

Unified quantum walk model for internal crystal effects in dynamical diffraction

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The theory of dynamical diffraction (DD) in perfect crystals is the backbone of high-precision neutron and x-ray diffraction experiments, enabling accurate determination of crystal-structure factors and the realization of perfect-crystal interferometers. In practice, however, real crystals exhibit deformations and imperfections, including surface roughness, defects, temperature gradients, angled crystal faces, and curvature, that degrade interferometer performance and are difficult to model using conventional DD theory, particularly in complex geometries. To address these challenges, a quantum information (QI) model for DD has been under development, with demonstrated experimental agreement both for ideal crystals and in the presence of some imperfections such as surface roughness and defects. Here, we present a unified quantum walk model that is now suitable for reproducing a broad range of established DD effects. We demonstrate this by incorporating several diverse internal crystal effects influencing DD intensity distributions, including linear temperature gradients, the DD Talbot effect, and angled or miscut crystals. These results establish the QI model as a comprehensive and flexible framework for experimental analysis, as well as for the design of next-generation perfect-crystal neutron interferometers and neutron optical components, such as condensing monochromators.

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I. INTRODUCTION

Bragg diffraction plays a fundamental role in neutron and x-ray experiments, particularly in applications involving perfect-crystal interferometers, which have been integral to research across multiple fields for over six decades [1–4]. These interferometers have enabled significant advancements in the development of phase-contrast imaging [5–7], high-precision lattice-constant measurements for redefining the kilogram [8–10], and the search for fifth forces [11,12].

Achieving high-contrast perfect-crystal interferometers is challenging due to the rigorous demands they place on fabrication tolerances and environmental control [13,14]. For instance, crystal-blade lattice planes must be aligned to within a few angstroms [15–17], and angular deviations from the Bragg condition must remain within the narrow constraints of the Darwin width, typically limited to just tens of microradians [3,18]. Furthermore, the crystal must be effectively isolated from external disturbances, as even low-frequency vibrations or temperature fluctuations on the order of a few millikelvins will reduce contrast [19–21].

Advancements in reproducible, high-contrast perfect-crystal interferometer fabrication methods [14,22,23] could enable novel high-precision experiments, such as tests of gravity modifications [24], large-area phase measurements [25], and neutron magnetic and electric dipole moment measurements [26–31]. This underscores a need to improve our understanding of experimental imperfections so that we can characterize and mitigate them.

To achieve this, a quantum information (QI) model for dynamical diffraction (DD) which simulates both neutron and x-ray propagation through perfect crystals as a quantum walk through a lattice of nodes has been under development [31–36]. To establish a comprehensive simulation framework for modeling high-precision experiments, it is essential to incorporate the effects of crystal imperfections, as well as strain and stress. Initial efforts in this direction applied the QI model to a neutron cavity formed by two Bragg blades, introducing a toolbox for modeling crystals with rough surfaces, which is often impractical using conventional DD [36].

In this work, we present a unified quantum walk framework for both neutron and x-ray Bragg diffraction experiments suitable for reproducing a broad range of established DD effects within a single model. We demonstrate this capability by incorporating several diverse internal crystal effects and deformations. We analyze elastically deformed crystals subject to a uniform temperature gradient and compare the results with experimental data [37]. We also consider angled crystal faces, which may arise from fabrication errors or may be intentionally introduced [38], and demonstrate

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how crystal asymmetry strongly modifies the diffracted intensity and beam divergence. Finally, we investigate the DD analog of the Talbot effect, which significantly modifies neutron or x-ray wave-function self-interference within the crystal [39–44]. To understand this effect, we introduce how coherent plane-wave DD results can be implemented within the QI model, in contrast to previous spherical-wave approaches [31–36].

II. THEORETICAL FRAMEWORK

A. Pendellösung oscillations

In the Laue geometry of DD theory, defined by Bragg planes perpendicular to the crystal surface, an incident beam of neutrons or x rays enters one face of the crystal and exits through the opposite one, with both the transmitted (O beam) and Bragg-diffracted (H beam) beams propagating in the forward direction. Unlike the simpler kinematic approximation, which assumes single scattering, DD theory accounts for multiple scattering events within the crystal volume and the coupling between incident and diffracted wave fields due to the periodic crystal potential. Under the two-wave approximation, where only one set of Bragg planes contributes significantly to the scattering, the neutron or x-ray wave equation within the crystal admits two Bloch wave solutions. Each Bloch wave is a coherent superposition of a transmitted component and a diffracted component, and together they form the complete solution for the internal wave field. Thus, four plane waves propagate inside the crystal (two transmitted and two diffracted), grouped into two Bloch wave eigenstates with distinct wave vectors (k^α and k^β) [3,18].

As these two Bloch waves propagate through the crystal, their differing longitudinal wave-vector components lead to a periodic modulation of the relative phase between them. This produces an interference effect observable as a spatial redistribution of intensity between the transmitted and diffracted beams, known as Pendellösung oscillations. These oscillations occur as a function of crystal thickness t or incident wavelength λ and are a direct consequence of the coherent superposition of the two Bloch waves [45]. The Pendellösung period is given as

$$\Delta_H = \frac{2\pi}{|k^\alpha - k^\beta|} = \frac{1}{C} \frac{\pi V \cos(\theta_B)}{\lambda |F_H|}, \quad (1)$$

where V is the unit cell volume, θ_B is the Bragg angle, λ is the wavelength, C is the polarization factor (unity for neutrons, polarization dependent for x rays), and F_H is the structure factor. The nature of F_H depends on the scattering mechanism: For x rays it is related to the electron density, while for neutrons it depends on the nuclear scattering length density [3,4].

