Problem 1

The Bragg Condition exists when the electrons are diffracted off the crystal plane and interfere with other incident electron beams. As shown in Figure 1, the simplest case is when two beams are incident on the crystal structure with interatomic spacing d and one beam is diffracted off the top layer of atoms while the second is diffracted off an adjacent layer.

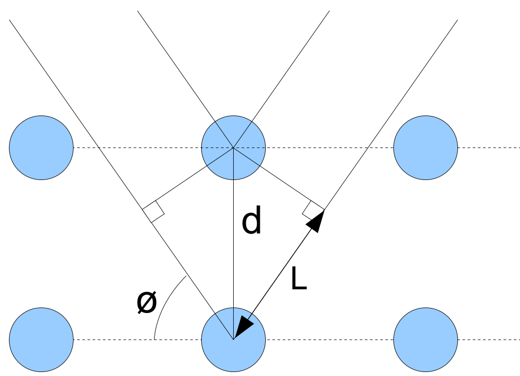

Figure 1: Electron interference from a crystal structure.

Constructive interference occurs when the additional path length of the second beam is an integer multiple of the wavelength, λ. The additional path length is $2L$, so constructive interference occurs when:

$$2L = n\lambda \qquad n = 1, 2, 3... \tag{1}$$

The path length L can be written in terms of the angle of incidence:

$$\cos\left(\frac{\pi}{2} - \theta\right) = \frac{L}{d}$$
$$\sin(\theta) = \frac{L}{d}$$
$$d\sin(\theta) = L$$

Introducing L from Equation 1 into the above expression, we have the Bragg Condition:

$$\boxed{2d\sin(\theta) = n\lambda \qquad n = 1, 2, 3...}$$

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Problem 2

Two slit diffraction experiments do not result in patterns of uniform intensity due to the wave nature of particles and photons. With two slits that have a finite size a and spacing b, waves incident on the two slits will interfere with each other as they emerge from the slits and propagate. Under Fraunhofer conditions, this interference results in intensity maxima and minima that correspond to the single slit diffraction envelope multiplied by an interference pattern. See Figure 2 for an example.

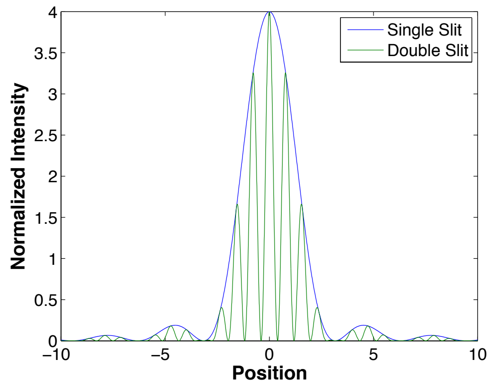

Figure 2: Single slit and double slit intensity pattern for λ = 632 nm and a 100μm slit width. Slit spacing is 400μm in the double slit plot.

Bonus For N slits, the pattern will resemble a diffraction grating with evenly spaced "modes" that have a sharper intensity distribution as N increases. The intensity of the principal diffraction mode is $N^2 I_o$ and there are $N-2$ smaller peaks between the main modes of the grating. These properties stem from the diffraction grating equation:

$$I(\theta) = I_o \left[\frac{\sin^2(\beta)}{\beta^2} \right] \left[\frac{\sin^2(N\gamma)}{\sin^2(\gamma)} \right] \tag{2}$$

where

$$\beta = \frac{\pi a \sin(\theta)}{\lambda}$$
$$\gamma = \frac{\pi b \sin(\theta)}{\lambda}$$

Plotting Equation 2 for $N = 6$ and $N = 10$ illustrates the intensity distribution for N slits. This is shown in Figure 3.

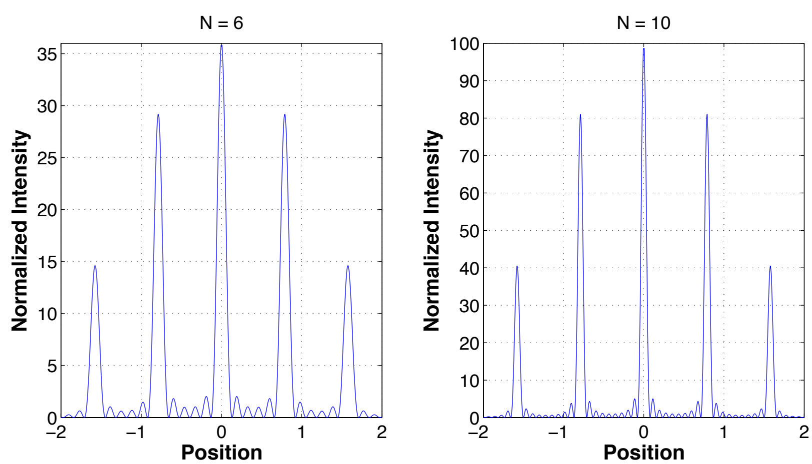

Figure 3: Intensity pattern for N = 6 and 10 slits with λ = 632 nm and a 100μm slit width. Slit spacing is 400μm.

