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An Extremum Principle for a Neutron Diffraction Experiment

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An extremum principle was postulated by Horne, Finkelstein, Shull, Zeilinger, and Bernstein in order to derive the physically allowable parameters for sinusoidal standing waves governing a neutron in a crystal which is immersed in a strong external magnetic field: "the expectation value of the total potential $\langle V \rangle$ is an extremum." We show that this extremum principle can be obtained from the variational principle used by Schrödinger to derive his nonrelativistic wave equation. We rederive the solutions found by the above-mentioned authors as well as some additional solutions.

1. DEDICATION

Dan Greenberger is passionately devoted to research in the foundations of physics and, at the same time, is fascinated with the explanation of concrete physical phenomena. It is appropriate, consequently, to dedicate to him a note showing that a variational formulation of the Schrödinger equation provides a direct justification of a practical rule for analyzing a neutron diffraction experiment. Dan exhibits another duality, which no scientific paper could adequately illustrate: he has both a strong critical intellect and a wonderfully warm and generous character—two features seldom exhibited in the same person.

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2. A NEUTRON DIFFRACTION EXPERIMENT

Since the strong interaction of a thermal neutron with a nucleus in a crystal is four orders of magnitude larger than the typical spin-orbit interaction with the radial electric field of a nucleus or a complete atom, it is surprising to learn that the effect of the latter is greatly enhanced when the neutrons fulfill Bragg's condition in entering a crystal and the crystal is immersed in a strong external magnetic field. This enhancement is a resonance effect that has been analyzed by Horne *et al.*[1] and exhibited experimentally by Finkelstein.[2]

In the experimental arrangement (Fig. 1) analyzed by Horne *et al.*,[1] the plane $z = 0$ is the entrance plane of a perfect crystal, the crystal occupying the region $z > 0$. The set of crystal planes responsible for the Bragg scattering of interest lie perpendicular to the xy-plane, parallel to the z-direction, with spacing d. The neutrons propagate in the xz-plane and enter the crystal at the Bragg angle β for the designated set of scattering planes,

$$\beta = \sin^{-1}(\pi/kd) \qquad (1)$$

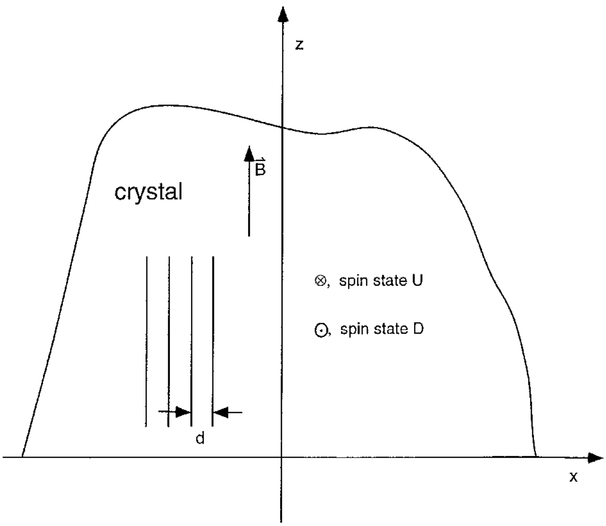

Fig. 1. The plane $x = 0$ is the entrance surface of a perfect crystal. The crystal planes of interest are perpendicular both to the plane of the figure and to the x-axis and have spacing d. The magnetic field **B** is along the z-axis. The "up" spin state U is out of the plane of the figure, and the "down" spin state D is into the plane.

Here k is the neutron's wave number, and the angle β is measured from the z-axis in the xz-plane. A basis for the spin states is U (up along the y-axis) and D (down along the y-axis). The external magnetic field of strength B is imposed in the z-direction. There are three effective contributions to the potential experienced by the neutron: First,

$$V_{\rm N} = V_0 + 2V_1 \cos(Gx), \qquad G = 2\pi/d \tag{2}$$

This formula is derived by keeping the two lowest-order terms associated with the designated set of planes in the Fourier series expansion in reciprocal lattice vectors of the periodic array. The array consists of delta-function spikes located (by an idealization) at each nucleus of the crystal. Second,

$$V_{\rm SO} = \pm 2\ V_2 \sin(Gx), \qquad + \text{ for spin state U}, \quad - \text{ for spin state D} \tag{3}$$

which is due to the interaction of the neutron's magnetic moment μ with the $\mathbf{v} \times \mathbf{E}$ magnetic field. Third,

$$V_{\rm ext} = \pm\ V_3, \qquad + (-) \text{ for spin up (down) along } \mathbf{B} \tag{4}$$

where $V_3 = \mu\mathbf{B}$.