B. Quantum information model

The QI model describes neutron and x-ray propagation through perfect crystals as a quantum walk through a two-dimensional lattice of nodes [31–36]. The beam input state to a single node (indexed with η) is given by the two-level system

state vector:

$$\psi_\eta = \alpha_\eta |a_\eta\rangle + \beta_\eta |b_\eta\rangle \quad \text{or} \quad \begin{pmatrix} \alpha_\eta \\ \beta_\eta \end{pmatrix}, \quad (2)$$

where $|a_\eta\rangle$ and $|b_\eta\rangle$ are the states propagating upward and downward, respectively, into the η th node. For a column of h nodes, the input beam wave function is represented as

$$\psi = \begin{pmatrix} \vdots \\ \alpha_\eta \\ \beta_\eta \\ \vdots \\ \alpha_h \\ \beta_h \end{pmatrix}, \quad (3)$$

where the nodes act as unitary operators on the input wave function, resulting in transmission and reflection to the neighboring nodes. The unitary operator for a node is given by

$$U_\eta = \begin{pmatrix} \cos \gamma & \sin \gamma \\ -\sin \gamma & \cos \gamma \end{pmatrix}, \quad (4)$$

where γ controls the transmission and reflection amplitude. Equation (4) is a reduced form of the general SU(2) beam-splitting operator. The omitted phases correspond to an overall unobservable phase and a global lattice translation, neither of which affects the single-crystal simulations considered here. Consequently, these phases are set to zero for the present work, consistent with previous implementations of the QI model in Refs. [32,35].

Following the convergence analysis introduced in Ref. [35], there is an equivalence relation between simulation and experimental parameters given by

$$N\gamma = \frac{\pi t}{\Delta_H}, \quad (5)$$

where N is the number of nodes in simulation space to simulate the corresponding crystal thickness t for Pendellösung length Δ_H from Eq. (1). This relation provides the connection between the coarse-grained numerical simulation parameters and experimentally relevant crystal properties, generalizing the original QI formulation introduced in Ref. [32]. For further discussion of the effects of the discretization parameter γ on simulation results and convergence to the DD limit, see the Appendix.

Throughout prior QI model developments [31–36], the focus was on spherical-wave formulations of DD, consistent with the Takagi-Taupin equations originally developed to analyze strain in x-ray diffraction experiments [3]. While this approach naturally captures real-space intensity profiles of diffracted beams, it does not directly reveal the angular-spectrum structure underlying many fundamental DD phenomena. In particular, effects that depend explicitly on well-defined plane-wave components, such as miset-angle dependence (rocking curves) and the DD Talbot effect, are most transparently described in the plane-wave limit. Motivated by this, here, we develop the coherent plane-wave formulation within the QI model, completing its exact connection to foundational DD results [3] and enabling exploration of the internal crystal Talbot effect in Sec. III C.

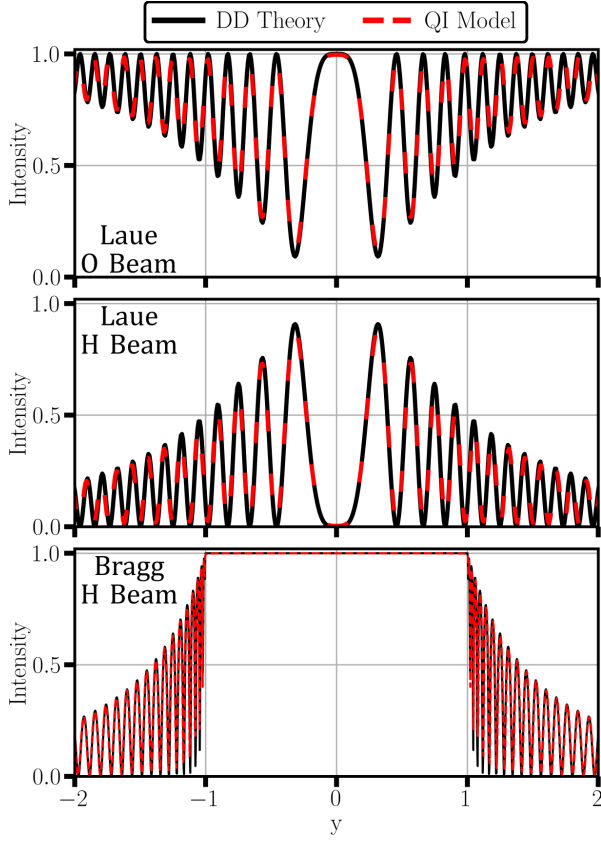


FIG. 1. Transmitted (O beam) and diffracted (H beam) intensity profiles in both the Laue and Bragg geometries for an incident misset monochromatic plane wave. The misset angle $\delta\theta$ is related to the conventional dimensionless misset parameter y according to $y = 2\Delta_H \sin(\theta_B)\delta\theta/\lambda$ [3,4]. The crystal thickness is $t = 10\Delta_H$ (220), $\lambda = 2.72 \text{ \AA}$, $\gamma = \pi/52$, and $0 \leq \eta \leq 4000$. The QI model and DD equations [Eqs. (7) and (8)] are in excellent agreement.

