# NEUTRON SPIN–PENDELLÖSUNG RESONANCE

Michael A. HORNE*, K.D. FINKELSTEIN, C.G. SHULL, Anton ZEILINGER** and
Herbert J. BERNSTEIN***

*Department of Physics, Massachusetts Institute of Technology, Cambridge, MA 02139, USA*

A novel resonant enhancement of the spin–orbit scattering of thermal neutrons in a perfect crystal is predicted. The effect occurs when the Larmor precession distance for the neutron in an externally applied magnetic field coincides with the pendellösung distance in the crystal. The potential is described, the wave functions are derived, and an experiment is proposed.

## 1. Introduction

As a neutron moves through matter, its magnetic moment senses the electric charges via the $v \times E$ magnetic field (spin–orbit interaction). This electromagnetic interaction scatters the neutron wave function, but for a thermal neutron the scattered intensity per atom is four orders smaller than the strong-interaction scattering by the nucleus and hence not easily observed [1]. However, we show here that when the matter is a crystal immersed in a suitable external magnetic field and the neutron wave function fulfills Bragg's condition, the electromagnetic scattering is dramatically enhanced and becomes comparable to the nuclear scattering. The enhancement is a resonant effect which occurs when the Larmor precession distance in the external field coincides with the pendellösung distance in the crystal [2]. Hence we call the effect neutron spin-pendellösung resonance.

Fig. 1 depicts the arrangement under consideration. The plane $z = 0$ is the entrance surface of a perfect crystal; the region $z > 0$ is the crystal and the region $z < 0$ is empty. The particular set of crystal planes of interest is also indicated. These planes are perpendicular to both the plane
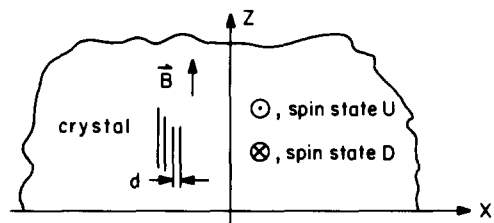


Fig. 1. The crystal position, the lattice planes, the $B$ field, the coordinates, and the two spin states used in our discussion.

of the figure and the $x$ axis and have spacing $d$. The adjustable strength external magnetic field $B$ is parallel to $z$ as indicated [3]. The choice of basis states for the spin is also shown: The "up" spin state $U$ is out of the plane of the figure and the "down" spin state $D$ is into the plane. Finally, we will be considering a neutron whose momentum lies in the plane of the figure, i.e., the plane of the figure is the scattering plane of the Bragg diffraction process.

## 2. Potential

The total potential considered here consists of three parts: the nuclear, the spin–orbit and the potential arising from the external magnetic field.

The nuclear interaction potential $V_N$ of a neutron with a *single nucleus* is usually described as simply a delta-function spike with an adjustable parameter to be determined by experiment. This

description is due to Fermi, who wrote the factor multiplying the delta function as $(2\pi\hbar^2/m)b$ so that, then, the adjustable parameter is the scattering length, $b$. Experiment reveals that $b \simeq 10^{-15}$ m and that both positive and negative values occur. Note that the potential function for a single nucleus (i.e., delta) is an *even* function about the position of the nucleus.

To describe the complete nuclear potential seen by a neutron in a perfect *crystal*, one initially imagines a periodic array of Fermi spikes, one at each nucleus. In the theory of crystal diffraction, this potential is first Fourier-expanded over all reciprocal lattice vectors and then inserted in Schrödinger's equation. When one is studying diffraction from a particular set of lattice planes, as we are, all coefficients in the Fourier series are ignored except the mean potential $V_0$ and a coefficient $V_1$ associated with the particular set of planes. Then the nuclear interaction potential $V_N$ is effectively just

$$V_N = V_0 + 2V_1 \cos(Gx) . \qquad (1)$$

Here, the factor 2 has been inserted for convenience in later expressions. The origin of the $x$ axis has been placed at one of the crystal planes (hence the *even* cosine function) and $G = 2\pi/d$. The values of $V_0$ and $V_1$ can be calculated from the structure of the crystal, the temperature, and $b$. To summarize, the array of Fermi spikes has been replaced by a simple corrugation potential.

