Marking Scheme: Diffraction of X-rays by Structured and Evolving Targets

General marking instructions

- A global phase factor multiplying a complex amplitude is not penalized, because it does not change intensity.
- In Part A, an overall sign change in a path or phase difference is acceptable only if the subtraction convention is stated or used consistently.
- In Part B, I_0 is the single-electron time-averaged intensity. Expressions using f_0^2 may receive full credit only if the identification $I_0 = f_0^2$ is explicit or clear from context.

Part A: Diffraction from two electrons treated as point particles [2.0 points]

A.1 [0.6 points]

Target result:

$$\Delta L_{\text{out}} = |\mathbf{P} - \mathbf{r}_1| - |\mathbf{P} - \mathbf{r}_2| \simeq \mathbf{r} \cdot \frac{\mathbf{k}_f}{k_f}.$$

Award marks only for the following identifiable equations or equivalent expressions:

(a) States the reference distance

$$|\mathbf{P} - \mathbf{r}_1| = |\mathbf{R}| = R.$$

[0.10 pt]

(b) Rewrites the second path length using the separation vector

$$|\mathbf{P} - \mathbf{r}_2| = |\mathbf{R} - (\mathbf{r}_2 - \mathbf{r}_1)| = |\mathbf{R} - \mathbf{r}|.$$

[0.10 pt]

(c) Uses the first-order far-field expansion

$$|\mathbf{R} - \mathbf{r}| \simeq R - \hat{\mathbf{s}}_f \cdot \mathbf{r} \quad \text{with} \quad \hat{\mathbf{s}}_f = \frac{\mathbf{R}}{R}.$$

[0.20 pt]

(d) Identifies the far-field detector direction with the outgoing wavevector direction

$$\hat{\mathbf{s}}_f \simeq \frac{\mathbf{k}_f}{k_f}.$$

[0.10 pt]

(e) Obtains the final path difference

$$\Delta L_{\text{out}} \simeq \hat{\mathbf{s}}_f \cdot \mathbf{r} = \mathbf{r} \cdot \frac{\mathbf{k}_f}{k_f}.$$

[0.10 pt]

If the student defines the path difference in the reverse order and obtains $-\mathbf{r} \cdot \mathbf{k}_f / k_f$, award full credit if the convention is stated or used consistently.

A.2 [0.4 points]

Target result:

$$\Delta\phi = \mathbf{q} \cdot \mathbf{r}.$$

Award marks only for the following identifiable equations or equivalent expressions:

(a) Writes the incident-wave phase difference in the chosen convention, for example

$$\Delta\phi_{\text{in}} = \mathbf{k}_i \cdot \mathbf{r}_1 - \mathbf{k}_i \cdot \mathbf{r}_2 = -\mathbf{k}_i \cdot \mathbf{r}.$$

[0.10 pt]

(b) Writes the outgoing propagation phase contribution using A.1,

$$\Delta\phi_{\text{out}} = k\Delta L_{\text{out}} = k\,\mathbf{r} \cdot \frac{\mathbf{k}_f}{k_f} = \mathbf{k}_f \cdot \mathbf{r}.$$

[0.10 pt]

(c) Combines the two phase contributions as

$$\Delta\phi = \Delta\phi_{\text{in}} + \Delta\phi_{\text{out}} = (-\mathbf{k}_i + \mathbf{k}_f) \cdot \mathbf{r}.$$

[0.10 pt]

(d) Uses $\mathbf{q} = \mathbf{k}_f - \mathbf{k}_i$ to obtain

$$\Delta\phi = (\mathbf{k}_f - \mathbf{k}_i) \cdot \mathbf{r} = \mathbf{q} \cdot \mathbf{r}.$$

[0.10 pt]

Accept $-\mathbf{q} \cdot \mathbf{r}$ for full credit only if the student has explicitly adopted the opposite phase-difference convention.

