \rangle^2 \Rightarrow \langle x^2 \rangle \geq \langle (\Delta x)^2 \rangle \quad \langle (\Delta p)^2 \rangle = \langle p^2 \rangle - \langle p \rangle^2 \Rightarrow \langle p^2 \rangle \geq \langle (\Delta p)^2 \rangle$$

$$E = \frac{p_x^2}{2m} + \frac{1}{2} m \omega_0^2 x^2 \Rightarrow \langle E \rangle = \frac{\langle p_x^2 \rangle}{2m} + \frac{1}{2} m \omega_0^2 \langle x^2 \rangle \geq \frac{\langle p_x^2 \rangle}{2m} + \frac{1}{2} m \omega_0^2 \langle x^2 \rangle$$

$$(a-b)^2 = a^2 + b^2 - 2ab \geq 0 \Rightarrow a^2 + b^2 \geq 2ab$$

$$\Rightarrow \frac{\langle p_x^2 \rangle}{2m} + \frac{1}{2} m \omega_0^2 \langle x^2 \rangle \geq 2\sqrt{\frac{\langle p_x^2 \rangle}{2m} \cdot \frac{1}{2} m \omega_0^2 \langle x^2 \rangle} = \sqrt{m \omega_0^2 \langle p_x^2 \rangle \langle x^2 \rangle} \geq \sqrt{m \omega_0^2 \cdot \frac{\hbar^2}{4}} = \frac{m \hbar \omega_0}{2}$$

$$\textcircled{5} \quad x_{nm} = \int_x x f_n y_m dx \quad y_n = \int_0^L \sin \frac{n\pi}{L} x \Rightarrow x_{nm} = \frac{2}{L} \int_0^L x \sin \frac{n\pi}{L} x \sin \frac{m\pi}{L} x dx$$

$$x_{jk} = x_{2,1} = \frac{2}{L} \int_0^L x \sin \frac{2\pi}{L} x \sin \frac{\pi}{L} x dx \quad \frac{\pi}{L} x = t \Rightarrow dx = \frac{L}{\pi} dt$$

$$\Rightarrow x_{2,1} = \frac{2L}{\pi^2} \int_0^\pi t \sin 2t \sin t dt \quad \cos(\alpha + \beta) = \cos \alpha \cos \beta - \sin \alpha \sin \beta \\ \cos(\alpha - \beta) = \cos \alpha \cos \beta + \sin \alpha \sin \beta \Rightarrow \sin \alpha \sin \beta = \frac{1}{2} [\cos(\alpha - \beta) - \cos(\alpha + \beta)]$$

$$\Rightarrow x_{2,1} = \frac{L}{\pi^2} \int_0^\pi t (\cos t - \cos 3t) dt = \frac{L}{\pi^2} \int_0^\pi t \cos t dt - \frac{L}{3\pi^2} \int_0^\pi t \cos 3t dt$$

$$= \frac{L}{\pi^2} (t \sin t \Big|_0^\pi - \int_0^\pi \sin t dt) - \frac{L}{3\pi^2} (t \sin 3t \Big|_0^\pi - \int_0^\pi \sin 3t dt) \\ = \frac{L}{\pi^2} \cos t \Big|_0^\pi - \frac{L}{3\pi^2} \cos 3t \Big|_0^\pi = -\frac{2L}{\pi^2} + \frac{2L}{3\pi^2} = -\frac{4L}{3\pi^2}$$

$$f_{nm} = \frac{2m}{\hbar} |u_{nm}| |x_{nm}|^2 = \frac{2m}{\hbar} \frac{E_n - E_m}{\hbar} |x_{nm}|^2 \Rightarrow f_{2,1} = \frac{2m}{\hbar} \frac{E_2 - E_1}{\hbar} |x_{2,1}|^2; \quad E_n = \frac{\hbar^2 n^2}{8mL^2} \quad E_2 = \frac{4\hbar^2}{8mL^2} \quad E_1 = \frac{\hbar^2}{8mL^2}$$

$$\Rightarrow f_{2,1} = \frac{2m}{\hbar^2} \frac{3h^2}{8mL^2} \cdot \frac{(h^2 L^2)^2}{81\pi^4} = \frac{8\hbar^2 \cdot 3}{81\pi^4} \cdot \frac{16^2}{81\pi^4} = \frac{16^2}{27\pi^2} = 0.86$$

$$\textcircled{6}) \quad [F, G] = i\hbar \quad \Rightarrow \text{Var}(F) \text{Var}(G) \geq \left[\frac{1}{2\hbar} [F, G] \right]^2 = \frac{\hbar^2}{4} \quad \sigma^2 = \langle (\Delta j)^2 \rangle = \langle j^2 \rangle - \langle j \rangle^2$$

$$\text{thus } [x, p_x] = i\hbar \quad \Rightarrow \text{Var}(x) \text{Var}(p_x) \geq \frac{\hbar^2}{4} \quad \text{Var}(x) = \langle x^2 \rangle - \langle x \rangle^2 = \langle \Delta x^2 \rangle \quad \text{Var}(p_x) = \langle p_x^2 \rangle - \langle p_x \rangle^2 = \langle \Delta p_x^2 \rangle$$

$$\Rightarrow \langle \Delta x^2 \rangle \geq \langle \Delta p_x^2 \rangle \geq \frac{\hbar^2}{4}$$

$$\varphi_n = \int_0^L \sin \frac{n\pi}{L} x \quad \langle F \rangle = \int_V \varphi^* F \varphi dr \Rightarrow \frac{2}{L} \int_0^L \sin \frac{n\pi}{L} x \cdot F \sin \frac{m\pi}{L} x dx \quad p_x = -i\hbar \frac{d}{dx}$$

