26/26

Structure of matter: Homework to exercise 7

PARTICLE IN THE BOX/OPERATORS

Due on november 21st 2023 at noon!

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

The ground state (n = 1) wavefunction of a particle in a rectangular potential box is	Even with respect to symmetry centre	✓
	odd with respect to symmetry centre	
	Neither even or odd	
$[\hat{p}_z, \hat{y}] = ?$ $\hat{p}_z = -i\hbar \frac{\partial}{\partial z}$ $\hat{y} = y$ $[\hat{p}_z, \hat{y}] = \hat{p}_z \hat{y} - \hat{y}\hat{p}_z$ $u = u(x, y, z)$ $\hat{p}_z \hat{y} u = -i\hbar \frac{\partial}{\partial z} y u$ $\hat{y}\hat{p}_z u = y -i\hbar \frac{\partial}{\partial z} u$	0	✓
	$i\hbar$	
	$-i\hbar$	

1

2. true or wrong? Make your decision! (tick the appropriate box):

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

Statement	true	wrong
All linear operators are self-adjoint.		✓
All eigenvalues of a self-adjoint operator are real.	✓	

2

3. Consider a particle trapped in a one-dimensional box potential with length L and infinitely high potential walls, i.e.

$$U = 0; \quad 0 \le x \le L$$
$$U \to \infty; \quad x < 0 \text{ or } x > L$$

The stationary states of this system are described by the normalized wavefunctions:

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi}{L} x; \quad n = 1,2,3,\ldots$$

Derive the normalization factor $\sqrt{\frac{2}{L}}$! (3 points)

4. Assume a 3D cubic potential box with edge length L=2nm. How many electrons with energy E $\le$ 1eV may be placed into this box, when each quantum state characterized by n_x, n_y, n_z may be occupied by two electrons? (6 points)

5. $\left[\hat{p}_z^2, \hat{z}\right] = ?$ (4 points)

6. The calculation of quantum mechanical expectation values, as well as the calculation of the efficiency of light absorption processes in manageable model quantum systems demands the calculation of integrals of certain complexity. In this connection, solve the following integral that becomes later relevant for the particle-in the-box model system:

$$\frac{2}{L}\int_0^L x\sin\left(\frac{n\pi x}{L}\right)\sin\left(\frac{m\pi x}{L}\right)dx = ?? \qquad n,m \text{ integer} > 0$$

Discriminate between the cases:

a) $n = m$

b) $n \neq m$ and $(n-m)$ – odd and

c) $n \neq m$ and $(n-m)$ – even! (10 points)

(3.) $\psi = e^{-i(\omega t - kx)}$ $\quad E = \hbar\omega = pc \Rightarrow \omega = \frac{E}{\hbar}$ $\quad p = \frac{\hbar\omega}{c}$ $\quad k = \frac{2\pi}{\lambda} = \frac{2\pi\nu}{c} = \frac{\omega}{c} \Rightarrow p = \hbar k$

$\Rightarrow \psi = e^{-\frac{i}{\hbar}(Et - px)}$ $\quad \frac{\partial}{\partial t}\psi = -\frac{i}{\hbar}E\psi \Rightarrow E\psi = i\hbar\frac{\partial}{\partial t}$ $\quad \frac{\partial}{\partial x}\psi = \frac{i}{\hbar}p\psi \Rightarrow p\psi = -i\hbar\frac{\partial}{\partial x} \Rightarrow p = -i\hbar\frac{\partial}{\partial x}$

$E = T_{kin} + U = \frac{p^2}{2m} + U = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + U \Rightarrow E\psi = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + U\right)\psi$

$x = L$ $\quad U = 0 \Rightarrow E\psi = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi \Rightarrow \psi \propto \sin kx \Rightarrow \psi = A\sin kx$

$x = L$ $\quad \psi(L) = A\sin kL = 0 \Rightarrow kL = n\pi \Rightarrow k = k_n = \frac{n\pi}{L} \Rightarrow \psi_n = A\sin\frac{n\pi}{L}x$

$\psi_n = \frac{A}{2i}\left(e^{i\frac{n\pi}{L}x} - e^{-i\frac{n\pi}{L}x}\right)$ $\quad \psi_n^* = \frac{A}{-2i}\left(e^{-i\frac{n\pi}{L}x} - e^{i\frac{n\pi}{L}x}\right) = A\sin\frac{n\pi}{L}x$

$\int_0^L \psi_n\psi_n^* dx = A^2\int_0^L \sin^2\frac{n\pi}{L}x\,dx = \frac{A^2}{2}\int_0^L\left(1-\cos\frac{2n\pi}{L}x\right)dx = -\frac{A^2}{2}\int_0^L\cos\frac{2n\pi}{L}x\,dx + \frac{A^2}{2}\int_0^L dx$