A.3 [0.6 points]

Target result, up to a global phase:

$$\widetilde{A}_{\text{tot}} = f_0 \left(1 + e^{i\mathbf{qr}}\right).$$

Award marks only for the following identifiable equations or equivalent expressions:

(a) Writes a valid single-electron amplitude, e.g.

$$\widetilde{A}_n = f_0 e^{-i\mathbf{q}\cdot\mathbf{r}_n} \quad \text{or} \quad \widetilde{A}_n = f_0 e^{+i\mathbf{q}\cdot\mathbf{r}_n}$$

with a consistent sign convention. [0.20 pt]

(b) Sums the two electron contributions, e.g.

$$\widetilde{A}_{\text{tot}} = f_0 e^{-i\mathbf{q}\cdot\mathbf{r}_1} + f_0 e^{-i\mathbf{q}\cdot\mathbf{r}_2}.$$

[0.20 pt]

(c) Factors out a common phase and expresses the relative phase using $\mathbf{r} = \mathbf{r}_2 - \mathbf{r}_1$, e.g.

$$\widetilde{A}_{\text{tot}} = f_0 e^{-i\mathbf{q}\cdot\mathbf{r}_2}\left(1 + e^{i\mathbf{q}\cdot(\mathbf{r}_2-\mathbf{r}_1)}\right) = f_0 e^{-i\mathbf{q}\cdot\mathbf{r}_2}\left(1 + e^{i\mathbf{q}\mathbf{r}}\right).$$

[0.10 pt]

(d) Gives a final equivalent form after dropping the global phase, for example

$$\widetilde{A}_{\text{tot}} = f_0(1 + e^{i\mathbf{q}\mathbf{r}}) \quad \text{or} \quad \widetilde{A}_{\text{tot}} = 2f_0 e^{i\mathbf{q}\mathbf{r}/2}\cos\left(\frac{\mathbf{q}\cdot\mathbf{r}}{2}\right).$$

[0.10 pt]

The complex conjugate form $f_0(1 + e^{-i\mathbf{q}\mathbf{r}})$ receives full credit because it gives the same intensity.

A.4 [0.4 points]

Target result:

$$I(\mathbf{q},\mathbf{r}) = 2f_0^2[1 + \cos(\mathbf{q}\cdot\mathbf{r})] = 4f_0^2\cos^2\left(\frac{\mathbf{q}\cdot\mathbf{r}}{2}\right).$$

Award marks only for the following identifiable equations or equivalent expressions:

(a) Uses the intensity definition

$$I = |\widetilde{A}_{\text{tot}}|^2 = f_0^2|1 + e^{i\mathbf{q}\mathbf{r}}|^2.$$

[0.10 pt]

(b) Evaluates the modulus squared correctly,

$$|1 + e^{ix}|^2 = (1 + e^{ix})(1 + e^{-ix}) = 2 + 2\cos x.$$

[0.20 pt]

(c) Gives one of the final forms

$$I = 2f_0^2[1 + \cos(\mathbf{q}\cdot\mathbf{r})] \quad \text{or} \quad I = 4f_0^2\cos^2(\mathbf{q}\cdot\mathbf{r}/2).$$

[0.10 pt]

Part B: Finite longitudinal coherence (phase-jump model) [2.3 points]

Target result:

$$\langle I(\mathbf{q},\mathbf{r},\lambda_0,L_0)\rangle_t = 2I_0\left[1 + \mu(\mathbf{q},\mathbf{r};L_0)\cos(\mathbf{q}\cdot\mathbf{r})\right],$$

where

$$\mu(\mathbf{q},\mathbf{r};L_0) = \begin{cases} 1 - \dfrac{\lambda_0}{2\pi L_0}|\mathbf{q}\cdot\mathbf{r}|, & |\mathbf{q}\cdot\mathbf{r}| \le \dfrac{2\pi L_0}{\lambda_0}, \\ 0, & |\mathbf{q}\cdot\mathbf{r}| > \dfrac{2\pi L_0}{\lambda_0}. \end{cases}$$

