Indian Institute of Technology Kanpur
Department of Physics
PHY114: Quantum Physics

Max. Marks: 120 MidSem Max. Time: 120 min.

Name Model Solⁿ Roll No. YNM Section No.___

All scoring has been out of 20X6 = 120, double of marks indicated.

- There are six questions and each carry 10 marks. The answers must be placed only in the designated space. There are __14___ pages in the booklet. One blank sheet is attached at the back for Rough Work.)
- Rough work can be done at the blank space provided at the end.
- Exchange of any material or borrowing of any device such as calculator or cell phone is strictly prohibited.
- No Pages (including Rough Work) must be detached from this booklet at any stage.

Honour Pledge

I pledge that I shall not resort to any unfair means during the examination including helping others in any manner. I understand that I will be liable to strict disciplinary action if I am found to be involved any such means.

(Signature)

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Q. No.	Marks
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2	
3.	
4.	
5.	
6.	
TOTAL	

1. a) A conjugate polymer of 11 carbon atoms with alternate single and double bonds has 22 pi electrons. The length of the molecule can be taken to be 3.2nm. Find the largest wavelength corresponding first absorption band (in nm). [3]

Highest filled level $n = 11 \Rightarrow \nu = \frac{\Delta E}{h} = \frac{(12^2-11^2)h}{8mL^2}$

$$\lambda = \frac{c}{\nu} = \frac{8mL^2 \cdot c}{h(12^2-11^2)}$$

$$= \frac{8 \times 9.1 \times 10^{-31} \times (3.2)^2 \times 10^{-18} \times 3 \times 10^8}{6.626 \times 10^{-34} (144-121)}$$

$$\boxed{\lambda \approx 1467 \text{ nm}}$$

b) Consider a cubic box of side a with all its walls impenetrable (i.e. V=∞). Let $\epsilon_0 = \frac{\hbar^2\pi^2}{2ma^2}$, where m is the mass of the electron. If only the lowest two energy states are fully occupied by electrons in the box, find the total energy (in terms of ϵ_0). [2]

$$\psi(x,y,z) \sim \sin\left(\frac{\pi n_x}{a}\right) \sin\left(\frac{\pi n_y}{a}\right) \sin\left(\frac{\pi n_z}{a}\right)$$

where $n_x, n_y, n_z : 1, 2, 3 \ldots$

(n_x, n_y, n_z) $(1,1,1) \longrightarrow 1$ state : $2e^-$

$(1,1,2) \longrightarrow 3$ states : $2e^- \times 3$

$$E_{n_x,n_y,n_z} = (n_x^2 + n_y^2 + n_z^2)\,\epsilon_0$$

$$\text{Total } E = (2 \times 3\epsilon_0) + (2 \times 3 \times 6\epsilon_0) = \boxed{42\,\epsilon_0}$$

c) Given the following wavefunction

$$\psi(x) = \frac{1}{\sqrt{2L}} e^{\frac{ip_0 x}{\hbar}}, |x| \le L$$
$$= 0, \qquad |x| > L$$

Find the corresponding $\Phi(p)$, and find the probability at p_0. [3]

$$\Phi(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \psi(x)\, e^{-i\frac{p}{\hbar}x}\, dx$$

$$= \frac{1}{\sqrt{2\pi\hbar}\sqrt{2L}} \int_{-L}^{L} e^{\frac{i}{\hbar}(p_0 - p)x}\, dx$$

$$= \sqrt{\frac{\hbar}{\pi L}}\; \frac{\sin\left[(p_0 - p)\frac{L}{\hbar}\right]}{(p_0 - p)}$$

$$\lim_{p \to p_0} \Phi(p) = \sqrt{\frac{\hbar}{\pi L}} \cdot \left(\frac{L}{\hbar}\right) \Rightarrow |\Phi(p)|^2 \Big|_{p_0} = \frac{L}{\pi\hbar}$$

$$|\Phi(p)|^2 \text{ at } p_0 = \frac{L}{\pi\hbar}$$

d) A wavepacket representing an electron has a width of $\Delta x = 0.05$ nm, estimate the time in which the wave packet will spread to a width of 0.1 nm. [2]