Consider a neutron or x-ray plane wave with wave-vector magnitude $k_0 = 2\pi/\lambda$ incident on a Laue crystal, with the reciprocal lattice vector oriented along the x axis. For a small misset angle $\delta\theta$ relative to the Bragg angle θ_B , the wave-vector component along the crystal surface is $k_x = k_0 \sin(\theta_B + \delta\theta)$. The physical spatial coordinate along the crystal surface x takes on discrete values in the simulation space corresponding to the node positions. The node spacing is $d_{\text{nodes}} = \gamma \Delta_H / \pi$, from setting $N = 1$ in Eq. (5). Note that for small γ , d_{nodes} can approach the true physical lattice spacing of the crystal d_{crystal} . Altogether, the physical coordinate of a node along the crystal surface is given by $x = 2\eta d_{\text{nodes}}$, where $\eta \in \mathbb{Z}$ is the node index. Subbing in the expressions for k_x and x and approximating for small $\delta\theta$, we obtain

$$\psi_{\text{plane}} = A_0 \exp(ik_x x) \sim A_0 \exp\left(i \frac{2\pi \eta \delta\theta}{\tan(\theta_B)} \frac{d_{\text{nodes}}}{d_{\text{crystal}}}\right), \quad (6)$$

where A_0 is the incident wave amplitude. This expression represents a plane wave incident on the discretized crystal, with a phase gradient determined by the angular deviation $\delta\theta$ from the Bragg condition.

TABLE I. Internal crystal effects, deformations, and imperfections and the proposed implementation with the QI model, with the equations from this work listed. The references highlight experimental demonstrations of the effects. Surface roughness and defects were considered in previous work [31,36]; linear temperature gradients, the DD Talbot effect, and angled crystals are demonstrated in this work, and bent crystals and incorporating spin are directions for future work.

Internal crystal effect, deformation, or imperfection	QI model implementation	Ref.
Surface roughness plus defects	Modify γ , Eq. (4)	[36]
Linear temperature gradient	Scale N , Eq. (12)	[37]
Angled or miscut crystals	Shape crystal, Eq. (15)	[38]
DD Talbot effect	ψ_{plane} , Eq. (6)	[39–44]
Bent crystals	Phase gradients	[46–48]
Magnetic fields plus spin-orbit interaction (Schwinger)	Introduce U_{spin}	[30,49]

In Fig. 1, we plot the QI model results for incident monochromatic plane waves within DD theory for both Laue and Bragg geometries for a crystal thickness of $t = 10\Delta_H$. The results are compared with the standard DD expressions given by

$$I = \begin{cases} y^2 \frac{\sin^2(\pi t \sqrt{1+y^2})}{(1+y^2)} + \cos^2(\pi t \sqrt{1+y^2}), & \text{O beam,} \\ \frac{\sin^2(\pi t \sqrt{1+y^2})}{(1+y^2)}, & \text{H beam,} \end{cases} \quad (7)$$

for the Laue geometry and

$$I_H = \begin{cases} \frac{\sinh^2(\pi t \sqrt{1-y^2})}{(1-y^2) + \sinh^2(\pi t \sqrt{1-y^2})}, & |y| \leq 1, \\ \frac{\sin^2(\pi t \sqrt{y^2-1})}{(y^2-1) + \sin^2(\pi t \sqrt{y^2-1})}, & |y| \geq 1, \end{cases} \quad (8)$$

for the Bragg reflected beam, with the conventional dimensionless misset parameter $y = 2\Delta_H \sin(\theta_B)\delta\theta/\lambda$ [3,4]. Excellent agreement with theory is obtained: In the Bragg geometry, the characteristic unity reflectivity for $-1 < y < 1$ is recovered, while in the Laue geometry, the transmitted intensity reaches unity at $y = 0$. This formulation naturally extends to multiple-crystal configurations, such as interferometers.

This establishes the QI model as a valid, single framework for both plane-wave and spherical-wave regimes.

III. INTERNAL CRYSTAL EFFECTS, IMPERFECTIONS, AND DEFORMATIONS

The QI model is capable of simulating a wide range of internal crystal effects, imperfections, and deformations, as summarized in Table I. Previous work addressed the effects of surface roughness and defects [31,36]. In the present study, we consider linear temperature gradients, the DD Talbot effect, and angled crystal geometries. We also discuss further implementations, such as the treatment of bent crystals and the incorporation of spin.