$= -\frac{A^2}{2}\cdot\frac{L}{2n\pi}\sin\frac{2n\pi}{L}\Big|_0^L + \frac{A^2}{2}x\Big|_0^L = \frac{A^2}{2}L = 1$ – $A = \sqrt{\frac{2}{L}}$

3

(4) $\psi_n = \sqrt{\frac{2}{L}}\sin\frac{n\pi}{L}x \Rightarrow \psi_n(x,y,z) = \sqrt{\frac{8}{L_xL_yL_z}}\sin\frac{n_x\pi}{L}x\,\sin\frac{n_y\pi}{L}y\,\sin\frac{n_z\pi}{L}z$

$E\psi = \left(-\frac{\hbar^2}{2m}\nabla^2 + U\right)\psi$ $\quad U = 0 \Rightarrow E\psi = -\frac{\hbar^2}{2m}\nabla^2\psi = (n_x^2+n_y^2+n_z^2)\frac{\pi^2}{L^2}(-1)^3\cdot\left(-\frac{\hbar^2}{2m}\right)\psi = E\psi$

$\Rightarrow E_n = \frac{\hbar^2\pi^2}{2mL^2}(n_x^2+n_y^2+n_z^2) = \frac{h^2}{8mL^2}(n_x^2+n_y^2+n_z^2) = \frac{6.625^2\times10^{-68}W^2s^4}{8\times9.108\times10^{-31}kg\cdot4\times10^{-18}m^2}(n_x^2+n_y^2+n_z^2)$

$\Rightarrow E_n = 0.15\times10^{-18}J\cdot(n_x^2+n_y^2+n_z^2)$ $\quad 1eV = 1.602\times10^{-19}J$

$E_n \le 1eV \Rightarrow 0.15\times10^{-18}(n_x^2+n_y^2+n_z^2) \le 1.602\times10^{-18}J \Rightarrow (n_x^2+n_y^2+n_z^2) \le 10.68$

6

$\Rightarrow (n_x, n_y, n_z) = (1,2,2), (2,1,2), (2,2,1), (1,1,2), (1,2,1)(2,1,1)(1,1,1)$

Thus totaly 7 quantum states. and Number of Electron is $N = 14$

⑤ $\psi = e^{i(kz-\omega t)}$ $\quad \omega = \frac{E}{\hbar} \quad \omega\hbar = pc \quad k = \frac{2\pi}{\lambda} = \frac{2\pi\nu}{c} = \frac{\omega}{c} = \frac{p}{\hbar}$

$\psi = e^{\frac{i}{\hbar}(pz - Et)} \qquad \frac{\partial}{\partial z}\psi = \frac{i}{\hbar}p\psi \Rightarrow -i\hbar\frac{\partial}{\partial z}\psi = p\psi \Rightarrow \hat{p}_z = -i\hbar\frac{\partial}{\partial z}$

$\hat{p}_z^2 = -\hbar^2\left(\frac{\partial}{\partial z}\right)^2 \qquad [\hat{p}_z^2, \hat{z}] = \hat{p}_z^2\hat{z} - \hat{z}\hat{p}_z^2$

$\hat{z}\hat{p}_z^2 u = z\left(-\hbar^2\frac{\partial^2}{\partial z^2}u\right) = -\hbar^2 z\frac{\partial^2}{\partial z^2}u$

$\hat{p}_z^2\hat{z}u = -\hbar^2\frac{\partial}{\partial z}\cdot\frac{\partial}{\partial z}(zu) = -\hbar^2\frac{\partial}{\partial z}\left(u + z\frac{\partial}{\partial z}u\right) = -\hbar^2\frac{\partial}{\partial z}u - \hbar^2\frac{\partial}{\partial z}u - \hbar^2 z\frac{\partial^2}{\partial z^2}u = -2\hbar^2\frac{\partial}{\partial z}u - \hbar^2 z\frac{\partial^2}{\partial z^2}u$

$\hat{p}_z^2\hat{z}u - \hat{z}\hat{p}_z^2 u = -2\hbar^2\frac{\partial}{\partial z}u - z\hbar^2\frac{\partial^2}{\partial z^2}u + z\hbar^2\frac{\partial^2}{\partial z^2}u = -2\hbar^2\frac{\partial}{\partial z}u \Rightarrow \underline{[\hat{p}_z^2, \hat{z}] = -2\hbar^2\frac{\partial}{\partial z}}$

