

NAME: _____

STUDENT NUMBER: _____

TUTORIAL GROUP: _____

Time: 60 minutes

This is a closed-book exam worth a total of 60 points. Please answer all questions.

ONLY THE FOLLOWING ITEMS ARE ALLOWED ON YOUR DESK DURING THE EXAM:

1. **THIS EXAM BOOK** – It contains this cover page, three question pages and a formula sheet (which may be torn off). Make sure you start by putting your **NAME, ID NUMBER, and TUTORIAL GROUP** on the front (cover) page of the exam. The entire exam book (minus the formula sheet) **will be handed in** at the end of the exam and marked.

a. **FORMULA SHEET**, annotated on the printed page. The formula sheet has to be printed from Quercus.
2. **A CALCULATOR**, which can be anything that does NOT connect to wifi and does NOT communicate with other devices. **ACCEPTABLE** calculators include programmable, graphing and scientific calculators. **UNACCEPTABLE** calculators include: cell phones, tablets and laptops.
3. **A PEN OR PENCIL.**
4. **YOUR STUDENT ID CARD**, used to check your identity.

If you are missing anything from the above items, raise your hand and ask an exam supervisor to supply what is missing. If you are missing an item that should have been brought by you (e.g., calculator, pen/pencil) there is a limited supply of extras and are on a first come, first served basis.

COMPLETE SOLUTION INCLUDES:

- a) A sketch with a coordinate system, where appropriate. Where a diagram is provided, additional markings can be added to it.
- b) Clear and logical workings, including quoting the equations that were used, proper substitutions of numbers (when necessary) with all steps clearly indicated.
- c) The final answer with units and two significant figures.

QUESTION	FOR OFFICE USE ONLY			
	I	II	III	TOTAL
	20	20	20	60

Question I

1. X-ray diffraction is a powerful method to elucidate structure of solids. Because of wave-particle duality, one can also use other particles to carry out diffraction experiments, such as electrons and neutrons. In order to obtain similar diffraction pattern, the wavelengths of these particles should be the same. Consider electron, neutron, and photon, all having the same wavelength of 1 \AA . List these particles in the order of highest to lowest energy. (Hint: You can ignore the rest energy of the electron and neutron and only consider kinetic energy for these particles. You can also assume that the mass of a neutron is the same as the proton mass. $1 \text{ \AA} = 10^{-10} \text{ m}$) [10 points]

For particles like electrons and neutrons,

de Broglie wave length is $\lambda = \frac{h}{p}$, where p is the momentum and can be determined from the kinetic energy $E = \frac{p^2}{2m}$.

$$\therefore E = \left(\frac{h}{\lambda}\right)^2 \frac{1}{2m}$$

Photon energy and wavelength is related by $E = hf = \frac{hc}{\lambda}$

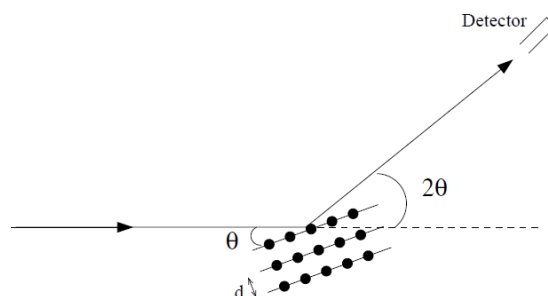
$$E_e = \left(\frac{6.626 \times 10^{-34}}{10^{-10}}\right)^2 \frac{1}{2 \cdot 9.1 \times 10^{-31}} = 2.4 \times 10^{-17} \text{ (J)}$$

$$E_n = \left(\frac{6.626 \times 10^{-34}}{10^{-10}}\right)^2 \frac{1}{2 \cdot 9.1 \times 10^{-31} \cdot 1836} = \frac{2.4 \times 10^{-17}}{1836} = 1.3 \times 10^{-20} \text{ (J)}$$

$$E_{ph} = \frac{6.626 \times 10^{-34} \cdot 3.0 \times 10^8}{10^{-10}} = 2.0 \times 10^{-15} \text{ (J)}$$