When $t\frac{\Delta p}{2m} \approx \Delta x$, the spreading will be significant i.e. Δx is same as original Δx.

$$\frac{t\,\Delta p}{2m} \approx \Delta x \quad (\Delta x \text{ is the initial width})$$

$$t_0 \approx \frac{2m\hbar}{(\Delta p)^2} \approx \frac{2m(\Delta x)^2}{\hbar} \approx \frac{2\times 9.1\times 10^{-31}}{1\times 10^{-34}}\left(5\times 10^{-11}\right)^2$$

$$\approx 450 \times 10^{-19}\ \text{s.}$$

$$\approx \underline{4.5\times 10^{-17}\ \text{s.}}$$

2. A wavefunction in momentum space is given as $\Phi(p) = A\, e^{-|p|/\alpha}$, where α is a positive constant.
   a) Find the normalization constant A.
   b) Find the symmetric p-interval (around the origin in p-space) in which the probability of finding the particle is 90%.
   c) Express $\hat{x}$ in p-space, and then use it to find $\hat{x}|\Phi(p)\rangle$.
   d) Obtain the corresponding $\psi(x)$, and provide a neat qualitative sketch of the wavefunction in real space. Find the positions at which $\psi(x)$ becomes half its peak value. [2+3+2+3]

a) $$A^2\int_{-\infty}^{\infty} |\phi(p)|^2 dp = A^2\int_{-\infty}^{0} e^{+2p/\alpha} dp + A^2\int_{0}^{\infty} e^{-2p/\alpha} dp$$

$$= 2A^2 \int_0^{\infty} e^{-2p/\alpha} dp = 1 \Rightarrow A = \frac{1}{\sqrt{\alpha}}$$

b) Prob. of finding $-p_1 < p < p_1$

$$\int_{-p_1}^{p_1} |\phi(p)|^2 dp = 2\int_0^{p_1} \frac{1}{\alpha} e^{-2p/\alpha} dp = \left(1 - e^{-2p_1/\alpha}\right)$$

$$1 - e^{-2p_1/\alpha} = 0.9 \Rightarrow p_1 = \frac{\alpha}{2}\ln 10 \approx 1.15\alpha$$

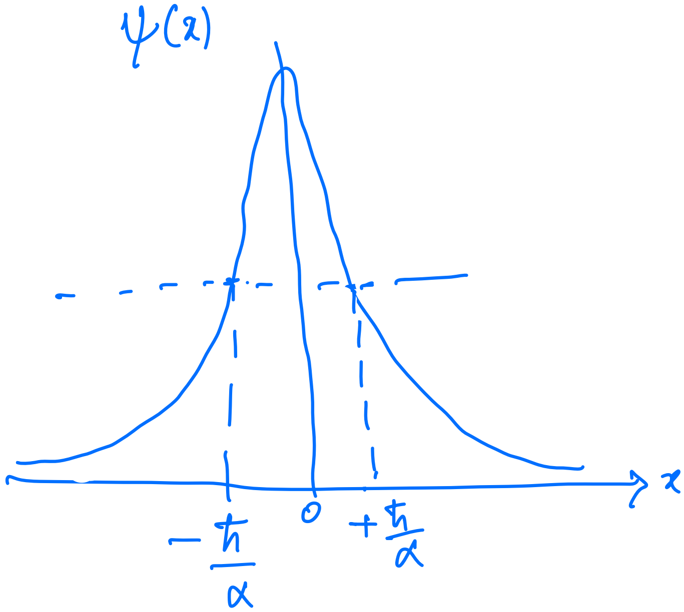
c) $$\langle p|\hat{x} = -i\hbar \frac{\partial}{\partial p} \Rightarrow \frac{-i\hbar}{\sqrt{\alpha}}\left(-\frac{1}{\alpha}\right) e^{-|p|/\alpha}$$