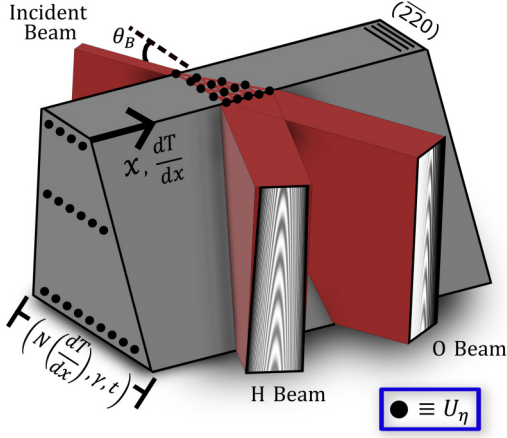


FIG. 2. Schematic of the QI model implementation of a temperature gradient dT/dx in a perfect silicon crystal wedge, with varying thickness t . A tall incident beam undergoes Bragg diffraction, producing Pendellösung interference fringes in the O and H beams observed at a 2D position-sensitive detector. The temperature gradient is normal to the Bragg planes and modifies the number of simulation nodes N with respect to the undeformed case [Eq. (12)]. The black circles represent the QI model nodes which apply the unitary Bragg operator [Eq. (4)].

A. Linear temperature gradients

Crystals can be elastically deformed by a uniform temperature gradient applied normal to the Bragg planes, which induces a phase difference between the coherently interfering wave fields within the crystal and modifies the resulting Pendellösung oscillations, as demonstrated by Hart [37].

To observe this effect, consider a tall incident beam to a crystal wedge at the Bragg angle, where the crystal thickness varies along the vertical extent of the beam (see Fig. 2). This thickness variation reveals the Pendellösung interference patterns in both the transmitted and diffracted beams, observable with a position-sensitive detector. Depending on the magnitude of the Pendellösung length, a precise number of intensity maxima will be visible within the wedge thickness range:

$$t = \bar{n}_0 \Delta_H, \quad (9)$$

where $\bar{n}_0$ is the interference order (or number of maxima). The Pendellösung oscillations shown at the two-dimensional (2D) position-sensitive detectors in Fig. 2 represent the perfect-crystal case where $dT/dx = 0$.

As shown in Ref. [37], computing the phase difference between interfering paths within the crystal reveals which interference order $\bar{n}$ will be observed as a function of the deformation $\frac{dT}{dx}$:

$$\bar{n} = \frac{1}{2} \bar{n}_0 \left(\sqrt{1 + \bar{p}^2} + \frac{\text{arcsinh}(\bar{p})}{\bar{p}} \right), \quad (10)$$

where

$$\bar{p} = \frac{\alpha t \tan \theta_B}{|C| |\chi_h|} \frac{dT}{dx}, \quad (11)$$

α is the thermal-expansion coefficient, $\frac{dT}{dx}$ is the linear temperature gradient, and $\chi_H = (-\lambda^2 F_H)/(\pi V)$. Notably, Eq. (10)

describes the observed fringe order $\bar{n}$ for a certain crystal thickness t and deformation $\frac{dT}{dx}$, relative to the fringe order with no deformation $\bar{n}_0$. The fringe order increases as the magnitude of the deformation increases, implying that the fringe spacing must decrease.

We now apply the QI model to simulate this temperature gradient. Using Eqs. (5), (9), and (10), we obtain

$$\frac{N}{N_0} \approx \frac{\bar{n}}{\bar{n}_0}, \quad (12)$$

where N_0 (N) defines the depth of the quantum walk for a crystal without (with) deformation. Consistent with the physical effect of elastic deformation, variation of N in Eq. (12) does not correspond to a change in the number of atomic sites but instead represents a change in the lattice spacing. Figure 3 shows the simulated Pendellösung oscillations for the diffracted (H-beam) and transmitted (O-beam) intensity profiles. The simulation considers incident $220 \text{ Ag } K\alpha_1$ x rays to a crystal wedge ranging in thickness from about 1.20 to 1.45 mm [37]. The interference order in the ideal (deformed) case is indicated by $\bar{n}_0$ ($\bar{n}$), and solid black lines connect identical interference orders across the different magnitude temperature gradients. The leftmost intensity profiles in the O and H beams represent the perfect-crystal case where $dT/dx = 0$. As the temperature gradient is introduced, we observe the movement of the fringes and the fringe spacing decreasing, in qualitative agreement with experiment [37].

To quantitatively compare the measurement results to experiment and DD theory [Eq. (10)], we choose fixed points of observation in the section patterns (i.e., $\bar{n}_0 = 26, 28, 30$) and then interpolate between interference orders to calculate $\bar{n}$ as the crystal deformation increases (as done in Ref. [37]). The horizontal line of black circles in Fig. 3 demonstrates where $\bar{n}$ is computed at the fixed observation point $\bar{n}_0 = 28$. Figure 4 shows the measured phase ratio $\bar{n}/\bar{n}_0$ versus the magnitude of the temperature gradient [Eq. (11)], as well as the prediction from DD theory [Eq. (10)] and the QI model simulation results.

As indicated by the relative residual, the QI model and DD theory agree within 0.2% over the full temperature range considered. The observed downward trend reveals a systematic deviation, with the QI model predicting an $\sim 0.2\%$ larger $\bar{n}/\bar{n}_0$ at the highest gradient ($dT/dx = 34.9 \text{ }^\circ\text{C/cm}$). The small oscillations in the residual are an artifact of the simulation resolution, defined by setting $\gamma = \pi/100$. We compute the rms error for both the QI model and DD theory compared to the $\bar{n}_0 = 28$ experimental data. While both models agree with the data at the 10^{-3} level, the QI model provides a slightly improved fit, with an rms error approximately 14% lower than that of DD theory. Overall, this agreement demonstrates that the QI model provides a simple yet quantitatively accurate framework for capturing the modification of Pendellösung oscillations under a linear temperature gradient.