The strategy of Horne *et al.*[1] is to use general physical considerations concerning Bragg diffraction to write solutions to the Schrödinger equation obtained by taking as the total potential

$$V = V_{\rm N} + V_{\rm SO} + V_{\rm ext} \tag{5}$$

The wave function is written as

$$\Psi(x, z, t) = X(x)\ Z(z)\ T(t) \tag{6}$$

where the geometry shows that there is no dependence upon y. If the neutron has a definite energy E and a definite z-component of linear momentum, then

$$T(t) = \exp(-iEt/h) \tag{7}$$

and

$$Z(z) = \exp(ik_z z) \tag{8}$$

The authors claim, furthermore, that because of $V_{\rm SO}$, the function $X(x)$ must be a superposition of multiples of the spinors U and D, which can be written (somewhat more generally than they do) as

$$X(x) = (\cos\alpha)\ X_{\rm U}(x)\ U + (\sin\alpha) \exp(i\phi)\ X_{\rm D}(x)\ D \tag{9}$$

The physics of Bragg diffraction requires that X_U and X_D are both standing waves, approximately of the general form[3]

$$X_U(x) = \sin[(Gx/2) - (\theta/2)] \tag{10}$$

$$X_D(x) = \sin[(Gx/2) - (\theta'/2)] \tag{11}$$

There are four parameters in Eqs. (8)–(11) for $X(x)$, which the authors of Ref. 1 propose to determine by the *extremum principle* that "the expectation value of the total potential $\langle V \rangle_X$ is an extremum." Actually, they state and use this extremum principle only for the purpose of determining the parameters θ and φ, since they invoke left–right/up–down symmetries in order to infer $\theta' = -\theta$, and they assert the equality of the amplitudes $\cos\alpha$ and $\sin\alpha$ on the grounds of the "physics of Bragg diffraction" without further explanation. We use the extremum principle to obtain constraints on all four parameters, but we also invoke physical considerations to eliminate some of the sets of parameters that satisfy the extremum principle. We also note that k_z, the z-component of the wave number, is constrained by the average value of the potential energy and hence by the parameters θ, θ', ϕ, and α, a constraint that is taken into account in the calculation below.

The main theoretical question which we address in this note is how to justify rigorously the extremum principle, which the authors of Ref. 1 justify only by a weak induction, noting that it holds in the already known cases when at least one of the three magnitudes V_1, V_2, and V_3 is zero. It is gratifying to report that a suitable generalization of the third equation of the first[4] of Schrödinger's initial series of papers on wave mechanics in 1926 provides the desired answer.

3. AN APPLICATION OF THE VARIATIONAL PRINCIPLE OF NONRELATIVISTIC QUANTUM MECHANICS

Schrödinger[4] writes a variational principle for his wave equation in the special case of a coulomb potential and spinless particle. Further details are given by Morse and Feshbach.[5] Generalizing to a spin-half particle with an arbitrary potential, we have the variational principle:

$$\delta J = \delta \int dx\, dy\, dz\, dt [(-\hbar^2/2m)(\mathrm{grad}\, \Psi^+)(\mathrm{grad}\, \Psi) - \Psi^+ V \Psi] = 0 \tag{12}$$