Equivalently,

$$\langle I\rangle_t = \begin{cases} 2I_0\left[1 + \left(1 - \dfrac{\lambda_0}{2\pi L_0}|\mathbf{q}\cdot\mathbf{r}|\right)\cos(\mathbf{q}\cdot\mathbf{r})\right], & |\mathbf{q}\cdot\mathbf{r}| \le \dfrac{2\pi L_0}{\lambda_0}, \\ 2I_0, & |\mathbf{q}\cdot\mathbf{r}| > \dfrac{2\pi L_0}{\lambda_0}. \end{cases}$$

Award marks only for the following identifiable equations or equivalent expressions:

(a) Sets up the two-field total field and time average:

$$E(t) = E_1(t) + E_2(t), \qquad \langle I \rangle_t = \langle |E_1(t) + E_2(t)|^2 \rangle_t.$$

[0.20 pt]

(b) Expands the intensity and identifies the interference term:

$$|E_1 + E_2|^2 = |E_1|^2 + |E_2|^2 + 2\Re(E_1 E_2^*),$$

$$\langle I \rangle_t = 2I_0 + 2\Re\langle E_1 E_2^* \rangle_t.$$

[0.30 pt]

(c) Writes the interference term as a phase average:

$$\langle E_1 E_2^* \rangle_t = E_0^2 \left\langle e^{i[\phi_1(t) - \phi_2(t)]} \right\rangle_t.$$

[0.25 pt]

(d) Separates deterministic and random phases and identifies the deterministic part:

$$\phi_1(t) - \phi_2(t) = \Delta\phi + \delta\phi(t), \qquad \Delta\phi = \mathbf{q} \cdot \mathbf{r}.$$

[0.30 pt]

(e) Defines the coherence factor explicitly as

$$\mu(\Delta t) = \left\langle e^{i\delta\phi(t)} \right\rangle_t, \qquad \langle E_1 E_2^* \rangle_t = E_0^2 \mu(\Delta t) e^{i\Delta\phi}.$$

[0.20 pt]

(f) Writes the same-interval probability for the phase-jump model:

$$P_{\text{same}}(\Delta t) = \begin{cases} 1 - |\Delta t|/t_0, & |\Delta t| < t_0, \\ 0, & |\Delta t| \geq t_0. \end{cases}$$

where

$$P_{\text{same}}(\Delta t) \equiv \Pr\{t \text{ and } t + \Delta t \text{ lie in the same interval of length } t_0\}.$$

[0.35 pt]

(g) Shows the averaging rule for the random phase:

$$e^{i\delta\phi} = 1 \quad \text{for same interval,} \qquad \left\langle e^{i\delta\phi} \right\rangle = 0 \quad \text{for different intervals,}$$

and hence

$$\mu(\Delta t) = P_{\text{same}}(\Delta t).$$

[0.25 pt]

(h) Relates time delay to path/phase difference:

$$\Delta\phi = \frac{2\pi}{\lambda_0} \Delta\ell = \mathbf{q} \cdot \mathbf{r}, \qquad |\Delta t| = \frac{|\Delta\ell|}{c} = \frac{\lambda_0}{2\pi c} |\mathbf{q} \cdot \mathbf{r}|, \qquad t_0 = \frac{L_0}{c}.$$

[0.20 pt]

(i) Gives the correct final intensity formula including the no-interference limit:

$$\langle I \rangle_t = 2I_0[1 + \mu \cos(\mathbf{q} \cdot \mathbf{r})],$$

with

$$\mu = 1 - \frac{\lambda_0}{2\pi L_0} |\mathbf{q} \cdot \mathbf{r}| \quad \text{inside the coherence window,} \qquad \langle I \rangle_t = 2I_0 \quad \text{outside it.}$$

[0.25 pt]

The random phase $\phi(t)$ represents the source phase carried by the incident wave. Therefore, at position $\mathbf{r}$, it should be understood as being evaluated at the retarded time $t - \hat{\mathbf{s}}_i \cdot \mathbf{r}/c$, where $\hat{\mathbf{s}}_i = \mathbf{k}_i/k$. Consequently, the two scattered contributions sample the random source phase at times separated by the total effective path delay corresponding to the full scattering phase difference $\Delta\phi = \mathbf{q} \cdot \mathbf{r}$, not only by the outgoing path difference.