Therefore $E_{ph} > E_e > E_n$

2. The spacing of the Bragg planes in a NaCl crystal is $d = 2.82 \text{ \AA}$. Consider a neutron diffraction experiment using the neutron with the wavelength 1 \AA . Schematic diagram of Bragg diffraction is shown in the figure below. At what angle (shown as 2θ in the figure) should we put the detector in order to observe the first-order diffraction maximum? [10 points]



Use Bragg's law $n\lambda = 2d \sin \theta$ with $n=1$, $d=2.82$, $\lambda=1$

$$\text{Then } \theta = \sin^{-1}\left(\frac{1}{2 \cdot 2.82}\right) = 10.2^\circ$$

$$\therefore \underline{2\theta = 20.4^\circ}$$

Question II

1. At time $t = 0$ an electron is represented by the wave function

$$\Psi(x, 0) = \begin{cases} A\frac{x}{a} & 0 \leq x \leq \frac{a}{2}, \\ A(1 - \frac{x}{a}) & \frac{a}{2} \leq x \leq a, \\ 0 & \text{elsewhere,} \end{cases}$$

where $a = 1.0$ nm and A is a constant to be determined.

- (a) Normalize Ψ (that is, find A , in terms of a). *Hint: Integration will be necessary. However, the integration becomes simpler if you use the symmetry of the wavefunction.* [5 points]

The normalization condition is $\int_{-\infty}^{\infty} |\Psi(x, 0)|^2 dx = 1$

The integrand is non-zero for $0 \leq x \leq a$.

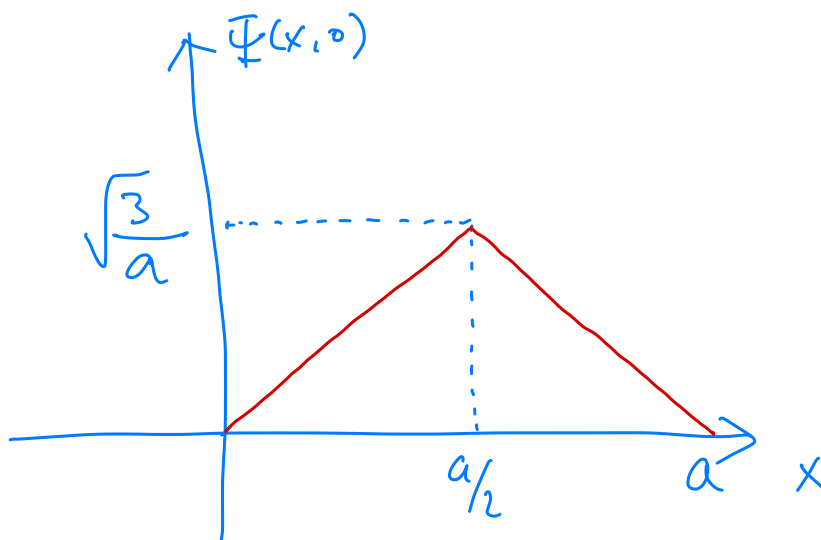
First, for $0 \leq x \leq \frac{a}{2}$

$$\frac{A^2}{a^2} \int_0^{a/2} x^2 dx = \frac{A^2}{a^2} \left[\frac{1}{3} x^3 \right]_0^{a/2} = \frac{A^2}{a^2} \frac{1}{3} \left(\frac{a}{2} \right)^3 = \frac{A^2 a}{24}$$

The integral for $\frac{a}{2} \leq x \leq a$ will be also the same as above, since the wave function is symmetric (See sketch below).

$$\therefore \frac{A^2 a}{24} \times 2 = 1 \quad A = \sqrt{\frac{12}{a}} = 2 \sqrt{\frac{3}{a}}$$

- (b) Sketch $\Psi(x, 0)$, as a function of x . Clearly label the graph including the x-intercept and the maximum value of $\Psi(x, 0)$. [5 points]



Question II continued on the next page.

Question II Continued.

- (c) What is the probability of finding the electron between $x = 0.0$ nm and $x = 0.5$ nm? [5 points]

Note $x = 0$ nm $\rightarrow x = 0$
 $x = 0.5$ nm $\rightarrow x = \frac{a}{2}$

We will use the probability density $|\Psi(x,0)|^2$.
 Then the probability to find the electron between $x=0$ and $a/2$ is $P = \int_0^{a/2} |\Psi(x,0)|^2 dx$

This is exactly the integral we did in part (a).

$$\therefore P = \frac{A^2 a}{24} = \frac{12}{a} \cdot \frac{a}{24} = \frac{1}{2}$$

We could have obtained this by recognizing that $x=0.5$ nm is exactly the midpoint of the wavefunction.