$$= \frac{i\hbar}{\alpha^{3/2}} e^{-|p|/\alpha}$$

d) $$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \Phi(p)\, e^{i\frac{p}{\hbar}x} dp$$

$$= \frac{1}{\sqrt{2\pi\hbar\,\alpha}} \int_{-\infty}^{\infty} e^{-|p|/\alpha}\, e^{i\frac{p}{\hbar}x} dp$$

$$= \sqrt{\frac{2\hbar^3}{\pi\alpha^3}}\ \frac{1}{x^2 + \left(\frac{\hbar}{\alpha}\right)^2}$$



$$\psi(0) = \sqrt{\frac{2\hbar^3}{\pi\alpha^3}}\left(\frac{\hbar}{\alpha}\right)^2$$

$$\psi(x_1) = $$

$$= \sqrt{\frac{2\hbar^3}{\pi\alpha^3}}\,\frac{1}{x_1^2+\left(\frac{\hbar}{\alpha}\right)^2}$$

$$\frac{\psi(x_1)}{\psi(0)} = \frac{1}{2}$$

$$\Rightarrow x_1^2 + \left(\frac{\hbar}{\alpha}\right)^2 = 2\left(\frac{\hbar}{\alpha}\right)^2$$

$$\Rightarrow \boxed{x_1 = \pm\frac{\hbar}{\alpha}}$$

It is a Lorentzian. (Need not be mentioned).

3. Consider a particle in an infinite potential well $V(x) = \begin{cases} 0, |x| < a/2 \\ \infty, |x| > a/2 \end{cases}$.

For all parts, use $x = 0$ as the origin.

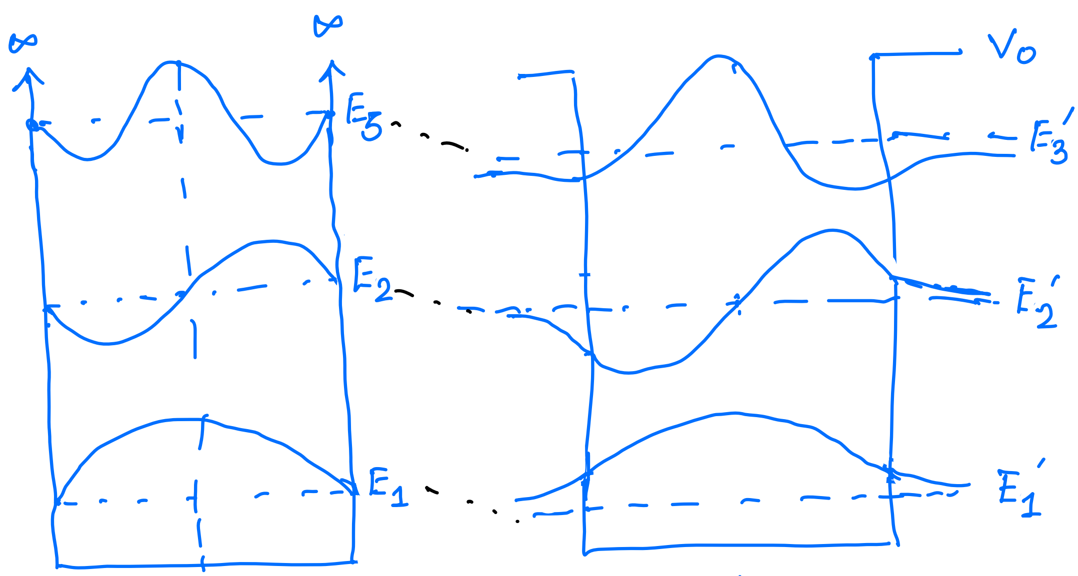
a) Write down the eigenfunctions i.e. the wavefunction and corresponding eigenvalues.

b) Sketch the first three eigenfunctions corresponding to lowest three energy states. Provide a comparative qualitative sketch of them if the barrier was finite instead.