Here Ψ is spinorial, and the symbol $^+$ stands for the hermitian adjoint. The variation δ is within the class of functions constrained by Eqs. (5)–(10), hence only over the parameters θ, θ', ϕ, and α occurring in those equations. (The first three of these parameters have values in the interval $[0, 2\pi)$, but the fourth is restricted to $[0, \pi/2]$.) Conservation of energy entails that the sum of the average of the kinetic energy $\langle KE \rangle$ and the average of the potential energy $\langle V \rangle$ is equal to the total energy E, where the former average is the integral of the first term in the brackets in Eq. (12) and the latter average is the integral of the second term in the brackets. The standard Lagrange multiplier technique deals with the constraint by replacing Eq. (12) with

$$\delta[J - \lambda(\langle KE \rangle + \langle V \rangle - E)]$$

$$= \delta \int dx\, dy\, dz\, dt[(1-\lambda)(-\hbar^2/2m)(\text{grad } \Psi^+)(\text{grad } \Psi)$$

$$-(1-\lambda)\, \Psi^+ V \Psi + \lambda E \psi^+ \psi] = 0 \tag{12a}$$

Because Ψ is independent of y, the y-integration in Eq. (12a) is trivial. Furthermore, Ψ is periodic in x, z, and t, and the integration with respect to these variables will be performed over a very large region comprising many equivalent cells. The integral of the kinetic energy density—i.e., the first term in the integrand of Eq. (12a)—is not explicitly dependent on the four parameters. Furthermore, the integration with respect to z and t of the potential energy density—i.e., the second term of the integrand of Eq. (11)—is trivial, leaving, after cancellation of $(1+\lambda)$,

$$\delta\langle V \rangle_X = \delta \int dx \{X(x)^+ \; V X(x)\} = 0 \tag{13}$$

This is exactly the extremum principle stated without proof in Ref. 1. The main purpose of this note is therefore accomplished. Since we have used more parameters than in Ref. 1, however, it is important to work out the consequences of the extremum principle in detail.

4. DETERMINATION OF THE PARAMETERS

We represent the spinor U by a column matrix with 1 as the upper element and 0 as the lower element, and D by a column matrix with 0 as the upper and 1 as the lower element; and we write the potentials of Eqs. (3) and (4) as

$$V_{SO} = [2V_2 \sin(Gx)]\, \sigma_3 \tag{14}$$

and

$$V_{\mathrm{ext}} = -V_3\sigma_1 \tag{15}$$

where σ_1 and σ_3 are conveniently chosen Pauli matrices. Then the integral of Eq. (13) becomes

$$\begin{aligned}\langle V\rangle_x = \int dx\{&\cos^2\alpha\sin^2[(Gx/2)-(\theta/2)][V_0+2V_1\cos(Gx)+2V_2\sin(Gx)]\\ &+\sin^2\alpha\sin^2[(Gx/2)-(\theta'/2)][V_0+2V_1\cos(Gx)-2V_2\sin(Gx)]\\ &+\cos\alpha\sin\alpha\sin[(Gx/2)-(\theta/2)]\\ &\times\sin[(Gx/2)-(\theta'/2)](-V_3)\,2\cos\phi\}\end{aligned} \tag{16}$$

By trigonometric identities,

$$\sin^2[(Gx/2)-(\theta/2)] = (\tfrac{1}{2})[1-\cos Gx\cos\theta-\sin Gx\sin\theta] \tag{17}$$

and likewise with θ' substituted for θ. Also by identities,

$$\begin{aligned}&\sin[(Gx/2)-(\theta/2)]\sin[(Gx/2)-(\theta'/2)]\\ &\quad=(\tfrac{1}{2})\cos[(\tfrac{1}{2})(\theta'-\theta)]-(\tfrac{1}{2})\cos[Gx-(\tfrac{1}{2})(\theta+\theta')]\end{aligned} \tag{18}$$

If Eqs. (17) and (18) are inserted in Eq. (16), the integration over a potential period of length d can be performed by inspection:

$$\begin{aligned}\langle V\rangle_X = \text{constant}+(d/2)\{&\cos^2\alpha[-V_1\cos\theta-V_2\sin\theta]\\ &+\sin^2\alpha[-V_1\cos\theta'+V_2\sin\theta']\\ &-V_3\cos\alpha\sin\alpha\,2\cos\phi\cos[(\tfrac{1}{2})(\theta'-\theta)]\}\end{aligned} \tag{19}$$

where the constant is independent of the four parameters.