- (d) Let's assume that the above wave function represents a wave packet for the electron matter wave at $t = 0$. Using the uncertainty relation, we can estimate the minimum uncertainty, $(\Delta p)_{\min}$, of the electron's momentum. Compare this to the momentum (p) of the matter wave with $\lambda = 1$ nm and find the ratio $(\Delta p)_{\min}/p$. [5 points]

Uncertainty relation: $(\Delta x)(\Delta p) \geq \frac{\hbar}{2}$

Δx can be estimated in several ways, but we will just take a . Then $\Delta p \geq \frac{\hbar}{2a}$.

Using $\lambda = \frac{h}{p}$, $p = \frac{h}{\lambda}$.

$$\begin{aligned} \text{Therefore } \frac{(\Delta p)_{\min}}{p} &= \frac{\frac{\hbar}{2a}}{\frac{h}{\lambda}} = \frac{\cancel{\hbar}}{4\pi a} \cdot \frac{\lambda}{\cancel{h}} \\ &= \frac{10^{-9}}{4\pi \cdot 10^9} = \frac{1}{4\pi} \text{ (or } 0.08) \end{aligned}$$

Question III

1. A particle of mass m , which moves freely inside an infinite potential well of length a , has the following initial wave function at $t = 0$:

$$\Psi(x, 0) = \sqrt{\frac{7}{5a}} \sin\left(\frac{\pi x}{a}\right) + \sqrt{\frac{2}{5a}} \sin\left(\frac{3\pi x}{a}\right) + \frac{1}{\sqrt{5a}} \sin\left(\frac{5\pi x}{a}\right).$$

- (a) What is the expectation value of the energy? Express your answer using \hbar , m , and a . [10 points]

First we can use the energy eigenstate of the infinite square well $\psi_n = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right)$ to rewrite the above wave function

$$\Psi(x, 0) = \sqrt{\frac{7}{10}} \psi_1(x) + \sqrt{\frac{2}{10}} \psi_3(x) + \sqrt{\frac{1}{10}} \psi_5(x)$$

In other words, $c_1 = \sqrt{\frac{7}{10}}$, $c_3 = \sqrt{\frac{2}{10}}$, $c_5 = \sqrt{\frac{1}{10}}$, $c_n = 0$ for all other n 's.

Then the expectation value

$$\langle \hat{H} \rangle = \sum_{n=1}^{\infty} |c_n|^2 E_n = \frac{7}{10} E_1 + \frac{2}{10} E_3 + \frac{1}{10} E_5$$

$$= \frac{\hbar^2 \pi^2}{2ma^2} \left(\frac{7}{10} + \frac{2}{10} \cdot 9 + \frac{1}{10} \cdot 25 \right) = \frac{\hbar^2 \pi^2}{2ma^2} \left(\frac{50}{10} \right) = \frac{5\hbar^2 \pi^2}{2ma^2}$$

- (b) Find the wave function $\Psi(x, t)$ at later time t . [5 points]

$$\begin{aligned} \Psi(x, t) = & \sqrt{\frac{7}{5a}} \sin\left(\frac{\pi x}{a}\right) e^{-i \frac{\hbar^2 \pi^2}{2ma^2} t} + \sqrt{\frac{2}{5a}} \sin\left(\frac{3\pi x}{a}\right) e^{-i \frac{9\hbar^2 \pi^2}{2ma^2} t} \\ & + \sqrt{\frac{1}{5a}} \sin\left(\frac{5\pi x}{a}\right) e^{-i \frac{25\hbar^2 \pi^2}{2ma^2} t} \end{aligned}$$

- (c) What is the probability of finding the system at a time t in the following state? [5 points]

$$\sqrt{\frac{2}{a}} \sin\left(\frac{2\pi x}{a}\right) e^{-i \frac{2\hbar^2 \pi^2}{ma^2} t}$$

This is a wave function describing $n=2$ state. Since $c_2 = 0$, the probability to find the system in $n=2$ is $|c_2|^2 = 0$.

