Étude on the one-dimensional periodic potential

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All the formulas pertinent to dynamic diffraction in either the Bragg geometry or the Laue geometry are derived for an arbitrary one-dimensional periodic potential for which the reflection amplitude (r) and the transmission amplitude (t) for a single period are known. These formulas are derived by strictly algebraic methods. The diffraction of neutrons by monatomic and diatomic ideal single crystals is analyzed as an example. A general relation between the phases of the reflection and transmission amplitudes is proved by a gedanken experiment for an arbitrary nonabsorbing potential barrier.

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1. INTRODUCTION

Periodic potentials are nearly ubiquitous in solid state physics. They are related most directly to crystals and multilayer systems, which are presently finding progressively more technological applications. In many cases, crystals themselves may be thought of as multilayer systems; i.e., they can be described by a one-dimensional periodic potential.

Although the solution of the problem of the behavior of a particle in a one-dimensional periodic potential (an electron in the band theory of solids or a netron, for example, in the scattering of a particle by a crystal) was found a long time ago, the method for solving this problem is still far from perfected. Since it was formulated by Mathieu,[1] Floquet,[2] and—for quantum mechanics—Block,[3] it has remained essentially unchanged. It is true that attempts have been made to solve this problem by recurrence relations (e.g., Refs. 4–6), but these attempts have also been far from perfect and have resulted in some rather cumbersome expressions. In the present note we make use of specifically the method of recurrence relations. Using it, we put the solution of the problem of the behavior of a particle in a one-dimensional periodic potential in its simplest form. We do make the assumption that the transmission and reflection amplitudes for a single period, t and r, are known and are scalar functions of the energy of the particle.

Actual problems are usually three-dimensional, but to some extent they can be reduced to one-dimensional problems. An example is the case of Laue diffraction by a single crystal, which we will examine briefly at the end of this note. In some cases, three-dimensional effects can be dealt with by transforming from scalar functions t and r to matrix functions.

2. RECURRENCE RELATIONS; SEMI-INFINITE PERIODIC POTENTIAL; REFLECTION AMPLITUDE

We imagine an ideal semi-infinite periodic potential (Fig. 1) in which the periods are separated by infinitely narrow gaps of widths ϵ, in which the potential vanishes. It is physically obvious that infinitely narrow gaps will have no effect of any sort on the behavior of a particle, but their introduction makes it possible to monitor the motion of a particle without regard to its actual wave function in some specific potential or other. (We should stipulate that although we are talking about a wave function here, i.e., although we are talking in terms of quantum mechanics for definiteness, the arguments below also hold in other fields of physics in which periodic layered media arise: optics, acoustics, hydrodynamics, etc.) A real potential is usually not perfectly periodic, since the outermost periods will differ from the inner periods if there are long-range forces. This point, however, can be dealt with by introducing a surface potential and calculating the scattering by that potential separately.

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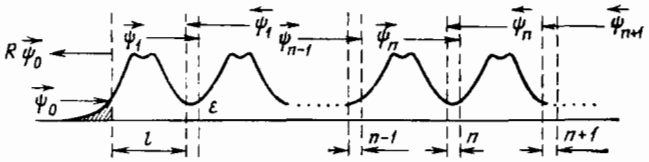

FIG. 1.

We assume that we know the outcome of scattering by an isolated period. In other words, we know the reflection amplitude $r(k)$ and the transmission amplitude $t(k)$ if the isolated period is flanked on its right and left by a vacuum; here k is the wave number of the incident neutron (for definiteness, we will be talking exclusively in terms of the scattering of neutrons, simply because that is the field of specialization of the author). If an isolated period is not symmetric with respect to its center, we need to distinguish between the cases of incidence on the potential from the left (we denote the corresponding amplitudes by $\vec{r}$ and $\vec{t}$) and from the right $\overleftarrow{r}$ and $\overleftarrow{t}$). In quantum mechanics we have the relations $\vec{t} = \overleftarrow{t} = t$, $\vec{r} = \overleftarrow{r} \times \exp(2i\eta) = re^{i\eta}$, in the case of an asymmetric potential,[7] where η is a phase which is real if the potential is real. We will show that this phase is inherited in the amplitude for reflection from the entire periodic potential with a finite or infinite number of periods.

