Quantum information approach to the implementation of a neutron cavity

O Nahman-Lévesque1,2, D Sarenac1,2, O Lailey1,2, D G Cory1,4, M G Huber5 and D A Pushin1,2,*

1 Institute for Quantum Computing, University of Waterloo, Waterloo, ON N2L3G1, Canada
2 Department of Physics and Astronomy, University of Waterloo, Waterloo, ON N2L3G1, Canada
3 Department of Physics, University at Buffalo, State University of New York, Buffalo, NY 14260, United States of America
4 Department of Chemistry, University of Waterloo, Waterloo, ON N2L3G1, Canada
5 National Institute of Standards and Technology, Gaithersburg, MD 20899, United States of America

* Author to whom any correspondence should be addressed.

E-mail: dmitry.pushin@uwaterloo.ca

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Abstract

Using the quantum information model of dynamical diffraction we consider a neutron cavity composed of two perfect crystal silicon blades capable of containing the neutron wavefunction. We show that the internal confinement of the neutrons through Bragg diffraction can be modelled by a quantum random walk. Furthermore, we introduce a toolbox for modelling crystal imperfections such as surface roughness and defects. Good agreement is found between the simulation and the experimental implementation, where leakage beams are present, modelling of which is impractical with the conventional theory of dynamical diffraction. Analysis of the standing neutron waves is presented in regards to the crystal geometry and parameters; and the conditions required for well-defined bounces are derived. The presented results enable new approaches to studying the setups utilizing neutron confinement, such as the experiments to measure neutron magnetic and electric dipole moments.

1. Introduction

The advancement of silicon fabrication techniques in the 20th century has enabled the use of perfect crystals in neutron science to resolve dynamical diffraction (DD) effects. The most successful application was perfect crystal neutron interferometry where three well-polished blades from a single ingot of silicon achieve centimeter-scale path separation and coherent superposition [1–5]. Hallmark experiments with a perfect crystal neutron interferometer (NI) include the first demonstration of gravity on a quantum particle [6], probing of dark energy/fifth forces [7, 8], observing the $4\pi$ symmetry of spinor rotation [9], and observing neutron orbital angular momentum [10–14].

The theory of DD models the neutron propagation through perfect crystals. Albeit powerful, it becomes impractical when considering complicated geometries. For example, neutron cavities that employ DD have been experimentally investigated for use as a neutron storage device [15–21], and work has been done to analyze Bragg reflection between two perfect crystal plates with DD [22, 23]. However, in-depth modelling of the neutron propagation through a cavity and parameter analysis is lacking.

The recently introduced quantum information (QI) model of DD attempts to simplify the mathematics by treating the neutron propagation as a quantum random walk [24–27]. Good agreement has been found between the model and the standard DD effects such as the Borrmann triangle, pendellösung oscillations, and the spatial intensity profiles of the NI paths.

Here we apply the QI model of DD to the case of a neutron cavity built from two perfect crystal silicon blades. We show that such an arrangement can contain the neutron wavefunction. The behaviour of the neutron modes inside the cavity is characterized with respect to the cavity geometry, and good agreement is found between an initial experimental implementation and the model. In addition to providing new insights
into neutron storage devices, the presented work lays the foundation for simulating the proposed measurements of the neutron magnetic and electric dipole moment [28–30].

2. QI model for DD

When considering neutron diffraction through crystals, DD effects must be considered. However, the standard theory of DD is limited to idealized perfect crystals (no impurities or defects) and practically limited to simple geometries. In [24], it was demonstrated that there exists a simpler, more computationally accessible QI based model in terms of a quantum random walk. In the QI model, the crystal is represented as a lattice of nodes which act as a unitary operator on the neutron state by either transmitting or reflecting it to its nearest neighbours (as seen in figure 1). The neutron input state to every node is given by a two-state vector:

$$\alpha|a\rangle + \beta|b\rangle \quad \text{or} \quad \begin{pmatrix} \alpha \\ \beta \end{pmatrix}, \quad (1)$$

where $|a\rangle$ and $|b\rangle$ are the states propagating onto the node in the up and down directions, respectively. The action of the $j$th node in figure 1 is given by:

$$U_j = |a_{j-1}\rangle(t_a|a_j\rangle + r_b|b_j\rangle) + |b_{j+1}\rangle(r_a|a_j\rangle + t_b|b_j\rangle), \quad (2)$$

with coefficients

$$t_a = e^{i\xi}\cos\gamma, \quad r_b = e^{i\zeta}\sin\gamma,$$
$$r_a = -e^{-i\zeta}\sin\gamma, \quad t_b = e^{-i\xi}\cos\gamma. \quad (3)$$

The parameter $\gamma$ controls the amplitude of reflection/transmission at each node, while $\xi$ and $\zeta$ are phase parameters.