B. Fankuchen cut crystals

In practice, crystal surfaces are not perfectly parallel (in Bragg geometry) or perpendicular (in Laue geometry) to the Bragg planes but deviate within certain tolerances depending on the application (approximately millirads). Such deviations

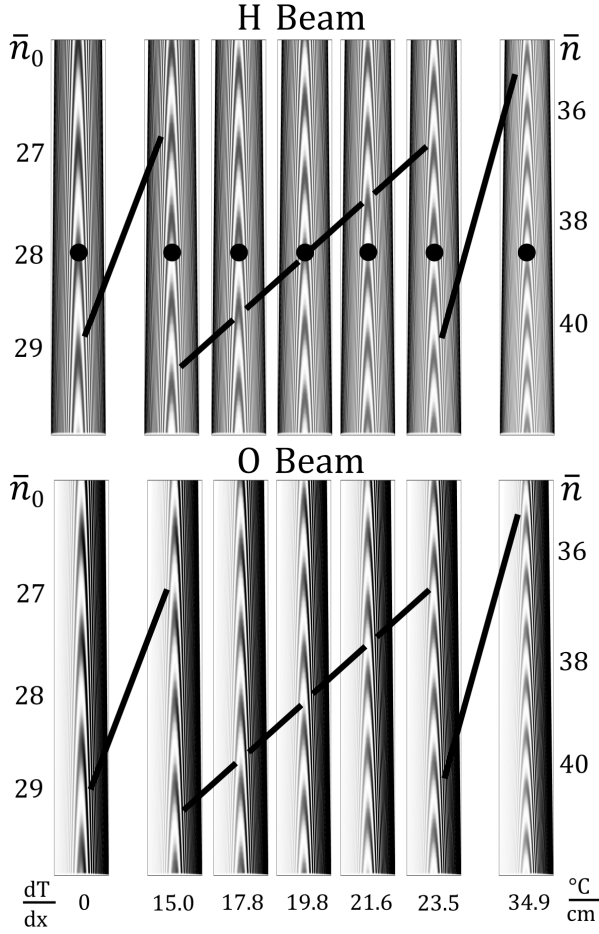


FIG. 3. Simulated O- and H-beam interference patterns for $\bar{2}20$ Ag $K\alpha_1$ incident on a crystal wedge subject to linear temperature gradients (see Fig. 2) with magnitudes ($0 \leq \frac{dT}{dx} \leq 34.9^\circ\text{C}/\text{cm}$). The interference order in the ideal (deformed) case is indicated by $\bar{n}_0$ ($\bar{n}$). The solid black lines across the interference patterns connect identical interference orders, a consequence of the fringe spacing decreasing as the deformation increases. From Eqs. (5) and (12), we set $\gamma = \pi/100$ and vary N according to the temperature gradient. The horizontal line of black circles in the H-beam intensity profiles indicate where the fringe-order ratio $\bar{n}/\bar{n}_0$ is computed for Fig. 4. The intensity profiles show qualitative agreement with those in Ref. [37]; a quantitative comparison is demonstrated in Fig. 4.

can arise from miscuts or polishing tolerances and must be accounted for to achieve quantitative agreement with experimental results [30,35,50].

Intentional angular offsets can also be introduced to tailor beam properties, as proposed by Fankuchen in the design of condensing x-ray monochromators [38]. In this approach, the crystal surface is cut at an angle α relative to the Bragg planes [see Fig. 5(a)], placing it within the broader framework of asymmetric Bragg diffraction [51–53]. These angled crystal geometries have been studied for both x rays and neutrons [54–56].

Such controlled asymmetry is particularly valuable for neutron optics, where shaping or focusing beams without losses is challenging. In contrast to aperture-based or Fresnel-zone plate-based methods, asymmetric crystal geometries

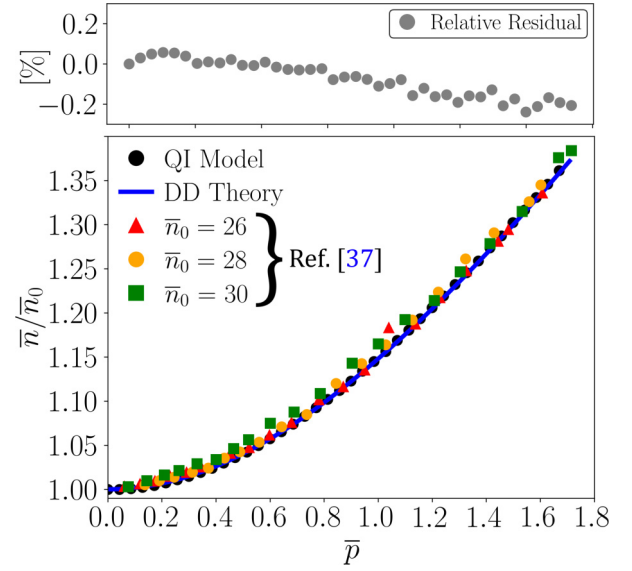


FIG. 4. The measured fringe-order ratio $\bar{n}/\bar{n}_0$ for $\bar{2}20$ Ag $K\alpha_1$ at various observation points $\bar{n}_0$ as a function of temperature gradient dT/dx [Eq. (11)] from Ref. [37], as well as the prediction from DD theory given by Eq. (10) and the QI model simulation (from Fig. 3). The relative residual percentage between the QI model results and the DD theoretical curve is shown above the data: $(\text{QI-DD})/\text{DD}$.