c) If the particle is initially in the ground state, and there is a sudden and rapid doubling of the width of the infinite barrier potential well symmetrically (i.e. new barriers are at $-a$ and a). Obtain the probability of finding the particle in the ground and the first excited of the new potential well. [3+3+4]

$$\psi_n(x) = \begin{cases} \sqrt{\frac{2}{a}} \cos\left(\frac{n\pi x}{a}\right), & n = 1, 3, 5, \ldots \\ \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right), & n = 2, 4, 6, \ldots \end{cases} \quad |x| < \frac{a}{2}$$

$$E_n = \frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2 n^2, \quad n = 1, 2, 3, \ldots$$



Infinite Barrier Well

Finite Barrier Well

$$E_{n'} < E_n$$

$$\langle E_1^{2a} | x \rangle = [\psi_1^{2a}(x)] = \begin{cases} \sqrt{\frac{1}{a}} \cos\frac{\pi x}{2a}, & |x| < \frac{a}{2} \\ 0 & |x| > a \end{cases}$$

$$\langle E_1^{2a} | E_1^{a} \rangle = \int dx \, \langle E_1^{2a} | x \rangle \langle x | E_1^{a} \rangle$$

$$= \int_{-a/2}^{a/2} dx \, \sqrt{\frac{1}{a}} \cos\left(\frac{\pi x}{2a}\right) \sqrt{\frac{2}{a}} \cos\left(\frac{\pi x}{a}\right)$$

$$= \frac{8}{3\pi}$$

(Note the integration limits are $-a/2$ to $a/2$ since it is non-zero only in this region).

$$\left| \langle E_1^{2a} | E_1^{a} \rangle \right|^2 = \frac{64}{9\pi^2} = 0.72$$

$$\left| \langle E_2^{2a} | E_1^{a} \rangle \right|^2 = 0 ,$$

integrand odd. symmetry considerati

4. a) Given $|\chi\rangle = i|\varphi_1\rangle - 2|\varphi_2\rangle - i|\varphi_3\rangle$ and $|\xi\rangle = i|\varphi_1\rangle + 2|\varphi_3\rangle$, where $|\varphi_j\rangle$, $j = 1,2,3$ are a set of complete orthonormal basis states.

i) Determine $\langle\chi|\xi\rangle$.

ii) Determine $\sum_{j=1}^{3}\langle\varphi_2|\chi\rangle\langle\xi|\varphi_j\rangle$. [2]

i) $+1+2i$

(ii) $2i+0-4 = 2i-4$

$= \langle 2|\chi\rangle\langle\xi|1\rangle + \langle 2|\chi\rangle\langle\xi|2\rangle + \langle 2|\chi\rangle\langle\xi|3\rangle$

b) Find if the differentiation operator in one dimension $\hat{D} \equiv \frac{d}{dx}$ is Hermitian by determining $\hat{D}^\dagger$. ~~[2]~~ [3]

$$\left\langle g \middle| \frac{d}{dx} f \right\rangle = \int_{-\infty}^{\infty} g^* \frac{df}{dx}\, dx = \cancel{g^* f \Big|_{-\infty}^{\infty}}^{\,0} - \int_{-\infty}^{\infty} \frac{dg^*}{dx} f(x)\, dx$$

Integration by parts

$$= -\int_{-\infty}^{\infty} \left(\frac{dg}{dx}\right)^* f\, dx = -\left\langle \frac{dg}{dx} \middle| f \right\rangle$$

$\therefore$ Anti-Hermitian. [$\langle\psi|\frac{d}{dx}|\psi\rangle$ can also be used.]

c) A one-dimensional translational operator $\hat{T}(a)$ is defined as $\hat{T}(a)|x\rangle = |x+a\rangle$. For any $\psi(x)$, find the wavefunction resulting from $\hat{T}(a)|\psi\rangle$. [2]

$$\psi'(x) = \langle x|\psi'\rangle = \langle x|\hat{T}(a)|\psi\rangle$$
$$= \int dx' \langle x|x'+a\rangle\langle x|\psi\rangle$$
$$= \int dx'\, \delta[x-(x'+a)]\langle x'|\psi\rangle$$
$$= \langle x-a|\psi\rangle = \psi(x-a)$$