The full state vector $\psi$ at every simulation layer $i$ is represented by a size $2h$ column vector, where $h$ is the number of nodes in the layer $i$. The $2m$ entry of $\psi$, where $m \in [0, h-1]$, represents the upwards input to node $j = 2m + 1$ ($j = 2m$) for even (odd) $i$ of the simulation grid. Similarly, the $2m + 1$ entry of $\psi$ is the downwards input to the corresponding node $j$. Following the notation of equation (1) and figure 1, $\psi$ is written as:

$$\psi = \begin{pmatrix} \vdots \\ \alpha_j \\ \beta_j \\ \alpha_{j+2} \\ \beta_{j+2} \\ \vdots \end{pmatrix}, \quad (4)$$

where $\alpha_j, \beta_j$ are transmitted and reflected components into the $j$th node. Every lattice column of nodes has a corresponding unitary scattering operator $C_i$ which is built of diagonal blocks of equation (2)

$$C_i = \begin{pmatrix} t_a & r_b & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & t_a & r_b & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \ldots , \quad (5)$$

The state vector after $n$ layers is given by

$$\psi_n = \prod_{i=0}^{n-1} C_{n-i}\psi_0. \quad (6)$$

In [27], it was shown that there is an equivalence between the simulation parameters and a given experimental configuration in both the Laue and Bragg geometry, given by

$$n \cdot \gamma = \frac{\pi d}{\Delta H}, \quad (7)$$
where \( n \) is the number of simulation layers needed to simulate a real-space distance \( d \) with parameter \( \gamma \). \( \Delta_H \) is the pendellösung period inside the crystal, and for the Bragg geometry is given by

\[
\Delta_H = \frac{\pi V_{\text{cell}} \sin \theta_B}{\lambda |F_H|},
\]

where \( V_{\text{cell}} \) is the volume of a crystal unit cell, \( \theta_B \) is the Bragg angle, \( \lambda \) is the neutron wavelength and \( F_H \) is the crystal structure factor. For a material such as silicon, with common wavelengths used in experiments, \( \Delta_H \) is on the order of 50 \( \mu \)m.

3. Modelling of a neutron cavity

DD theory predicts that in the Bragg geometry, neutrons falling within a narrow range of momentum centered around the Bragg condition (the Darwin width) are reflected with close to 100% probability. In a neutron cavity composed of two perfect crystals, neutrons outside the Darwin width will escape through the crystals within the first few bounces. Conversely, neutrons inside this width are effectively confined, allowing for a great number of bounces. Interestingly, the QI model predicts that this result can be explained purely as a consequence of a quantum random walk: the total neutron wavefunction is expressed as a sum over all the possible paths through the Bragg lattice. The difference in phase accumulated by the different paths results in constructive interference only for the paths which stay confined in a small region close to the gap.

To model a neutron cavity consisting of two silicon blades separated by a gap, we use a single column matrix where the nodes outside (inside) the crystals are free space (Bragg diffracting) operators. The operator for the free space nodes is given by the matrix

\[
U_{\text{free}} = |a_{j-1}\rangle\langle a_j| + |b_{j+1}\rangle\langle b_j|,
\]

while the operator for the Bragg diffracting nodes are given by equation (2). As shown in figure 2, without any information about transverse momentum, boundary conditions, or incident angle, the model predicts that only after a few bounces, the intensity within the blades is almost entirely localized in a narrow band around the inter-crystal gap. Most neutrons that do not settle within this band are either transmitted straight through the top of the crystal interferometer, or bounce at most once and transmit through the bottom.

Shown in figure 3(a) is the neutron average intensity inside the top crystal as a function of the penetration depth upwards into the top crystal. The intensity drops sharply within the first \( \Delta_H \), showing that the confined neutrons do not penetrate very deeply inside the crystal.
Figure 2. The simulated neutron intensity inside two perfect crystal silicon blades acting as a neutron cavity. Incident neutrons hit the bottom corner of the top crystal (Bragg case). In the simulation, this is where the first excited node begins the quantum random walk. Given that most of the beam gets initially transmitted, the range of the colour bar is limited to emphasize the confined intensity. The crystals are placed a distance $D$ apart, have thickness $t$ and length $L$. After the first few bounces, most of the leftover neutron intensity inside the blades is contained within a small band on the inside edges of the crystals. This intensity is preserved with further propagation. A detector can be placed at the exit of the crystals to capture the neutrons exiting the cavity. This simulation ($\Delta H = 50 \mu m$, $t = 0.5 \ mm$, $D = 0.2 \ mm$, $L = 3 \ cm$) considers a very thin crystal slice to better illustrate the behaviour near the gap. The position at which a neutron would have classically bounced 110 times is indicated in this figure as it is relevant for figure 3(a).