We consider the nth gap. We denote by $\vec{\psi}_n$ the amplitude of a wave which is incident on the right wall of the gap, beyond which there is another infinite number of periods. We denote the amplitude for reflection from the semi-infinite periodic potential by $\vec{R}$. A wave reflected from the right wall of the n-th gap is then

$$\overleftarrow{\psi}_n = \vec{R}\vec{\psi}_n. \tag{1}$$

The wave $\vec{\psi}_n$ can be expressed in terms of $\vec{\psi}_{n-1}$ through the use of the recurrence relation

$$\vec{\psi}_n = \vec{t}\,\vec{\psi}_{n-1} + \overleftarrow{r}\,\overleftarrow{\psi}_n. \tag{2}$$

The first term corresponds to a wave which has passed from left to right through a single period, between the nth and the $(n-1)$st gaps; the second term corresponds to a wave which is reflected from the same period from the left. It follows from (1) and (2) that we have

$$\frac{\vec{\psi}_n}{\vec{\psi}_{n-1}} = (1 - \overleftarrow{r}\vec{R})^{-1}\,\vec{t}. \tag{3}$$

We now seek the wave $\overleftarrow{\psi}_{n-1}$, for which we can write relations similar to (1) and (2):

$$\overleftarrow{\psi}_{n-1} = \vec{R}\vec{\psi}_{n-1} = \vec{r}\vec{\psi}_{n-1} + \overleftarrow{t}\,\overleftarrow{\psi}_n. \tag{4}$$

Using (3), we then find

$$\frac{\overleftarrow{\psi}_{n-1}}{\vec{\psi}_{n-1}} = \vec{R} = \vec{r} + \overleftarrow{t}\vec{R}\,(1 - \overleftarrow{r}\vec{R})^{-1}\,\vec{t}. \tag{5}$$

For $\vec{R}$ and, similarly, for $\overleftarrow{R}$, we thus have the equations

$$\vec{R} = \vec{r} + \overleftarrow{t}\vec{R}\,(1 - \overleftarrow{r}\vec{R})^{-1}\vec{t}, \tag{6a}$$

$$\overleftarrow{R} = \overleftarrow{r} + \vec{t}\overleftarrow{R}\,(1 - \vec{r}\,\overleftarrow{R})^{-1}\vec{t}. \tag{6b}$$

Substituting into Eq. (6a,b) $\overleftarrow{r} = \vec{r}\exp(2i\eta) = r\exp(i\eta)$, we find $\overleftarrow{R} = \vec{R}\exp(2i\eta)$, i.e., the phase η is indeed inherited.

Multiplying both sides of Eq. (6a) by $\exp(i\eta)$, and using the notation $R = \vec{R}\exp(i\eta)$, we can put (6a) in the form

$$R = r + tR\,(1 - rR)^{-1}t, \tag{6c}$$

which is characteristic for a symmetric potential. In the case of a scalar potential, Eq. (6) is a quadratic algebraic equation:

$$R^2 - \frac{2R\,(r^2+1-t^2)}{2r} + 1 = 0. \tag{7}$$

The roots of the equation

$$x^2 - 2px + 1 = 0 \tag{8}$$

can be written

$$x_{1,2} = [(p+1)^{1/2} \mp (p-1)^{1/2}] \times [(p+1)^{1/2} \pm (p-1)^{1/2}]^{-1}. \tag{9}$$

Clearly, these roots are mutually reciprocal $x_2 = 1/x_1$. In the case of Eq. (7) we have

$$p \pm 1 = \frac{(r \pm 1)^2 - t^2}{2r}, \tag{10}$$

so we can write

$$R = \frac{[(r+1)^2 - t^2]^{1/2} - [(r-1)^2 - t^2]^{1/2}}{[(r+1)^2 - t^2]^{1/2} + [(r-1)^2 - t^2]^{1/2}}. \tag{11a}$$

Of the two possible roots we have selected that which leads to a zero reflection amplitude if the periods are fictitious, i.e., $r = 0$. If, on the other hand, we have $r = \pm 1$ and $t = 0$, then we also have $R = \pm 1$.

For an asymmetric scalar potential it is easy to verify that the following relations hold:

$$\vec{R} = \left(\frac{\vec{r}}{\overleftarrow{r}}\right)^{1/2} R, \quad \overleftarrow{R} = \left(\frac{\overleftarrow{r}}{\vec{r}}\right)^{1/2} R, \tag{11b}$$

where R is given by (11a) with

$$r = (\vec{r}\,\overleftarrow{r})^{1/2}. \tag{12}$$

3. BLOCH WAVE VECTOR

The complete wave function within a periodic potential is written in the form $\Psi(x) = \varphi(x)\exp(iqx)$, where $\varphi(x)$ is a periodic function, and q is a so-called Bloch wave vector. To find its magnitude, we need only compare the wave functions in two adjacent periods. It is not always possible to find the wave function in a single period for an arbitrary potential. Here again, however, we make use of the gap, since it is a part of a period, and in it, in the nth gap, for example, the wave function is

$$\psi_n = \vec{\psi}_n + \overleftarrow{\psi}_n = \exp(iql)\,\psi_{n-1} = \exp(iql)\,(\vec{\psi}_{n-1} + \overleftarrow{\psi}_{n-1}). \tag{13a}$$