d) Let $\hat{H} = \frac{\hat{p}_x^2}{2m} + \alpha\hat{x}^n$, where α is a positive constant and n integer. Find the rate of change of $\langle p_x\rangle$ in terms of the expectation value of a function of $\hat{x}$. Indicate all steps with reasoning. [3]

$$[\hat{H}, \hat{p}_x] = [V(\hat{x}), \hat{p}_x] = i\hbar \frac{dV}{dx}(\hat{x})$$

$$\frac{d\langle p_x\rangle}{dt} = \frac{i}{\hbar}\langle\psi|[\hat{H}, \hat{p}_x]|\psi\rangle$$

$$= \frac{i}{\hbar}\langle\psi|i\hbar\frac{dV}{dx}(\hat{x})|\psi\rangle = \left\langle -\frac{dV}{dx}\right\rangle$$

$$= \alpha n \langle -x^{n-1}\rangle$$

5.

a) For a one-dimensional harmonic oscillator, starting from known properties of the lowering ladder operator, *derive* explicitly the ground state $\langle x|0\rangle$. [2]

$$\hat{a} = \frac{1}{\sqrt{2}}(\hat{X} + \hat{P}) \qquad x_0 = \sqrt{\frac{\hbar}{m\omega}}$$

$$= \frac{1}{\sqrt{2}}\left(\frac{\hat{x}}{x_0} + x_0\frac{d}{dx}\right) = \frac{1}{\sqrt{2}\,x_0}\left(\hat{x} + x_0^2\frac{d}{dx}\right)$$

$$\langle x|\hat{a}|0\rangle = 0$$

$$= \frac{1}{\sqrt{2}\,x_0}\langle x|\left(\hat{x} + x_0^2\frac{d}{dx}\right)|0\rangle = \frac{1}{\sqrt{2}x_0}\left[x\,\psi_0(x) + x_0^2\frac{d\psi_0}{dx}\right]$$

$$\Rightarrow \frac{d\psi_0}{dx} = -\frac{x}{x_0^2}\psi_0(x)$$

$$\Rightarrow \psi_0(x) = A\, e^{-\frac{x^2}{2x_0}}; \quad A^2\sqrt{\pi}\,x_0 = 1 \quad \text{i.e. } A = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}$$

$$\boxed{\langle x|0\rangle = \psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-x^2/2x_0}}$$

b) In a harmonic oscillator, the particle is in the ground state. The spring-constant is abruptly changed to 4 times of its original value. Find the probability of finding the particle still in the ground state. [3]

$$\omega_1 = \sqrt{\frac{k}{m}}, \quad \omega_2 = \sqrt{\frac{4k}{m}} = 2\omega_1$$

$$\psi_{10}(x) = \left(\frac{m\omega_1}{\pi\hbar}\right)^{1/4} e^{-\frac{1}{2}\frac{m\omega_1}{\hbar}x^2}$$

$$\psi_{20}(x) = \left(\frac{2m\omega_1}{\pi\hbar}\right)^{1/4} e^{-\frac{1}{2}\frac{2m\omega_1}{\hbar}x^2}$$

$$\langle\psi_{20}|\psi_{10}\rangle = \int_{-\infty}^{\infty} (2)^{1/4}\left(\frac{m\omega_1}{\pi\hbar}\right)^{1/2} e^{-\frac{1}{2}\cdot\frac{3m\omega_1}{\hbar}x^2}\,dx$$

$$= (2)^{1/4}\left(\frac{m\omega_1}{\pi\hbar}\right)^{1/2}\sqrt{\frac{2\pi\hbar}{3m\omega_1}} = 2^{1/4}\sqrt{\frac{2}{3}}.$$

$$\therefore \langle\psi_{20}|\psi_{10}\rangle = \frac{2\sqrt{2}}{3} \approx 0.94$$

c) For a one-dimensional harmonic oscillator, using operator methods, find σ_x, σ_p and their product for the eigenstate $|3\rangle$. [3]

$$\langle E\rangle = \frac{\langle p_x^2\rangle}{2m} + \frac{1}{2}m\omega^2\langle x^2\rangle = \frac{(\Delta p_x)^2 + \cancel{\langle p_x\rangle}^{2}}{2m} + \frac{1}{2}m\omega^2\left[(\Delta x)^2 + \cancel{\langle x\rangle}^{2}\right]$$