Setting to zero the derivatives of Eq. (19) with respect to each of the four parameters yields

$$\begin{aligned}&\cos^2\alpha[+V_1\sin\theta-V_2\cos\theta]\\ &\qquad-V_3\cos\alpha\sin\alpha\sin[(\tfrac{1}{2})(\theta'-\theta)]\cos\phi=0\end{aligned} \tag{20}$$

$$\begin{aligned}&\sin^2\alpha[V_1\sin\theta'+V_2\cos\theta']\\ &\qquad+V_3\cos\alpha\sin\alpha\sin[(\tfrac{1}{2})(\theta'-\theta)]\cos\phi=0\end{aligned} \tag{21}$$

$$V_3\cos\alpha\sin\alpha\cos[(\tfrac{1}{2})(\theta'-\theta)]\sin\phi=0 \tag{22}$$

$$\begin{aligned}&\cos\alpha\sin\alpha\{(V_1\cos\theta+V_2\sin\theta)+(-V_1\cos\theta'+V_2\sin\theta')\\ &\qquad+V_3(-\sin^2\alpha+\cos^2\alpha)\cos[(\tfrac{1}{2})(\theta'-\theta)]\cos\phi\}=0\end{aligned} \tag{23}$$

We consider several cases in seeking solutions to Eqs. (20)–(23).

Case (1):

$$\cos\alpha = \sin\alpha, \qquad \text{and} \qquad \sin\phi = 0 \tag{24}$$

Then Eq. (22) is satisfied, the last term of Eq. (23) vanishes, and Eqs. (20) and (21) yield

$$-V_1 \sin\theta + V_2 \cos\theta = V_1 \sin\theta' + V_2 \cos\theta' \tag{25}$$

By introducing the notation

$$\sin\gamma = V_1/(V_1^2 + V_2^2)^{1/2}, \qquad \cos\gamma = V_2/(V_1^2 + V_2^2)^{1/2} \tag{26}$$

we can rewrite Eq. (25) as

$$\cos(\gamma + \theta) = \cos(\gamma - \theta') \tag{27}$$

Hence, either

$$\theta' = -\theta \tag{28a}$$

or

$$\theta' = \theta + 2\gamma \tag{28b}$$

Now using Eqs. (24) and (16) in Eq. (23), we have

$$\sin(\gamma + \theta) = \sin(\gamma - \theta') \tag{29}$$

whence either Eq. (28a) is obtained again or

$$\theta' = \theta + 2\gamma - \pi \tag{29a}$$

Since Eq. (29a) is inconsistent with Eq. (28b), the only way to satisfy both Eq. (27) and Eq. (29) is by taking the option Eq. (28a). Since Eq. (24) allows two values of ϕ, namely, 0 and π, the insertion of these values in Eq. (20), or equivalently into Eq. (21), yields four choices of the parameters ϕ, θ, and θ' ($\cos\alpha = \sin\alpha = 1/\sqrt{2}$ in all subcases):

$$\phi = 0, \qquad \theta = \tan^{-1}[V_2/(V_1 + V_3)] + \eta \tag{30a,b}$$

$$\phi = \pi, \qquad \theta = \tan^{-1}[V_2/(V_1 - V_3)] + \eta \tag{30c,d}$$

where η is either 0 or π, and $\tan^{-1}(\ldots)$ lies in the interval $[0, \pi)$. Equations (30a)–(30d) state solutions obtained in Ref. 1.

Case (2):

$$\cos[(\tfrac{1}{2})(\theta' - \theta)] = 0, \qquad \sin[(\tfrac{1}{2})(\theta' - \theta)] = \pm 1 \tag{31a}$$

Then Eq. (22) is satisfied without any assumptions about ϕ or α. Equation (31) implies

$$\theta - \theta = \pi \text{ or } 3\pi \tag{31b}$$

so that

$$\cos\theta' = -\cos\theta, \qquad \sin\theta' = -\sin\theta \tag{31c}$$

If Eqs. (31a) and (31c) are inserted into Eq. (23), we obtain

$$\cos\alpha \sin\alpha \, 2V_1 \cos\theta = 0 \tag{32}$$

whence either

$$\cos\alpha = 0 \qquad \text{or} \qquad \sin\alpha = 0 \tag{32a}$$

or

$$\theta = \pi/2 \quad (\text{and } \theta' = 3\pi/2) \qquad \text{or} \qquad \theta = 3\pi/2 \quad (\text{and } \theta' = \pi/2) \tag{32b}$$