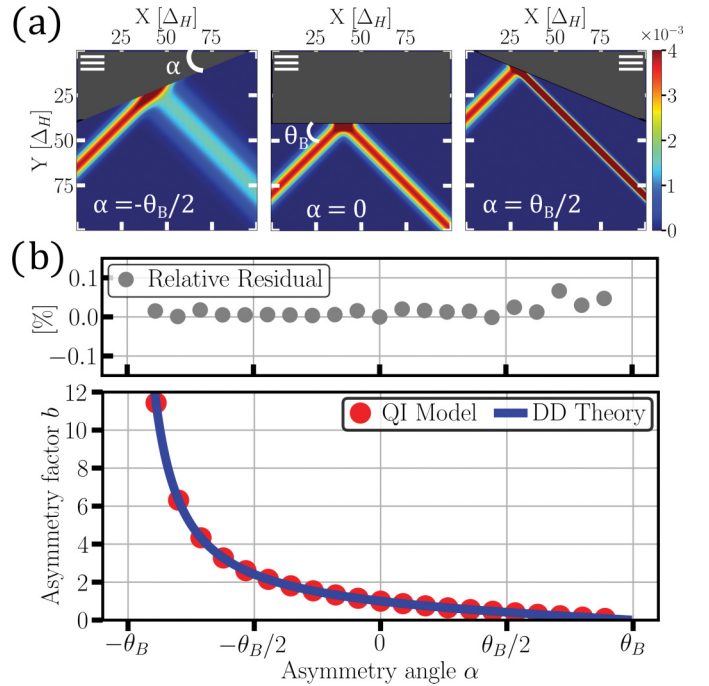


FIG. 5. (a) QI model simulations of Bragg diffraction at $\theta_B = 45^\circ$ from crystals with asymmetry angles $\alpha = -\theta_B/2$, $\alpha = 0$, and $\alpha = \theta_B/2$. The input Gaussian width is $w_{\text{in}} = 4\Delta_H$, and $\gamma = \pi/100$ from Eq. (5). (b) Comparison of the QI model and DD theory for $w_{\text{out}}/w_{\text{in}} = |b|$, where $\theta_B = 45^\circ$ and α is varied from $-\theta_B$ to θ_B . The relative residual $(\text{QI} - \text{DD})/\text{DD}$ demonstrates agreement at the 0.1% level.

enable phase-space transformations that preserve beam intensity and enable beam expansion or condensing.

From DD theory, the crystal asymmetry factor b is

$$b = \frac{\sin(\theta_B - \alpha)}{\sin(\theta_B + \alpha)}, \quad (13)$$

transforming the beamwidth as

$$w_{\text{out}} = |b|w_{\text{in}}, \quad (14)$$

where w_{in} (w_{out}) are the input (output) beamwidths from the crystal. In accordance with Liouville's theorem, the angular divergence scales as $1/|b|$, such that a compressed beam becomes more divergent. Multiple asymmetric crystals can be arranged in sequence to enable enhanced control over beam shaping and collimation.

In Fig. 5, we model Fankuchen cut crystals using the QI framework and obtain excellent agreement with DD theory. Analogous to the double-Bragg-blade cavity geometry considered in previous work [36], the crystal geometry is implemented by introducing free-space nodes,

$$U_{\text{free}} = U_i(\gamma = 0), \quad (15)$$

which allow the crystal surface to be oriented according to the asymmetry angle α .

We simulate an incident Gaussian beam with rms beamwidth $w_{\text{in}} = 4 \Delta_H$ impinging on a crystal with Bragg angle $\theta_B = 45^\circ$ while varying the asymmetry angle over the range $-\theta_B < \alpha < \theta_B$. The output beam is fit to a Gaussian profile to extract w_{out} . The plotted relative residual between the QI model and Eq. (14) shows agreement within 0.1%. As expected, taking the Fourier transform of the reflected beam profiles confirms that the angular divergence scales as $1/|b|$.

Notably, the QI model reveals that the DD interference responsible for reshaping the beam occurs directly at the crystal surface, with minimal penetration into the crystal. Identity nodes [Eq. (15)] represent free-space propagation, while the standard Bragg diffraction operators [Eq. (4)] describe the crystal, as indicated by the gray regions in Fig. 5. This capability to model imperfect or arbitrarily shaped crystals is critical for characterizing beam size and divergence in the design and analysis of neutron and x-ray crystal optics.