$0 \qquad 0$

$$\Rightarrow \langle E\rangle = \frac{(\Delta p_x)^2}{2m} + \frac{1}{2}m\omega^2(\Delta x)^2$$

$$\hat{x} = \frac{\hat{a} + \hat{a}^\dagger}{\sqrt{2}}$$

$$\hat{p} = \frac{\hat{a} - \hat{a}^\dagger}{\sqrt{2}\, i}$$

$$(\Delta x)^2 = \langle n|\frac{(\hat{a} + \hat{a}^\dagger)^2}{2}|n\rangle$$

$$= \frac{1}{2}\langle n|\left[\hat{a}^2 + (\hat{a}^\dagger)^2 + \hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a}\right]|n\rangle$$

$$= \frac{1}{2}\left(\langle n|\hat{a}\hat{a}^\dagger|n\rangle + \langle n|\hat{a}^\dagger\hat{a}|n\rangle\right)$$

$$= \frac{1}{2}\left(\langle n|(\hat{N}+1)|n\rangle + \langle n|\hat{N}|n\rangle\right) = \frac{1}{2}(2n+1)$$

square terms $\to 0$ since $\langle n|n'\rangle = \delta_{nn'}$

$\hat{a}\hat{a}^\dagger = 1 + \hat{a}^\dagger\hat{a}$

$$(\Delta p)^2 = -\frac{1}{2}\langle n|\hat{a} - \hat{a}^\dagger|n\rangle = \frac{1}{2}(2n+1)\langle n|n\rangle$$

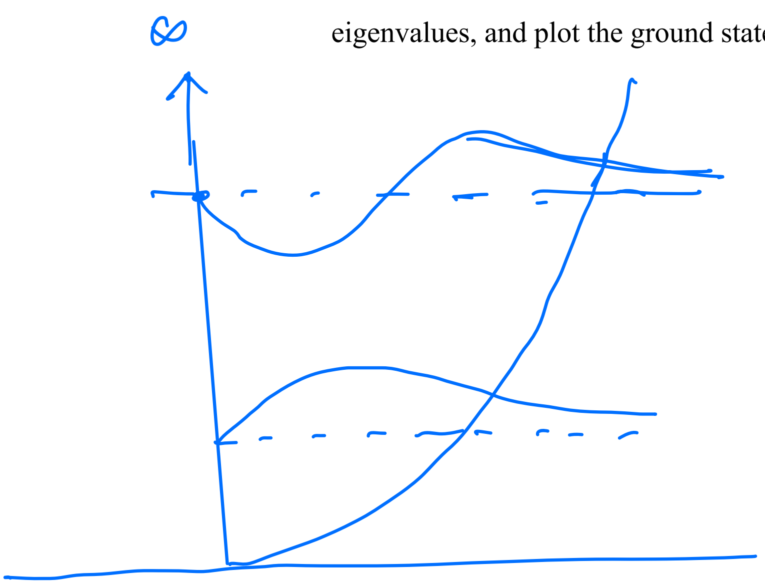
$$\boxed{(\Delta p)^2 = \frac{1}{2}m\hbar\omega(2n+1)}$$

$$\Delta x = \sqrt{\left(n+\frac{1}{2}\right)\frac{\hbar}{m\omega}}$$

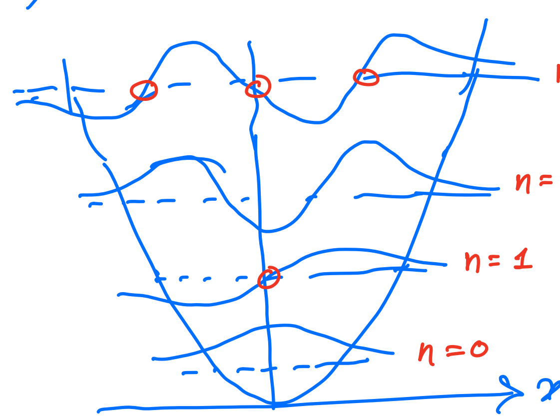
$$\Delta p = \sqrt{\left(n+\frac{1}{2}\right)\hbar\omega m}$$