The existence of the neutron magnetic moment implies [4] that the spatially even, spin-independent nuclear potential must be augmented by a spatially odd and spin-dependent electromagnetic potential. This potential arises because, as the neutron passes the nucleus, its magnetic moment senses the radial electric field of the nucleus via the $v \times E$ magnetic field (spin–orbit interaction). The oddness of this spin–orbit potential $V_{SO}$ follows from the fact that, since $E$ is radial, $v \times E$ just to the right of the nucleus is into the plane of fig. 1 and just to the left it is out of the plane.

This picture of the spin–orbit potential $V_{SO}$ (i.e., spatially odd and with a sign change upon spin reversal from $U$ to $D$) applies not only to a

bare nucleus but also to a complete atom and hence to each site of the crystal array. If one is interested in Bragg diffraction from a particular set of planes, one again retains only the lowest order Fourier components. Hence one can write simply

$$V_{SO} = \begin{cases} + 2V_2 \sin(Gx), & \text{for spin state } U , \\ -2V_2 \sin(Gx), & \text{for spin state } D . \end{cases} \qquad (2)$$

Again, the factor 2 is included for convenience later. The required spatial oddness of the interaction is reflected in the use of sine instead of cosine. For a neutron of specified energy, and a particular reflection in a particular crystal, the value of $V_2$ may be calculated from the magnetic moment and speed of the neutron, and from the total $E(r)$ field of the atomic nucleus and electrons. (The electronic contribution to $E(r)$ may be obtained from either quantum theoretical values or those effectively determined by X-ray diffraction data which reflect the electron charge distribution of the atom). For a thermal neutron in silicon, $V_2 \simeq 10^{-2}V_1$.

Finally, an externally produced homogeneous magnetic field contributes the external potential

$$V_{ext} = \begin{cases} +V_3, & \text{for spin state along } B , \\ -V_3, & \text{for spin state along } -B . \end{cases} \qquad (3)$$

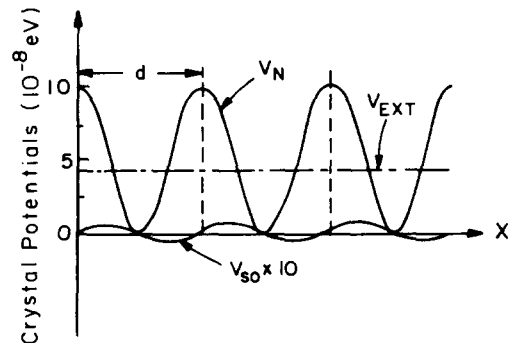Here $V_3 = \mu B$, $\mu$ being the neutron magnetic moment. Note that the spin states appearing in



Fig. 2. The three potentials are the nuclear potential $V_N$ and the spin–orbit potential $V_{SO}$ of the crystal, and the external potential $V_{ext}$ due to the applied magnetic field. The magnitudes shown for $V_N$ and $V_{SO}$ are for a typical reflection in silicon. The $V_{ext}$ is of course adjustable and the $V_{SO}$ and $V_{ext}$ as shown are for specific spin states (See eqs. (2) and (3)).

(3) are *not* the base states $U$ and $D$. Fig. 2 depicts the three parts of the total potential.

## 3. Wave functions

We will now construct a set of four base states suitable for describing any [5] Bragg diffraction experiment in the total potential

$$V = V_N + V_{SO} + V_{ext} . \qquad (4)$$

Let $\Psi(x, z, t)$ denote one of the base states associated with the potential (4). We assume that this $\Psi$ factors, describes a neutron of *definite energy* $E$, and describes a neutron of *definite z-momentum*. Hence, we write

$$\Psi(x, z, t) = X(x)Z(z)T(t) , \qquad (5)$$

$$T(t) = \exp[-iEt/\hbar] , \qquad (6)$$

$$Z(z) = \exp[iK_z z] . \qquad (7)$$

Here $E$ is considered a single known value, but the allowed values of $K_z$ are unknown and will be determined below, after the $X(x)$ functions have been first determined.