C. Internal Talbot effect

The Talbot effect, in which a periodic object produces self-images at specific propagation distances, has found broad applicability across a range of fields [57,58]. The corresponding self-imaging distance, or Talbot distance z_T , is given by

$$z_T = \frac{\lambda}{1 - \sqrt{1 - \frac{\lambda^2}{D^2}}}, \quad (16)$$

where λ is the wavelength and D is the periodicity of the object or grating. In the limit $\lambda \ll D$, this reduces to $z_T \approx 2D^2/\lambda$. Recently, the Talbot effect was theoretically investigated by Balyan as an internal crystal phenomenon within DD theory [39–44]. In this context, the effect modulates the Pendellösung oscillations, generating interference “carpets” in the transmitted and reflected beams when an incident neutron or x-ray plane wave is structured by a periodic grating. Here,

we show that this internal interference modulation is captured exactly within the QI framework.

The corresponding Talbot distance in a crystal is

$$z_{\text{td}}^{\text{cr}} = \frac{2\Delta_H}{\sqrt{1 + 4\left(\frac{\Delta_H \tan(\theta_B)}{D}\right)^2} - 1}. \quad (17)$$

If the condition $\Delta_H \tan(\theta_B) \ll D$ is satisfied, then Eq. (17) can be approximated as $z_{\text{td}}^{\text{cr}} \approx D^2/[\Delta_H \tan^2(\theta_B)]$. Similarities with the optical case are clear, with the characteristic Pendellösung length scale replacing wavelength as the parameter of interest.

With plane-wave DD validated within the QI model (see Sec. II B), we can incorporate the internal DD Talbot effect [39]. We modulate an incident plane wave with a periodic amplitude grating of the form

$$T(x) = \frac{1 + \cos(2\pi x/D)}{2}, \quad (18)$$

with period $D = 40 \mu\text{m}$. The resulting simulated Talbot carpets in both the O and H beams are shown in Fig. 6. We consider (220) silicon with Mo $K\alpha$ radiation ($\lambda = 0.71 \text{ \AA}$) and σ polarization, yielding a Pendellösung length of $36.6 \mu\text{m}$ and a Talbot distance of $z_{\text{td}}^{\text{cr}} \approx 1.3 \text{ mm}$. The O-beam carpet appears tilted due to asymmetry in the transmitted DD wave field [40].

At the Talbot distance, the reflected intensity reproduces the incident grating $T(x)$, confirming the expected self-imaging behavior and agreeing with DD predictions [40]. At half the Talbot distance, $z_{\text{td}}^{\text{cr}}/2$, the carpet pattern exhibits the characteristic $D/2$ lateral shift.

Complementary to the results for a linear temperature gradient (see Fig. 3), this internal Talbot effect can be experimentally verified using wedged crystals to produce interference fringes on a 2D position-sensitive detector, as proposed in Ref. [39]. Notably, the Talbot distance in Fig. 6 is approximately 35 times larger than the Pendellösung period. This magnified spatial scale is ideal for utilizing neutron imaging detectors, where typical pixel sizes ($\sim 50 \mu\text{m}$) are well suited to resolve the Talbot structure but not for the much finer Pendellösung oscillations. As a result, the Talbot effect provides a practical route for imaging internal DD behavior, where we propose that the Pendellösung length can be retrieved from the measured carpet periodicity.

IV. DISCUSSION AND CONCLUSION

In this work, we established a comprehensive quantum walk model capturing known dynamical diffraction phenomena. While traditional analytical DD approaches become impractical when confronted with complex crystal geometries, deformations, and imperfections, our quantum walk framework naturally accommodates these real-world experimental environments. By successfully integrating the coherent plane-wave and spherical-wave regimes into a single model, this work provides an accurate and highly accessible tool kit for simulating both macroscopic crystal diffraction and complex internal crystal effects. Rather than merely reproducing individual diffraction effects, our framework demonstrates a robust capacity to naturally implement common crystal deformations and arbitrary crystal geometries. We validated this by accurately capturing the modified Pendellösung oscillations

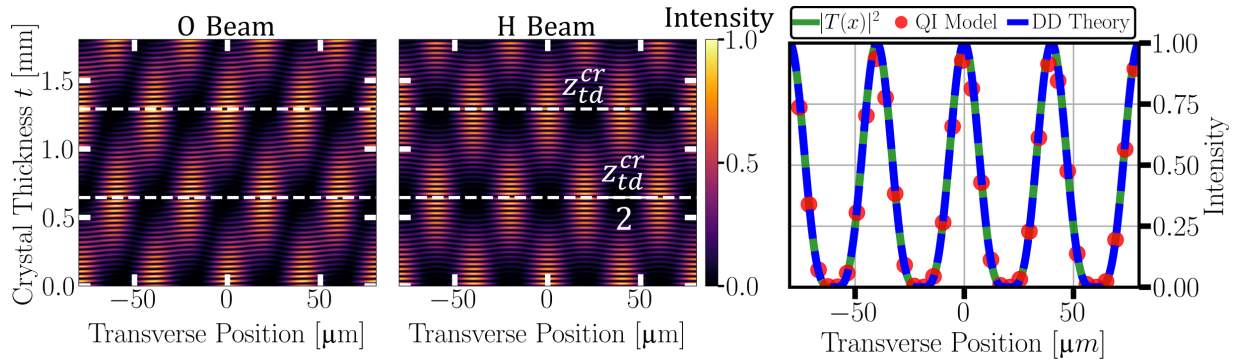


FIG. 6. Simulated DD Talbot carpets in both the O and H beams in the Laue geometry for a periodic amplitude grating with $D = 40 \mu\text{m}$. The Talbot distance is $z_{td}^{cr} \approx 1.3 \text{ mm}$. As shown in the rightmost plot, the QI model self-image (transverse intensity at $t = z_{td}^{cr}$ in the H beam) matches the incident grating periodicity and DD theory result. These simulations neglect the effects of absorption.

induced by linear temperature gradients and by demonstrating the tunable beam transformations inherent in asymmetric Fankuchen cut crystals. Furthermore, we utilized the plane-wave formulation to simulate the internal crystal DD Talbot effect. Notably, since this effect produces spatial-intensity modulations on a scale resolvable by modern neutron imaging detectors, our model serves as an ideal predictive tool for the experimental design and verification of these internal interference carpets, offering a practical route to directly extract the orders of magnitude smaller Pendellösung length.