$$\Rightarrow (\Delta x)(\Delta p) = \left(n+\frac{1}{2}\right)\hbar \Rightarrow \boxed{\frac{7}{2}\hbar} \text{ for } |3\rangle$$

d) Consider a potential given by $V(x) = \begin{cases}\frac{1}{2}m\omega^2x^2, \cancel{|}x\cancel{|} > 0 \\ \infty, \cancel{|}x\cancel{|} \le 0\end{cases}$. Find the spectrum of energy eigenvalues, and plot the ground state and the first excited the state. [2]



Full Symmetric H.O.



All allowed wavefunctions must vanish at $x = 0$

$\psi_{2n+1}(x=0) = 0$

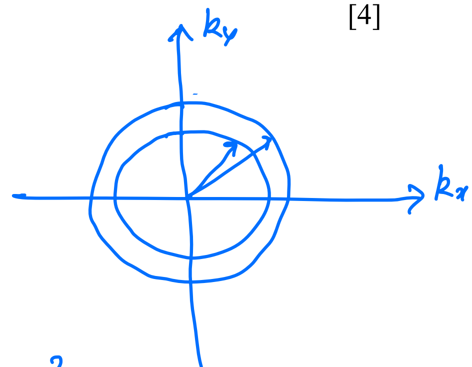
only these are allowed.

$$E_n = \left[(2n+1) + \frac{1}{2}\right]\hbar\omega = \left(2n + \frac{3}{2}\right)\hbar\omega$$

$$n = 0, 1, 2, 3, \ldots\ldots$$

6.

a) Obtain the density of states of a two-dimensional free electron metal under periodic boundary conditions. Use it to find the average energy per electron in terms of E_F, the highest occupied energy in the ground state. [4]



$$dn = 2 \cdot \frac{2\pi k\, dk}{(2\pi)^2} = \frac{k\, dk}{\pi}$$

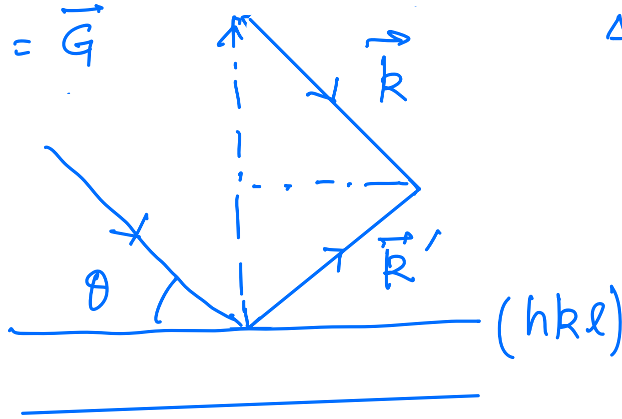
$$E = \frac{\hbar^2 k^2}{2m} \Rightarrow dE = \frac{\hbar}{m} k\, dk$$

$$\frac{dn}{dE} = g_{2D}(E) = \frac{m}{\pi \hbar^2}$$

$$\frac{E_{TOT}}{n} = \frac{\int_0^{E_F} E\, g_{2D}(E)\, dE}{\int_0^{E_F} g_{2D}(E)\, dE} = \frac{\frac{E_F^2}{2}}{E_F} = \frac{E_F}{2}.$$

b) Starting from Laue condition for diffraction, obtain the Bragg condition for diffraction due to elastic scattering in a periodic lattice. [2]