The options of Eq. (32a) are shown in Sec. 5 to be unphysical. Either of the options of Eq. (32b), when applied to Eqs. (20) and (21), yields

$$\sin^2\alpha = \cos^2\alpha \tag{33}$$

Using Eq. (33) and Eq. (32b) in Eq. (20) implies

$$\cos\phi = V_1/V_3 \tag{34}$$

Hence another set of solutions of Eqs. (20)–(23), not mentioned in Ref. 1, is

$$\begin{aligned} &\phi = \cos^{-1} V_1/V_3, \quad \theta = \pi/2 \text{ or } 3\pi/2, \quad \theta' = (\pi + \theta)(\text{mod } 2\pi) \\ &\alpha = \pi/4 \end{aligned} \tag{35}$$

Case (3):

$$\cos^2\alpha \neq \sin^2\alpha \tag{36}$$

We do not attempt to find the parameters satisfying Eqs. (20)–(23) for this case, because the checking in Sec. 5 of physical possibility poses problems which go beyond the scope of this paper. However, the special case of Case 3 stated in Eq. (32a), in which the neutrons are completely spin polarized, is discussed in Sec. 5.

5. THE SCHRÖDINGER EQUATION

If the expressions for the potential of Eqs. (5), (2), (14), and (15) are used in the variational principle Eq. (12), then the standard Euler–Lagrange method yields the Schrödinger equation,

$$(i\hbar)\,\partial\Psi/\partial t = (-\hbar^2/2m)\,\mathrm{grad}^2\,\Psi + [V_0 + 2V_1\cos(Gx) + 2V_2\sin(Gx)\,\sigma_3 - V_3\sigma_1]\,\Psi \tag{37}$$

If we insert the trial functions given by Eqs. (6)–(11) and perform the t, y and z integrations, we obtain the coupled equations

$$\begin{aligned}&\cos\alpha\{(-\hbar/2m)(d^2/dx^2) + (\hbar^2/2m)\,k_z^2\\ &\quad - E + V_0 + 2V_1\cos(Gx) + 2V_2\sin(Gx)\}\,\sin[(Gx/2) - (\theta/2)]\\ &= \sin\alpha\sin[(Gx/2) - (\theta'/2)]\exp(i\phi)\end{aligned} \tag{38a}$$

$$\begin{aligned}&\sin\alpha\{(-\hbar^2/2m)(d^2/dx^2) + (\hbar^2/2m)\,k_z^2 - E + V_0\\ &\quad + 2V_1\cos(Gx) - 2V_2\sin(Gx)\}\,\sin[(Gx/2) - (\theta'/2)]\exp(i\phi)\\ &= +\cos\alpha\sin[(Gx/2) - (\theta/2)]\end{aligned} \tag{38b}$$

Equations (38a) and (38b) imply that $\phi = 0$.

We do not expect these equations to be satisfied exactly for any values of the parameters, because in the case that has been investigated rigorously,[3] when V_2 and V_3 are zero, the exact solutions for the uncoupled equations are not sine functions but Mathieu functions. In Ref. 3 it is shown that the sine functions of Eqs. (10) and (11) are good approximations when the kinetic energy of the neutrons greatly exceeds the average potential energy. Rigorous solutions of the coupled Eqs. (38a) and (38b) are beyond the scope of this note, but we anticipate that they, too, will involve Mathieu functions.

We can, however, treat the subcase mentioned in Sec. 4, in which either $\cos\alpha$ or $\sin\alpha$ is zero, i.e., the neutrons are spin polarized along either U or D. For concreteness assume the former. Then the left-hand side of

Eq. (38a) is zero, while the right-hand side is a sine function with amplitude unity. Thus, Eq. (38a) is grossly violated. Hence one of the choices of parameters which satisfies the extremum principle of Secs. 3 and 4 is shown by a direct inspection of the Schrödinger equation to be physically impossible. Of course, spin-polarized solutions of Eqs. (38a) and (38b) are not precluded if the wave functions are taken to be linear combinations of the sine functions of the form of Eqs. (10) or (11), or linear combinations of Mathieu functions, but these possibilities are not investigated here.

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