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Problem 3

The Heisenberg uncertainty principle for momentum (p) and position (x) is the following:

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

With $\Delta x = \frac{R}{2}$ and $\Delta p = p$, we can find an expression for p in terms of R:

$$\begin{aligned} \Delta x \Delta p = \frac{Rp}{2} &\geq \frac{\hbar}{2} \\ p &\geq \frac{\hbar}{R} \end{aligned}$$

In order to find minimum momentum for any atomic size R, we set momentum to be the lower bound of the inequality

$$p = \frac{\hbar}{R} \tag{3}$$

Total energy can be written as the sum of kinetic and potential energy, and potential energy is provided in the problem. Total energy is then:

$$\begin{aligned} E_{total} &= KE + PE \\ &= \frac{p^2}{2m} - \frac{e^2}{4\pi\epsilon R} \end{aligned}$$

Substituting in p from Equation 3 and differentiating with respect to R

$$\begin{aligned} E_{total} &= \frac{\hbar^2}{2mR^2} - \frac{e^2}{4\pi\epsilon R} \\ \frac{dE_{total}}{dR} &= \frac{1}{dR}\left(\frac{\hbar^2}{2mR^2} - \frac{e^2}{4\pi\epsilon R}\right) \\ &= -\frac{\hbar^2}{mR^3} + \frac{e^2}{4\pi\epsilon R^2} \end{aligned}$$

Letting $\frac{dE_{total}}{dR} = 0$ and solving for R produces a size that results in minimal total energy.

$$\begin{aligned} 0 &= \frac{1}{R^2}\left(-\frac{\hbar^2}{mR} + \frac{e^2}{4\pi\epsilon}\right) \\ \frac{\hbar^2}{mR} &= \frac{e^2}{4\pi\epsilon} \end{aligned}$$

$$\boxed{R = \frac{4\pi\epsilon\hbar^2}{me^2}}$$

This value for R is commonly known as the Bohr radius.

Bonus As shown above, the uncertainty principle governs the stability and stable size of an atom. This can be understood by taking into account the implications of the classical atomic model and minimization of energy. In the classical model, electrons continuously lose energy and spiral towards the nucleus as they orbit. According to the uncertainty principle, localizing the electron near the nucleus ($\Delta x \approx 0$) requires that $\Delta p \to \infty$. It is very unlikely that an electron would still be bound to an atom with that large of a momentum, so there exists a balance between Δx and Δp which results in atomic stability. ■

Problem 4

The argument for $\psi(x)$ and $\frac{d\psi(x)}{dx}$ being continuous and finite can be made by understanding the meaning of expectation values, such as momentum and position.

$\psi(x)$ and $\frac{d\psi(x)}{dx}$ are finite: We know that the expectation value for momentum can be written as:

$$\bar{p} = -i\hbar \int_{-\infty}^{\infty} \Psi^*(x,t) \frac{\partial \Psi(x,t)}{\partial x} dx$$

Since momentum, a measurable quantity, is expected to be finite, $\frac{\partial \Psi(x,t)}{\partial x}$ should be finite as well. Expectation for position results in the requirement that $\Psi(x,t)$ is finite as well. The finite properties of the $\frac{\partial \Psi(x,t)}{\partial x}$ and $\Psi(x,t)$ will also be true for the time-independent eigenfunction, $\psi(x)$.

$\psi(x)$ is continuous: If $\frac{d\psi(x)}{dx}$ is finite, then $\psi(x)$ must be continuous. This property is inherent to the derivative of a function.

$\frac{d\psi(x)}{dx}$ is continuous: This property can be explain by investigating the Schröedinger wave equation. From the wave equation:

$$\frac{d^2\psi(x)}{dx^2} = \frac{2m}{\hbar^2} \left[V(x) - E \right] \psi(x)$$

having a finite $V(x)$, E, and $\psi(x)$ implies that $\frac{d^2\psi(x)}{dx^2}$ is also finite. For $\frac{d^2\psi(x)}{dx^2}$ to be finite, $\frac{d\psi(x)}{dx}$ must be continuous by the same argument stated before. ■