$\Delta\vec{k} = \vec{G}$



$\overline{\Delta\vec{k}}$ $\quad |\vec{k}| = |\vec{k}'|$

$\vec{G}_{hkl} \perp (hkl)$

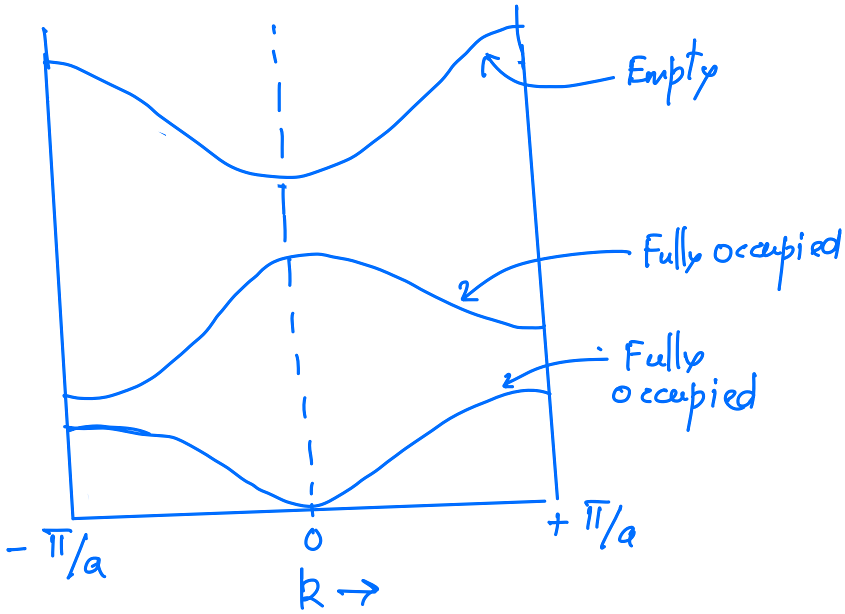
$|\vec{G}_{hkl}| = \frac{2\pi}{d_{hkl}}$.

$$|\vec{G}_{hkl}| = |\Delta\vec{k}| = 2k\sin\theta = \frac{2\pi}{d_{hkl}}$$

$$\Rightarrow 2 \cdot \frac{\cancel{2\pi}}{\lambda} \sin\theta = \frac{\cancel{2\pi}}{d_{hkl}}$$

$$\Rightarrow \boxed{2 d_{hkl} \sin\theta = n\lambda}$$

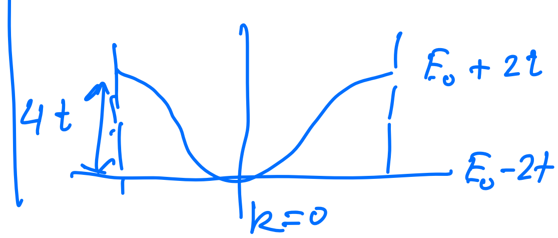
c) For a linear chain of atoms with a lattice constant a, and each contributing 4 loosely bound (nearly free) electrons, sketch a neatly labelled E-k diagram in the first Brillouin zone indicating the occupied bands, and the lowest unoccupied band. [2]



d) An isolated atomic level E_0 spreads into a band due to a periodic potential under tight binding assumptions when assembled as a one-dimensional lattice with lattice constant a. Find the $E(k)$ relationship if the effective mass at the bottom of the band is m^*. [2]

$$E(k) = E_0 - 2t\cos(ka)$$

$$\frac{1}{m^*} = \frac{1}{\hbar^2}\frac{d^2E}{dk^2}$$



$$\frac{d^2E}{dk^2} = 2a^2 t\cos(ka)$$

Bottom of band at $k = 0$.

$$m^* = \frac{\hbar^2}{2a^2 t} \Rightarrow t = \frac{\hbar^2}{2a^2 m^*}$$

$$\boxed{E(k) = E_0 - 2\left(\frac{\hbar^2}{2a^2 m^*}\right)\cos(ka)}$$

$$= \boxed{E_0 - \left(\frac{\hbar^2}{a^2 m^*}\right)\cos(ka)}$$

-----------------------------ROUGH WORK------------------------------

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