Figure 3. (a) The average neutron intensity inside the top crystal shown in figure 2 is plotted as a function of the penetration depth upwards into the top crystal. Note that the region from figure 2 that is considered here is from bounce 110 until the end of the crystal in order to avoid the initial high intensity region. The intensity drops sharply within the first pendellösung period, indicating that the neutron is mostly confined within a band of width $\approx \Delta H$ inside the crystal’s inner surface. (b) Examining the crystal thickness necessary to achieve total confinement after a large number of bounces. Shown is the confined intensity after a length $L = 16000 \Delta H$ as a function of crystal thickness $t$ for gap thickness $D = 12 \Delta H$ and $D = 100 \Delta H$. It can be observed that crystal thickness should be $\geq 4 \Delta H$ to ensure confinement after a large number of bounces.

3.1. Confined intensity
With the QI model we can examine the neutrons which remain confined within the cavity. Figure 3(b) shows the confined intensity inside the cavity ($1 - \text{escaped intensity}$) after a length $L = 16000\Delta H$ for different crystal thickness $t$. For various gap widths, the model predicts that crystal thickness should be $\geq 4\Delta H$ for confinement of neutron intensity after a large number of bounces. Figure 4(a) shows the confined intensity inside the cavity as a function of the number of bounces, for cavity parameters $D = 12\Delta H$ and $t = 87.5\Delta H$. In this simulation we consider a length of crystal corresponding to a geometrical path of 1000 bounces. The intensity drops sharply as the direct beam transmits straight through the first crystal, and then drops slightly less at each subsequent reflection. Eventually, it settles to an effectively constant value of around 4% of the incoming intensity. An estimation for the reflectivity of the crystal as the number of bounces increases can be extracted from this curve, by fitting it to an inverse exponential. The reflectivity in the ‘stable’ region between 500 and 800 bounces is found to be ($\approx 1 - 1.6 \times 10^{-5}$).

In figure 4(b), the intensity remaining in the cavity after a length $L = 16000\Delta H$ is plotted as a function of $D$. The confined intensity oscillates with period $\Delta H$ as the gap width $D$ is varied. The QI model indicates that to maximize the number of bounces for a given set of crystals, the spacing can be made very small without losing much intensity at the exit. However, the spacing should be made no smaller than $D = \Delta H/4$, which is
the first maximum in figure 4(b). Note that this particular prediction of the model has not been experimentally verified.

3.2. Cavity modes
Simulation of the neutron cavity using the QI model shows that the neutrons inside the cavity settle in one of two regimes, depending on the inter-crystal distance $D$. It should be noted that in the limit where $D \to 0$, the system reduces to a simple Laue crystal of thickness $L$, in which case the neutron will diverge to the edges of the Bormann triangle as predicted by DD theory. However, for nonzero spacing, after the first few bounces, most of the neutron current is confined within the cavity, and bounces back and forth between the blades without penetrating very deeply into the crystal. Figure 5(a) shows the simulated reflected intensity on the surface of the top crystal throughout the cavity, for different values of $D$. For the $D < \Delta_H$ regime, the neutron behaves like a standing wave inside the cavity, with a period dependent on $D$. For the regime with larger values of $D$ ($> 2 \Delta_H$), the bounces are well-separated and localized at first. As the number of bounces increases, the neutron wave packets spread and induce interference effects. This behaviour is shown in figure 5(b): for small $D$, there is one dominant frequency which changes with $D$. As $D$ increases, more pairs of harmonics are introduced.

4. Experimental implementation
An experimental implementation of a neutron cavity was performed at the NIOF beamline at the National Institute of Standards and Technology (NIST) center for neutron research (NCNR). The setup is shown in figure 6(b). A beam of neutrons with wavelength 0.235 nm was propagated through a 10 mm wide silicon neutron cavity composed of two 10 mm thick perfect crystal silicon blades (220 reflection) attached to a common base. A slit upstream to the crystal was 2 mm (wide) by 6 mm (tall) which provides an underestimate of the beam size. The beam divergence was $\leq 0.5^\circ$. The theoretical Bragg pendellösung length for this configuration is found to be 38.98 $\mu$m. The Bragg lattice spacing is 1.92 Å and the simulation node size is 0.78 $\mu$m (using $\gamma = \pi/50$ in equation (7)). After the initial transmission through the top crystal, the neutrons underwent four well-defined bounces with the top blade before leaving the cavity at the exit. These four bounces off the top blade correspond to the four low intensity beams that are observed exiting the top crystal. A scanning slit and an integrating detector were placed above the top crystal at Bragg angle with respect to the crystal, and were used to map the spatial intensity of neutrons along the crystal cavity.