The wave function $X$ must be a *spinor*. The most general $x$-dependent spinor is a superposition of the base spinors $U$ and $D$,

$$X(x) = X_U(x)U + \exp[i\phi]X_D(x)D , \qquad (8)$$

where $X_U$ and $X_D$ are arbitrary functions of $x$ and a relative phase $\phi$ has been explicitly exhibited for convenience. The *physics of Bragg diffraction* dictates that $X_U$ and $X_D$ each must be a standing wave, i.e., a superposition of right-

running $(K_x = +G/2)$ and left-running $(K_x = -G/2)$ waves of equal amplitude. Thus, without loss of generality,

$$X_U(x) = \sin[(Gx/2) - (\theta/2)] , \qquad (9)$$

$$X_D(x) = \sin[(Gx/2) - (\theta'/2)] , \qquad (10)$$

where $\theta$ and $\theta'$ are phases to be determined. The left-right/up-down *symmetries* in figs. 1 and 2 imply that, if the $X_U$ standing wave is displaced to one side of the origin, the $X_D$ wave must be displaced equally far to the other side. Hence,

$$\theta' = -\theta . \qquad (11)$$

To determine the phases $\phi$ and $\theta$, we appeal explicitly to the potential (4) via the following *extremum principle*:

The phases $\phi$ and $\theta$ appearing in $X$ are to be adjusted so that the expectation value of the total potential $\langle V \rangle_X$ is an extremum.

One justification for this principle stems from the fact that it correctly yields already known base states when any one (two) of $V_1$, $V_2$, $V_3$ is (are) zero. Applying the principle to the general case, we find $\langle V \rangle_X$ has extrema at *four* points in the region $0 < \phi < 2\pi$, $0 < \theta < 2\pi$, of the $(\phi, \theta)$ phase plane. Thus the system has *four* natural base states; call them $\psi_1$, $\psi_2$, $\psi_3$, and $\psi_4$. These are listed in table I along with their associated phases and expectation values for the potential.

Finally, the $K_z$'s appearing in (7) are found from the *energy constraint*:

$$K_z = +[(2m/\hbar^2)(E - \langle V \rangle_X) - (G/2)^2]^{1/2} . \qquad (12)$$

Table I
Some phases and expectation values used in constructing the four base states.

| Base state $\psi$ | Phase $\phi$ | Phase $\theta$ | Expectation value $\langle V \rangle_X$ |
|---|---|---|---|
| $\psi_1$ | $\phi_1 = 0$ | $\theta_1 = \tan^{-1}[V_2/(V_1 + V_3)]$ | $\langle V \rangle_{X_1} = V_0 - [(V_1 + V_3)^2 + V_2^2]^{1/2}$ |
| $\psi_2$ | $\phi_2 = \pi$ | $\theta_2 = \tan^{-1}[V_2/(V_1 - V_3)]$ | $\langle V \rangle_{X_2} = V_0 - [(V_1 - V_3)^2 + V_2^2]^{1/2}$ |
| $\psi_3$ | $\phi_3 = \pi$ | $\theta_3 = \theta_2 + \pi$ | $\langle V \rangle_{X_3} = V_0 + [(V_1 - V_3)^2 + V_2^2]^{1/2}$ |
| $\psi_4$ | $\phi_4 = 0$ | $\theta_4 = \theta_1 + \pi$ | $\langle V \rangle_{X_4} = V_0 + [(V_1 + V_3)^2 + V_2^2]^{1/2}$ |

Since the four $\psi$'s have different $\langle V \rangle_X$, they have different $K_z$'s; call them $K_1$, $K_2$, $K_3$, and $K_4$.

To summarize, the four base states for describing Bragg diffraction in the potential (4) are each given by (5), together with eqs. (6) through (12) and the appropriate phases and expectation values in table I.