Part C: Non-point-particle effect [1.0 point]

C.1 [0.4 points]

Target result:

$$Q_0 = \rho_0 \pi^{3/2} R_0^3, \qquad \rho_0 = \frac{Q_0}{\pi^{3/2} R_0^3}.$$

Award marks only for the following identifiable equations or equivalent expressions:

(a) States or uses the total-charge equality for the extended distribution:

$$Q_0 = \int \rho_2(\mathbf{r})\, d^3\mathbf{r}.$$

[0.10 pt]

(b) Writes the Gaussian total-charge integral in spherical coordinates:

$$\int \rho_2(\mathbf{r})\, d^3\mathbf{r} = \rho_0 \int_0^\infty e^{-r^2/R_0^2} 4\pi r^2\, dr.$$

[0.10 pt]

(c) Uses the given radial Gaussian integral to obtain

$$\int \rho_2(\mathbf{r})\, d^3\mathbf{r} = \rho_0 \pi^{3/2} R_0^3.$$

[0.10 pt]

(d) Gives the normalization relation

$$Q_0 = \rho_0 \pi^{3/2} R_0^3 \quad \text{or} \quad \rho_0 = \frac{Q_0}{\pi^{3/2} R_0^3}.$$

[0.10 pt]

C.2 [0.4 points]

Target results:

$$A_2(\mathbf{q}) = Q_0 \exp\left(-\frac{q^2 R_0^2}{4}\right), \qquad \frac{A_2(\mathbf{q})}{A_1(\mathbf{q})} = \exp\left(-\frac{q^2 R_0^2}{4}\right),$$

where the problem gives the point-charge amplitude $A_1(\mathbf{q}) = Q_0$. Award marks only for the following identifiable equations or equivalent expressions:

(a) Sets up the Gaussian amplitude integral and applies the supplied Fourier-transform identity with $\alpha = 1/R_0^2$ and $k = q$:

$$A_2(\mathbf{q}) = \rho_0 \int_{\mathbb{R}^3} e^{-r^2/R_0^2} e^{i\mathbf{q}\cdot\mathbf{r}}\, d^3\mathbf{r}.$$

[0.10 pt]

(b) Obtains the Gaussian Fourier-transform factor:

$$\int_{\mathbb{R}^3} e^{-r^2/R_0^2} e^{i\mathbf{q}\cdot\mathbf{r}}\, d^3\mathbf{r} = \pi^{3/2} R_0^3 \exp\left(-\frac{q^2 R_0^2}{4}\right).$$

[0.12 pt]

(c) Uses the C.1 normalization $\rho_0 \pi^{3/2} R_0^3 = Q_0$ to obtain

$$A_2(\mathbf{q}) = Q_0 \exp\left(-\frac{q^2 R_0^2}{4}\right).$$

[0.13 pt]

(d) Compares with the point-charge amplitude $A_1(\mathbf{q}) = Q_0$, for example by writing

$$\frac{A_2(\mathbf{q})}{A_1(\mathbf{q})} = \exp\left(-\frac{q^2 R_0^2}{4}\right),$$

or by stating that the extended-charge amplitude is reduced at nonzero q while matching the point-charge amplitude at $q = 0$. [0.05 pt]

If the student derives or states $A_1(\mathbf{q}) = Q_0$ again, do not penalize; however, no separate credit is required for deriving A_1, because it is given in the problem statement.

C.3 [0.2 points]

Target result:

$$\frac{I_2}{I_1} = e^{-2} \simeq 0.14.$$

Award marks only for the following identifiable equations or equivalent expressions:

(a) Squares the amplitudes and obtains

$$\frac{I_2}{I_1} = \left|\frac{A_2}{A_1}\right|^2 = \exp\left(-\frac{q^2 R_0^2}{2}\right).$$

[0.10 pt]

(b) Substitutes $q = 2/R_0$ and obtains

$$\frac{I_2}{I_1} = \exp\left[-\frac{(2/R_0)^2 R_0^2}{2}\right] = e^{-2} \simeq 0.14.$$

[0.10 pt]

If the student gives the amplitude ratio e^{-1} instead of the intensity ratio, award **0.10**.