As previously mentioned, DD theory for perfect crystals predicts that neutrons outside the Darwin width will escape after few bounces. This implies that the intensity of the beams transmitted through the top crystal will rapidly decrease as the cavity length $L$ increases since a larger number of bounces within the gap will occur. However, the experimental results show four leakage beams each of comparable intensity. Likewise, the QI model predicts negligible intensity at the location of the observed leakage beams for perfect crystals. This implies that the experimental setup has some imperfections. We speculate that this is due to surface roughness and defects on the inner crystal walls, which induces decoherence.

Using the QI model we can simulate the experimental configuration in both the ideal setup and when there are crystal imperfections. The simulation parameters were chosen according to the equivalence relation of equation (7). As shown in [27] we can account for the experimental factors such as the spread of the incident beam, beam divergence, and slit size through the analysis of a Bragg diffraction peak. Similar to the
methods of [27] the intensity penetrating through the top crystal was convolved with the measured shape of the exit peak. The simulated intensity throughout the setup is shown as a false-colour map, and the simulated integrated intensity at the detector is shown above the setup in a solid red line. It can be observed that the majority of the contribution to the exiting beam of the cavity comes from the classical bouncing path.

To model decoherence due to surface roughness and defects in the crystal, we introduce identity nodes near the blade surfaces. For these nodes, we replace the Bragg diffracting operators (equation (2)) with free space operators (equation (9)) as shown in figure 6(a). The free space nodes are randomly added to each unitary scattering operator $C_i$ (equation (5)) within a penetration depth of one $\Delta_H$ into the crystal blades.

Figure 5. (a) The intensity reflected from the bottom surface of the top crystal as a function of position, for different inter-crystal spacing distances $D$. There are two different regimes: when the spacing is smaller than the pendellösung length, the neutron state is represented by a standing wave, whose frequency depends on crystal spacing. The second regime is where the spacing is larger than the pendellösung length. Here the neutron bounces are well-separated at first followed by self interference after many bounces. There is a noticeable disruption around $175\Delta_H$ (indicated by a downwards arrow) caused by the first reflection from the back face of the top crystal. (b) The frequency spectrum of the intensity profiles shown in figure 5(a). In the region of $D < \Delta_H$, there is one dominant frequency, which varies with $D$. As the spacing increases, the neutron bounces become well-separated, and new frequencies appear corresponding to the higher harmonics of the main bounce frequency.
Figure 6. (a) A depiction of how surface roughness and defects are simulated with the QI model. Black nodes are Bragg diffracting operators representing the silicon crystal (equation (2)). Blue nodes are free space operators (equation (9)) that are used for the gap between the blades and crystal imperfections that induce decoherence. (b) The experimental implementation of a neutron cavity using two perfect crystal silicon blades and a position sensitive neutron detector above the top blade. Using the described QI model of DD we can simulate the neutron propagation through the cavity. Here the nodes outside the two crystals act as identity matrices, while a quantum random walk occurs inside the two crystals ($\gamma = \pi/50$ in equation (7)). No further physics or boundary conditions are present. Neutrons are incident to the bottom face of the top crystal at the Bragg angle. The geometric trajectory of the neutron as it bounces back and forth is clearly visible between the two crystals. Shown above in black is the experimental measurement corresponding to this geometry. Overlaid in the solid red line, is the intensity obtained via the QI model. Note that as shown in [27], the QI model accounts for experimental parameters by convolving the intensity output with the shape of the exiting beam. Good agreement is found between the simulation and experiment.

The simulated intensity profile in figure 6(b) is an average over 10 runs to avoid features from randomly located defects. We find good agreement with the measured intensity profile when 28% of the nodes within one $\Delta H$ (in this case $\Delta H = 38.98 \mu m$) of the four parallel crystal faces are identity nodes.

5. Conclusion and discussion

In conclusion, we have applied the QI model of DD to the case of a neutron cavity composed of two perfect crystal silicon blades. The model enables us to study the dependence of the cavity modes on the system geometry. Full analysis is provided and good agreement is found between an experimental implementation and the simulation of the particular setup.

Several exciting applications and proposed measurements rely on neutron confinement inside such cavities. Our work presents an in-depth analysis of the neutron behaviour inside the crystal blades and the crystal spacing. Therefore, we expect that the QI model will become a standard and easily-accessible tool used for experimental analysis that relies on neutron DD.
Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

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ORCID iDs

O Nahman-Lévesque https://orcid.org/0000-0003-2413-3556
D Sarenac https://orcid.org/0000-0001-8575-3367
O Lailey https://orcid.org/0000-0003-1051-1683
M G Huber https://orcid.org/0000-0002-3795-8445
D A Pushin https://orcid.org/0000-0002-4594-3403

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