6) $I = \frac{2}{L}\int_0^L x\sin\left(\frac{n\pi x}{L}\right)\sin\left(\frac{m\pi x}{L}\right)dx \qquad \frac{\pi x}{L} = \xi \Rightarrow x = \frac{L}{\pi}\xi \quad dx = \frac{L}{\pi}d\xi \qquad x = L \Rightarrow \xi = \pi$

$= \frac{2L}{\pi^2}\int_0^\pi \xi\sin(n\xi)\sin(m\xi)\,d\xi = \frac{2L}{\pi^2}\int_0^\pi -\frac{1}{4}\left(e^{in\xi} - e^{-in\xi}\right)\left(e^{im\xi} - e^{-im\xi}\right)\xi\,d\xi$

$= -\frac{L}{2\pi^2}\int_0^\pi\left[e^{i(n+m)\xi} - e^{i(n-m)\xi} - e^{-i(n-m)\xi} + e^{-i(n+m)\xi}\right]\xi\,d\xi$

$= \frac{L}{2\pi^2}\int_0^\pi 2\left[\frac{e^{i(n-m)\xi} + e^{-i(n-m)\xi}}{2} - \frac{\left(e^{i(n+m)\xi} + e^{-i(n+m)\xi}\right)}{2}\right]\xi\,d\xi$

$= \frac{L}{\pi^2}\int_0^\pi\left[\cos(n-m)\xi - \cos(n+m)\xi\right]\xi\,d\xi$

$= \frac{L}{\pi^2}\int_0^\pi \cos[(n-m)\xi]\,\xi\,d\xi - \frac{L}{\pi^2}\int_0^\pi\cos[(n+m)\xi]\,\xi\,d\xi$

$= \frac{L}{\pi^2(n-m)}\int_0^\pi \xi\,d\sin[(n-m)\xi] - \frac{L}{\pi^2(n+m)}\int_0^\pi\xi\,d\sin[(n+m)\xi]$

$= \frac{L}{\pi^2(n-m)}\left(\xi\sin(n-m)\xi\Big|_0^\pi - \int_0^\pi\sin[(n-m)\xi]\,d\xi\right) - \frac{L}{\pi^2(n+m)}\left(\xi\sin[(n+m)\xi]\Big|_0^\pi - \int_0^\pi\sin[(n+m)\xi]\,d\xi\right.$

$= \frac{L}{\pi^2(n-m)^2}\cos[(n-m)\xi]\Big|_0^\pi - \frac{L}{\pi^2(n+m)^2}\cos[(n+m)\xi]\Big|_0^\pi$

$\Rightarrow I = \frac{L}{\pi^2}\left\{\frac{1}{(n-m)^2}[\cos(n-m)\pi - 1] - \frac{1}{(n+m)^2}[\cos(n+m)\pi - 1]\right.$

(a) $n = m \Rightarrow I = \frac{L}{\pi^2}\int_0^\pi[\cos(n-m)\xi - \cos(n+m)\xi]\,\xi\,d\xi = \frac{L}{\pi^2}\int_0^\pi[1 - \cos(2n\xi)]\,\xi\,d\xi$

$= \frac{L}{\pi^2}\int_0^\pi\xi\,d\xi - \frac{L}{\pi^2}\int_0^\pi\cos(2n\xi)\,\xi\,d\xi = \frac{L}{\pi^2}\cdot\frac{\xi^2}{2}\Big|_0^\pi - \frac{L}{2n\pi^2}\int_0^\pi\xi\,d\sin(2n\xi)$

$= \frac{L}{2} - \frac{L}{2n\pi^2}\left(\xi\sin 2n\xi\Big|_0^\pi - \int_0^\pi\sin 2n\xi\,d\xi\right) = \frac{L}{2} - \frac{L}{4n^2\pi^2}\cos 2n\xi\Big|_0^\pi = \frac{L}{2}$

(b) $n - m = 2k+1$ $\quad k$ is integer $\quad n+m = 2k+1+2m = 2k'+1$ $\quad k'$ is also integer

$$\Rightarrow I = \frac{L}{\pi^2}\left[\frac{-2}{(2k+1)^2} + \frac{2}{(2k'+1)^2}\right] = \frac{2L}{\pi^2}\left[\frac{1}{(2k'+1)^2} - \frac{1}{(2k+1)^2}\right] \quad k', k \text{ are integer}$$

$$= \frac{2L}{\pi^2}\left[\frac{1}{(n+m)^2} - \frac{1}{(n-m)^2}\right]$$

(4) $n-m=2k \quad n+m=2k+2m=2k' \quad k, k'$ are integer

$$I = \frac{L}{\pi^2}\left[\frac{1}{4k^2}(\cos 2k\pi - 1)\right] - \frac{L}{\pi^2}\left[\frac{1}{4k'^2}(\cos 2k'\pi - 1)\right] = 0$$

10