Part D: Diffraction from a film with non-flat surface morphology [2.4 points]

Target results:

$$\frac{I(q_z = \pi/2d, \sigma = 0.4, \bar{N} = 5)}{I(q_z = \pi/2d, \sigma = 0, \bar{N} = 5)} = \frac{1 + e^{-\pi^2/25}}{2} \simeq 0.84,$$

$$\frac{I(q_z = 2\pi/d, \sigma = 0.4, \bar{N} = 5)}{I(q_z = 2\pi/d, \sigma = 0, \bar{N} = 5)} = 1.$$

Award marks only for the following identifiable equations or equivalent expressions:

(a) Writes the column amplitude as a geometric sum and closed form:

$$A_N(q_z) = \sum_{n=0}^{N-1} e^{iq_z nd} = \frac{1 - e^{iq_z Nd}}{1 - e^{iq_z d}}.$$

[0.25 pt]

(b) Uses the coherent average, not the incoherent average:

$$\langle A(q_z)\rangle = \int P(N) A_N(q_z)\, dN, \qquad I(q_z) = |\langle A(q_z)\rangle|^2.$$

[0.25 pt]

(c) Substitutes the closed form into the coherent average:

$$\langle A(q_z)\rangle = \frac{1 - \langle e^{iq_z Nd}\rangle}{1 - e^{iq_z d}}.$$

[0.20 pt]

(d) Decomposes the scattering vector near a Bragg point:

$$q_z = Q_z + \Delta q_z, \qquad Q_z = \frac{2\pi m}{d},$$

and, for integer N, uses

$$e^{iQ_z Nd} = e^{i2\pi mN} = 1,$$

so that

$$\langle e^{iq_z Nd}\rangle = \langle e^{i\Delta q_z Nd}\rangle.$$

[Reason for using Δq_z rather than q_z: For an integer number of layers, writing $q_z = Q_z + \Delta q_z$ with $Q_z = 2\pi m/d$ gives

$$e^{iq_zNd} = e^{iQ_zNd}e^{i\Delta q_zNd} = e^{i2\pi mN}e^{i\Delta q_zNd} = e^{i\Delta q_zNd}.$$

Thus, in the underlying integer-layer model, the Bragg-periodic part contributes only a trivial phase factor, and the thickness-dependent dephasing is governed by the deviation Δq_z from the Bragg point. In the present continuous-extension model for Gaussian roughness, we apply the Gaussian characteristic function to this residual phase $\Delta q_z Nd$. Therefore, the damping factor is written in terms of $(\Delta q_z d)^2\sigma^2$, not $(q_z d)^2\sigma^2$ as shown in (e).]

[0.25 pt]

(e) Evaluates the Gaussian characteristic function:

$$\left\langle e^{i\Delta q_zNd}\right\rangle = \int_{-\infty}^{\infty} P(N)e^{i\Delta q_zNd}\,dN.$$

[0.08 pt]

With $\xi = N - \bar{N}$, i.e. $N = \bar{N} + \xi$ and $dN = d\xi$,

$$\left\langle e^{i\Delta q_zNd}\right\rangle = e^{i\Delta q_z\bar{N}d}\int_{-\infty}^{\infty}\frac{1}{\sqrt{2\pi}\sigma}\exp\left[-\frac{\xi^2}{2\sigma^2} + i\Delta q_z d\,\xi\right]\,d\xi.$$

[0.10 pt]

Completes the square correctly:

$$-\frac{\xi^2}{2\sigma^2} + i\Delta q_z d\,\xi = -\frac{(\xi - i\sigma^2\Delta q_z d)^2}{2\sigma^2} - \frac{1}{2}(\Delta q_z d)^2\sigma^2.$$

[0.12 pt]

Therefore obtains the exact Gaussian characteristic function

$$\left\langle e^{i\Delta q_zNd}\right\rangle = e^{i\Delta q_z\bar{N}d}e^{-\frac{1}{2}(\Delta q_z d)^2\sigma^2}.$$

This Gaussian integral is exact for the assumed continuous Gaussian distribution; the use of Δq_z reflects the Bragg-periodic phase removal described in part (d), not a small-σ approximation.