Since the waves $\vec{\psi}$ and $\overleftarrow{\psi}$ are linearly independent, relation

(13a) holds for each of the waves separately:

$$\vec{\psi}_n = \exp(iql)\,\vec{\psi}_{n-1}, \quad \overleftarrow{\psi}_n = \exp(iql)\,\overleftarrow{\psi}_{n-1}. \tag{13b}$$

Making use of this circumstance, we rewrite Eq. (4) as

$$\overleftarrow{\psi}_{n-1} = [1 - \overleftarrow{t}\exp(iql)]^{-1}\vec{r}\vec{\psi}_{n-1}, \tag{14}$$

and by substituting (14) into (2) and using (13b) we find

$$\exp(iql) = \vec{t} + \overleftarrow{r}\exp(iql)\,[1 - \overleftarrow{t}\exp(iql)]^{-1}\vec{r}. \tag{15}$$

In the case of a scalar potential Eq. (15) becomes

$$X^2 - \frac{2X(t^2+1-r^2)}{2t} + 1 = 0, \tag{16}$$

where we have introduced $X = \exp(iql)$, $r = (\vec{r}\overleftarrow{r})$, and $t = \vec{t} = \overleftarrow{t}$. Of the two solutions of Eq. (16) we choose

$$\exp(iql) = \frac{[(t+1)^2-r^2]^{1/2}+[(t-1)^2-r^2]^{1/2}}{[(t+1)^2-r^2]^{1/2}-[(t-1)^2-r^2]^{1/2}}, \tag{17}$$

which, in empty space with a fictitious period $[r = 0,\ t = \exp(ikl)]$, leads to $q = k$, where k is the wave vector of the free neutron. Comparison of (17) and (11a) reveals

$$X(r, t) = R^{-1}(t, r). \tag{18}$$

4. PERIODIC POTENTIAL WITH A FINITE NUMBER OF PERIODS

To determine the reflection amplitude R_N and the transmission amplitude T_N of a periodic potential with N periods, we can make use of the fact that a potential which is periodic with a period l is also periodic with a period Nl. We can thus replace r and t by R_N and T_N in Eqs. (6), (7), (15), and (16). As a period l in (15) and (16) we should take Nl. As a result we find the equations

$$R^2 - \frac{2R(R_N^2+1-T_N^2)}{2R_N} + 1 = 0, \tag{19}$$

$$\exp(2iqlN) - 2\exp(iqlN)\,(T_N^2+1-R_N^2)\,(2T_N)^{-1} + 1 = 0. \tag{20}$$

Since R, $\exp(iql)$, and thus also $\exp(iqlN)$ are known and are given by expressions (11a) and (17), we can solve Eqs. (19) and (20) for R_N and T_N. After some simple algebraic manipulations we find

$$R_N = R\,[1 - \exp(2iqlN)]\,[1 - R^2\exp(2iqlN)]^{-1}, \tag{21a}$$

$$T_N = \exp(iqlN)\,(1 - R^2)\,[1 - R^2\exp(2iqlN)]^{-1}. \tag{21b}$$

These two expressions convert into each other upon the substitution $R \leftrightarrow \exp(iqlN)$ or $R \leftrightarrow \exp(-iqlN)$, as they should. In the case of an asymmetric potential, R in (21) should be replaced by $(\vec{R}/\overleftarrow{R})^{1/2}$. Furthermore, the reflection amplitudes $\vec{R}_N$ and $\overleftarrow{R}_N$ contains the factors $(\vec{R}/\overleftarrow{R})^{1/2}$ and $(\overleftarrow{R}/\vec{R})^{1/2}$, respectively.

If R and q are real, the phase R_N differs from the phase T_N by $\pm\pi/2$; we will need to make use of this relation below in proving a general theorem.