As with any physical model, the QI framework is based on several assumptions that define its limitations and range of applicability. The present model assumes coherent elastic DD and therefore models neutron and x-ray propagation through unitary evolution. As in conventional DD, it adopts the two-beam approximation and restricts scattering to nearest-neighbor nodes within the coarse-grained lattice. Rather than resolving every atomic plane, the crystal is represented by scattering nodes, each corresponding to the cumulative coherent scattering over a finite crystal thickness. Quantitative agreement with conventional DD is therefore obtained only when the discretization is sufficiently fine for the coarse-grained model to converge to the continuous DD limit (see Appendix), and all simulations presented here are performed within this regime.

Within these assumptions, the QI model provides a flexible framework for modeling neutron and x-ray DD in both ideal and imperfect crystals. In particular, it readily incorporates complex crystal geometries and spatially varying lattice properties, including defects, surface roughness, temperature gradients, and crystal miscuts, which are often difficult to treat using conventional DD. However, the present implementation also has several limitations. It neglects absorption, inelastic interactions, thermal diffuse scattering, and incoherent scattering. Furthermore, the lattice distortion modeling demonstrated here is currently restricted to linear temperature gradients perpendicular to the lattice planes rather than arbitrary three-dimensional strain fields. Finally, free-space propagation between crystals is treated as diffraction-free, such that neutron wave packets propagate without transverse spatial spreading or wavefront evolution.

Looking forward, the natural flexibility of the unified quantum model provides a straightforward path for incorporating

these missing dynamics and, as outlined in Table I, is readily extended to more complex scenarios. For example, intentionally bent crystals [59–61] are widely used to create focusing monochromators and to probe fundamental neutron-matter interactions, such as with neutron whispering-gallery states [62]. Analogous to the misset plane-wave approach shown in Fig. 1 and Eq. (6), these strain effects may be incorporated into the QI framework through position-dependent phase gradients across the node-discretized crystal. Additionally, magnetic fields and spin-orbit interactions are essential extensions for accurately describing neutron spin evolution both inside and outside the crystal [30,49]. These effects can be included by expanding the simulation space to apply a 2×2 unitary spin rotation operator U_{spin} at each node, analogous to the Bragg operator [Eq. (4)], but with the spin rotation angle arising from external magnetic fields or spin-orbit interactions.

Ultimately, by providing a precise, versatile, and unified alternative to standard DD theory, this framework will be instrumental in characterizing experimental diffraction experiments, optimizing large-area interferometers, and enabling high-precision measurements of fundamental interactions.

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DATA AVAILABILITY

The data that support the findings of this article are openly available [63].

APPENDIX

A summary of the quantum information (QI) model parameters used in this work, alongside their physical meaning and typical range of values used, is presented in Table II.

TABLE II. Summary of QI model parameters used in this work.

QI model parameter	Physical meaning	Typical values
γ	Simulation resolution	$\frac{\pi}{50} - \frac{\pi}{100}$
N	Simulation layers or depth	$10^2 - 10^4$
t	Crystal thickness	microns to centimeters
Δ_H	Pendellösung length	50 μm
d_{nodes}	Node spacing	1 μm
λ	Neutron or x-ray wavelength	10^{-10} m
θ_B	Bragg angle	$0^\circ - 90^\circ$
d_{crystal}	Lattice plane spacing	10^{-10} m
ψ	Input wave function	Spherical or plane
U_η	Unitary node operator	Bragg or free space
dT/dx	Linear temperature gradient	$0 - 34.9^\circ\text{C/cm}$
α	Crystal asymmetry angle	-45° to $+45^\circ$
D	Grating period	10–50 μm

In general, the choice of simulation parameters is critical for avoiding numerical artifacts and ensuring convergence to dynamical diffraction (DD) theory. As introduced in Ref. [35], the transmitted and reflected neutron intensity profiles from a perfect crystal in the Laue geometry are recovered exactly in the limit $\gamma \rightarrow 0$, provided that the product $N\gamma$ is held constant so that Eq. (5) is satisfied. The parameter γ controls the coarse-graining resolution of the simulated crystal: Larger values correspond to fewer, stronger beam-splitting nodes and produce increasingly coarse intensity profiles that cannot accurately resolve fine Pendellösung oscillations. As γ is reduced and the number of simulation planes N is increased accordingly, the QI model systematically converges to the DD solution. In practice, values of $\gamma \lesssim \pi/50$ already provide excellent agreement with DD while remaining computationally efficient.

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