$$\langle p_x \rangle = \frac{2}{L} \int_0^L \sin \frac{n\pi}{L} x \cdot (-i\hbar \frac{d}{dx} \sin \frac{m\pi}{L} x) dx = -\frac{2i\hbar}{L} \int_0^L \sin \frac{n\pi}{L} x \cdot \frac{d}{dx} \sin \frac{m\pi}{L} x dx = -\frac{i\hbar}{L} \int_0^L \frac{d}{dx} \sin \frac{n\pi}{L} x \sin \frac{m\pi}{L} x dx = -\frac{i\hbar}{L} \sin \frac{m\pi}{L} x \Big|_0^L = 0$$

$$\langle p_x^2 \rangle = \frac{2}{L} \int_0^L \sin \frac{n\pi}{L} x \cdot (-i\hbar^2 \frac{d^2}{dx^2} \sin \frac{m\pi}{L} x) dx = \frac{2\hbar^2 n^2 \pi^2}{L^3} \int_0^L \sin \frac{n\pi}{L} x dx = \frac{\hbar^2 n^2 \pi^2}{L^3} \int_0^L (1 - \cos \frac{2m\pi}{L} x) dx$$

$$= \frac{\hbar^2 n^2 \pi^2}{L^3} \left(\int_0^L dx - \int_0^L \cos \frac{2m\pi}{L} x dx \right) = \frac{\hbar^2 n^2 \pi^2}{L^3} \left(L - \frac{L}{2m\pi} \sin \frac{2m\pi}{L} x \Big|_0^L \right) = \frac{\hbar^2 n^2 \pi^2}{L^2}$$

$$\langle x \rangle = \frac{2}{L} \int_0^L x \sin \frac{n\pi}{L} x dx = \frac{1}{L} \int_0^L x (1 - \cos \frac{2m\pi}{L} x) dx = \frac{1}{L} \left[\int_0^L x dx - \int_0^L x \cos \frac{2m\pi}{L} x dx \right]$$

$$= \frac{1}{L} \left(\frac{1}{2} L^2 - \frac{L}{2m\pi} \int_0^L x \sin \frac{2m\pi}{L} x dx \right) = \frac{L}{2} - \frac{1}{2m\pi} \left(x \sin \frac{2m\pi}{L} x \Big|_0^L - \int_0^L \sin \frac{2m\pi}{L} x dx \right) = \frac{L}{2} - \frac{L}{4m^2 \pi^2} \cos \frac{2m\pi}{L} x \Big|_0^L = \frac{L}{2}$$

$$\langle x^2 \rangle = \frac{2}{L} \int_0^L x^2 \sin \frac{n\pi}{L} x dx = \frac{1}{L} \int_0^L (x^2 - x^2 \cos \frac{2m\pi}{L} x) dx = \frac{1}{L} \left(\int_0^L x^2 dx - \int_0^L x^2 \cos \frac{2m\pi}{L} x dx \right) = \frac{1}{L} \left(\frac{1}{3} L^3 - \frac{L}{2m\pi} \int_0^L x^2 \sin \frac{2m\pi}{L} x dx \right)$$

$$= \frac{1}{3}L^2 - \frac{1}{2n\pi} \left(x^2 \sin \frac{2n\pi}{L} x \Big|_0^L - 2 \int_0^L x \sin \frac{2n\pi}{L} x \, dx \right) = \frac{1}{3}L^2 + \frac{1}{n\pi} \int_0^L x \sin \frac{2n\pi}{L} x \, dx = \frac{1}{3}L^2 - \frac{L}{2n\pi^2} \int x \cos \frac{2n\pi}{L} x \, dx$$

$$= \frac{1}{3}L^2 - \frac{L}{2n\pi^2} \left(x \cos \frac{2n\pi}{L} x \Big|_0^L - \int_0^L \cos \frac{2n\pi}{L} x \, dx \right) = \frac{1}{3}L^2 - \frac{L^2}{2n\pi^2} + \frac{L}{4n\pi^3} \sin \frac{2n\pi}{L} x \Big|_0^L = \left(\frac{1}{3} - \frac{1}{2n\pi^2} \right) L^2$$

$$\text{Var}(x) = \langle \Delta x^2 \rangle = \langle x^2 \rangle - \langle x \rangle^2 = \left(\frac{1}{3} - \frac{1}{2n\pi^2} \right) L^2 - \frac{1}{2}L$$

$$\text{Var}(p_x) = \langle \Delta p_x^2 \rangle = \langle p_x^2 \rangle - \langle p_x \rangle^2 = \frac{\hbar^2 n^2 \pi^2}{L^2} = \frac{\hbar^2 n^2}{4L^2}$$

$$\langle \Delta x^2 \rangle \text{COP}_B^2 = \left(\left(\frac{1}{3} - \frac{1}{2n\pi^2} \right) L^2 - \frac{1}{2}L \right) \frac{\hbar^2 n^2 \pi^2}{L^2} = \frac{\hbar^2 n^2 \pi^2}{3} - \frac{\hbar^2}{2} - \frac{\hbar^2 n^2 \pi^2}{2L} = \left(\frac{n^2 \pi^2}{3} - \frac{n^2 \pi^2}{2L} - \frac{1}{2} \right) \hbar^2 = \frac{4n^2 \pi^2 L - 6n^2 \pi^2 - 6L}{12L} \hbar^2$$

$$= \frac{4n^2 \pi^2 L - 6n^2 \pi^2 - 6L}{3L} \cdot \frac{\hbar^2}{4} > \frac{\hbar^2}{4}$$