## 4. Proposed experiment

Illumination of the crystal with a polarized Bragg neutron of energy $E$ produces, in general, a superposition of $\psi_1 \ldots \psi_4$ inside the crystal. Because of the different values of $K_1 \ldots K_4$, beats occur in the various intensities [6] as a function of depth $z$. This oscillatory character survives even with an unpolarized incident beam. For example, if an unpolarized beam approaches the crystal from, say, left to right ($K_x = G/2$), the total (i.e., no spin analyzer present) intensity moving right to left (i.e., the Bragg intensity) at depth $z$ is

$$I = \tfrac{1}{2}[1 - \cos(\sigma z) \cos(\mu z)$$
$$+ \cos \eta \sin(\sigma z) \sin(\mu z)] , \qquad (13)$$

where $2\sigma = K_1 - K_4$, $2\mu = K_2 - K_3$ and $\eta = \theta_2 - \theta_1$.

In the special case of zero magnetic field ($\mu = \sigma$ and $\eta = 0$), eq. (13) reduces to

$$I = \tfrac{1}{2}[1 - \cos(2\sigma z)] \quad \text{(no magnetic field)} . \qquad (14)$$

Several years ago, one of us (CGS) observed [7] the interference fringes (14), known as pendellösung fringes. The characteristic distance (pendellösung length), $\Delta = 2\pi/\sigma$, is about 100 μm in silicon. The fringes were displayed by varying the incident neutron energy and thereby $\Delta$.

Returning to the general expression (13), we note the complicated dependence on magnetic field strength via $\sigma$, $\mu$, and $\eta$. Fig. 3 shows this dependence for three different crystal thicknesses, selected such that $I = 0$ at zero field. The resonance at $V_3 = V_1$ is caused by the spin–orbit interaction $V_2$; for with $V_2 = 0$, the resonance is not present. The condition for its appearance,
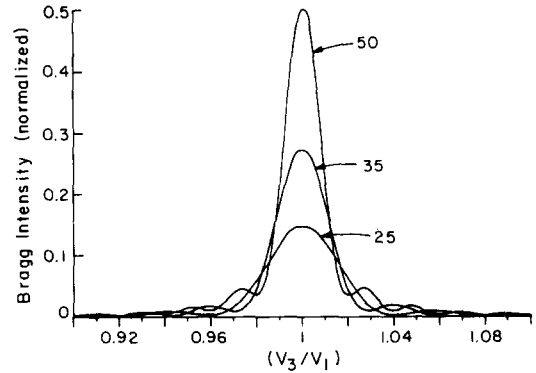


Fig. 3. Expected variation in intensity of Bragg diffracted radiation as a function of applied magnetic field strength. Results are given for three crystal thicknesses: 25, 35, and 50 pendellösung length units. Here $V_2 = 10^{-2}V_1$, typical of silicon. The intensity has been normalized to the incident intensity.

$V_3 = V_1$, is that the Larmor precession distance in the external field coincides with the pendellösung distance in the crystal. For silicon, the required magnetic field is about 6 kG, independent of neutron energy.

## References

[1] C.G. Shull, Phys. Rev. Lett. 10 (1963) 297.
[2] A. Zeilinger, M.A. Horne and H.J. Bernstein, J. de Physique 45 (1984) C3-209.
[3] The external field direction may be taken anywhere in the $(x, z)$ plane without altering our final result, eq. (13). However, the symmetry argument used to justify eq. (11) is simplest with the field parallel to $z$. Experimentally, the most convenient direction is along $x$.
[4] For simplicity we ignore the interaction of the neutron magnetic moment with the magnetic moments of the electrons and the nucleus.
[5] The wave functions presented here describe radiation which fulfills Bragg's condition *exactly*. More general wave functions will be published in Phys. Rev. B.
[6] At any depth $z$ the neutron may be found moving either left or right and its spin may be found either up or down. Thus there are 4 intensities.
[7] C.G. Shull and J.A. Oberteuffer, Phys. Rev. Lett. 29 (1972) 871.