Useful constants:

$$h = 6.626 \times 10^{-34} \text{ Js} = 4.14 \times 10^{-15} \text{ eV} \cdot \text{s} \text{ (Planck constant)}$$

$$c = 3 \times 10^8 \text{ m/s} \text{ (speed of light)}$$

$$e = 1.602 \times 10^{-19} \text{ C} \text{ (electron charge)}$$

$$m_e = 9.1 \times 10^{-31} \text{ kg} \text{ (electron mass)}$$

$$M_p/m_e = 1836 \text{ (Proton mass/ electron mass)}$$

$$k = 8.99 \times 10^9 \text{ Nm}^2/\text{C}^2 \text{ (Coulomb constant)}$$

$$k_B = 1.38 \times 10^{-23} \text{ J/K} = 8.6 \times 10^{-5} \text{ eV/K} \text{ (Boltzmann constant)}$$

$$N_A = 6.02 \times 10^{23} \text{ (Avogadro number)}$$

$$R_H = 1.096776 \times 10^7 \text{ m}^{-1} \text{ (Rydberg constant)}$$

Quantum Mechanics:

$$\rho(\lambda, T) = \frac{8\pi hc}{\lambda^5} \frac{1}{e^{hc/\lambda kT} - 1}$$

$$E_{ph.el.} = hf - \phi$$

$$E = hf = \hbar\omega$$

$$\Delta\lambda = \frac{h}{mc}(1 - \cos\theta) \text{ (Compton)}$$

$$\lambda_C = \frac{h}{mc} = 2.4263 \times 10^{-12} \text{ m}$$

$$\frac{1}{\lambda} = R_H \left(\frac{1}{n^2} - \frac{1}{m^2} \right)$$

$$n\lambda = 2d \sin\theta \text{ (Bragg's law)}$$

$$F_{cent} = \frac{mv^2}{r}$$

$$r_n = \frac{(n\hbar)^2}{kme^2}$$

$$r_1 = 0.053 \text{ nm} \text{ (Bohr radius)}$$

$$E_n = -\frac{m(ke^2)^2}{2\hbar^2} \frac{1}{n^2}$$

$$\lambda = \frac{h}{p}$$

$$\Delta x \Delta p \leq \frac{\hbar}{2}$$

$$\Delta E \Delta t \leq \frac{\hbar}{2}$$

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} = i\hbar \frac{\partial \Psi}{\partial t}$$

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x)$$

$$\hat{H}\psi(x) = E\psi(x)$$

$$\langle \hat{O} \rangle = \int \Psi(x, t)^* \hat{O} \Psi(x, t) dx$$

$$\langle x \rangle = \sum x P(x) \text{ (discrete)}$$

$$\langle x \rangle = \int x P(x) dx \text{ (continuous)}$$

$$\hat{p} = -i\hbar \frac{\partial}{\partial x}$$

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a}$$

$$E_n = \frac{\hbar^2 \pi^2}{2ma^2} n^2$$

$$\Psi(x, t) = \sum_{n=1}^{\infty} c_n \psi_n(x) e^{-iE_n t/\hbar}$$

$$c_n = \int \psi_n^*(x) \Psi(x, t) dx$$

$$\langle \hat{H} \rangle = \sum_{n=1}^{\infty} |c_n|^2 E_n$$

$$\Psi(x, 0) = \frac{1}{\sqrt{2\pi}} \int \phi(k) e^{ikx} dx$$

$$\phi(k) = \frac{1}{\sqrt{2\pi}} \int \Psi(x, 0) e^{-ikx} dx$$

Math formulae:

$$c = a + ib$$

$$c^* = a - ib$$

$$\sin x = \frac{e^{+ix} - e^{-ix}}{2i}$$

$$\cos x = \frac{|c|^2 = c^* c = a^2 + b^2}{e^{+ix} + e^{-ix}} \frac{1}{2}$$

$$e^{i\theta} = \cos\theta + i\sin\theta$$

$$\int_{-\infty}^{\infty} e^{-\alpha^2 x^2} dx = \frac{\sqrt{\pi}}{\alpha}$$

Special relativity: To be added