[0.10 pt]

(f) Obtains the averaged amplitude:

$$\langle A(q_z)\rangle = \frac{1 - e^{i\Delta q_z\bar{N}d}e^{-\frac{1}{2}(\Delta q_z d)^2\sigma^2}}{1 - e^{iq_zd}}.$$

[0.20 pt]

(g) Computes the coherent intensity:

$$I(q_z) = \frac{1 - 2e^{-\frac{1}{2}(\Delta q_z d)^2\sigma^2}\cos(\Delta q_z\bar{N}d) + e^{-(\Delta q_z d)^2\sigma^2}}{4\sin^2(q_zd/2)}.$$

[0.30 pt]

(h) For $q_z = \pi/(2d)$, identifies the required substitutions:

$$\Delta q_z d = \frac{\pi}{2}, \qquad \Delta q_z \bar{N} d = \frac{5\pi}{2}, \qquad \cos\left(\frac{5\pi}{2}\right) = 0, \qquad \sigma^2 = (0.4)^2 = 0.16.$$

[0.10 pt]

(i) Obtains the first intensity ratio:

$$\frac{I(\sigma = 0.4)}{I(\sigma = 0)} = \frac{1 + e^{-(\pi/2)^2(0.4)^2}}{2} = \frac{1 + e^{-\pi^2/25}}{2} \simeq 0.84.$$

[0.20 pt]

(j) For $q_z = 2\pi/d$, recognizes the limiting form:

$$q_z = \frac{2\pi}{d} \Rightarrow \Delta q_z = 0, \qquad \lim_{q_z \to 2\pi/d} A_N(q_z) = N.$$

[0.15 pt]

(k) Obtains the second requested ratio:

$$\frac{I(q_z = 2\pi/d, \sigma = 0.4, \bar{N} = 5)}{I(q_z = 2\pi/d, \sigma = 0, \bar{N} = 5)} = 1.$$

[0.10 pt]

Part E: Diffraction from a film with evolving surface morphology [2.3 points]

Target result:

$$\frac{I(0.8t_0)}{I(3.6t_0)} = 4.$$

Award marks only for the following identifiable equations or equivalent expressions:

(a) Identifies the alternating layer phase at $\mathbf{q} = (\pi/d)\hat{\mathbf{z}}$:

$$e^{iq_z nd} = e^{i(\pi/d)nd} = e^{in\pi} = (-1)^n.$$

[0.40 pt]

(b) Writes the amplitude for N completed layers plus fractional coverage θ:

$$A(N, \theta) = f_0 \left[\sum_{n=0}^{N-1} (-1)^n + \theta(-1)^N\right].$$

[0.50 pt]

(c) Identifies the two growth states:

$$t = 0.8t_0: \quad N = 0, \quad \theta = 0.8,$$

$$t = 3.6t_0: \quad N = 3, \quad \theta = 0.6.$$

[0.40 pt]

(d) Computes the first amplitude and intensity:

$$A(0,0.8) = 0.8f_0, \qquad I(0.8t_0) = |0.8f_0|^2 = 0.64f_0^2.$$

[0.35 pt]

(e) Computes the second amplitude and intensity:

$$\sum_{n=0}^{2}(-1)^n = 1, \qquad A(3,0.6) = f_0[1 + 0.6(-1)^3] = 0.4f_0,$$

$$I(3.6t_0) = |0.4f_0|^2 = 0.16f_0^2.$$

[0.35 pt]

(f) Gives the final ratio:

$$\frac{I(0.8t_0)}{I(3.6t_0)} = \frac{0.64f_0^2}{0.16f_0^2} = 4.$$

[0.30 pt]