5. EXAMPLE 1. RECTANGULAR POTENTIAL

If the potential of a single period is simple enough, we can find analytic expressions for the amplitudes r and t. We begin with the rectangular potential step of height U_0 shown by the solid line in Fig. 2. The Schrödinger equation for a scalar particle in such a potential is

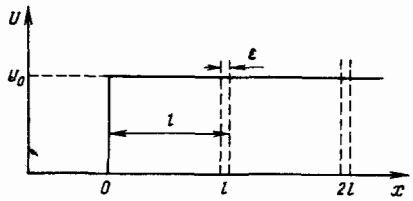

FIG. 2.

$$\frac{d^2\Psi(x)}{dx^2} - [u(x) - k^2]\,\Psi(x) = 0, \tag{22}$$

where the potential $U(x)$ can be represented by the unit step function θ:

$$u(x) = u_0\,\theta(x \geqslant 0). \tag{23}$$

This function is equal to one under the condition stated in the argument; otherwise it is zero. A solution of Eq. (22) can be sought in the form

$$\Psi(x) = (e^{ikx} + Re^{-ikx})\,\theta(x < 0) + \tau e^{ik'x}\theta(x > 0). \tag{24}$$

The coefficients R and τ are determined from the condition that the function and its derivative are continuous at the potential jump:

$$1 + R = \tau, \quad k(1 - R) = k'\tau. \tag{25}$$

Hence the reflection amplitude is

$$R = \frac{k-k'}{k+k'}, \quad k' = (k^2 - u_0)^{1/2}, \tag{26}$$

and the wave function inside the barrier is

$$\Psi(x) = \tau\exp(ik'x) = \frac{2k}{k+k'}\exp(ik'x). \tag{27}$$

Let us determine the amplitudes r and t for one rectangular barrier of width l, separated from the overall rectangular step by the first infinitely narrow gap shown by the dashed lines in Fig. 2. As before, we can seek these coefficients by requiring that the wave function and its derivative be continuous at both edges of the rectangular potential. We then find a system of four equations with four unknowns; this system is not difficult to solve, but the process is tedious. It is simpler again to make use of recurrence relations.

We denote by $\tilde{\psi}_1^+$ the wave which is incident on the right edge of the rectangular barrier from within the barrier. This wave consists of the wave which has been transmitted through the left edge of the potential, $\tau\exp(ik'l)$, and the waves which have been rereflected from both edges, etc.:

$$\tilde{\psi}_1^+ = \tau e^{ik'l} + e^{ik'l}\tilde{R}e^{ik'l}\tilde{R}\tilde{\psi}_1^+. \tag{28}$$

Here $\tilde{R}$ is the amplitude for reflection from the edge of the potential from within the barrier. This amplitude is defined in precisely the same way as (26):

$$\tilde{R} = \frac{k'-k}{k'+k} = -R. \tag{29}$$

Using (29), we easily find from (28)

$$\tilde{\psi}_1^\dagger = [1 - R^2 \exp(2ik'l)]^{-1} \tau \exp(ik'l). \tag{30}$$

We then determine the amplitude for reflection from the overall rectangular barrier

$$r = R + \tilde{\tau} e^{ik'l} \tilde{R} \tilde{\psi}_1^\dagger = R(1 - e^{2ik'l})(1 - R^2 e^{2ik'l})^{-1}, \quad \tilde{\tau} = 1 + \tilde{R} = \frac{2k'}{k' + k}. \tag{31}$$

The transmission amplitude t is

$$t = \tilde{\tau} \tilde{\psi}_1^\dagger = e^{ik'l}(1 - R^2)(1 - R^2 e^{2ik'l})^{-1}. \tag{32}$$

If the potential u_0 is real and if $k^2 > u_0$, the amplitude R is real, so that the phase of r differs from the phase of t by $\pm \pi/2$. If $k^2 < u_0$, then k' is purely imaginary, and R takes the form $\exp(-2i\chi)$. Consequently, the phases r and t again differ by $\pm \pi/2$, as can be seen easily from (31) and (32).

We also note that in the limit $l \to 0$ we find $r \to 0$ and $t \to 1$ from (31) and (32). In other words, an infinitely narrow barrier and also an infinitely narrow potential well have no effect on the behavior of a particle if the height of the barrier or the depth of the well is finite. This result proves that we are indeed justified in introducing infinitely narrow gaps in a potential, and in doing so we do not change the dynamics of a particle.

When we set up an infinite number of rectangular barriers of widths l side by side, separated by infinitely narrow gaps, we eventually obtain a semi-infinite potential, which is a simple potential step. The amplitude for reflection from it is the same as in (26). If we instead set up N such barriers side by side, we find that the amplitudes R_N and T_N calculated from (21) are the same as (31) and (32) after replacement of q by k', since the Bloch wave vector q calculated in accordance with (17) is exactly equal to k'.

6. EXAMPLE 2. KRONIG-PENNEY POTENTIAL

We now consider the potential shown in Fig. 3. We let the height of the rectangular barrier go to infinity, $U_0 \to \infty$, and the width a go to zero, in such a way that the product $U_0 a$ is a constant: $U_0 a = 2p_0$. In this case we find the potential

$$U(x) = 2p_0 \delta(x). \tag{33}$$

The wave function of the Schrödinger equation with potential (33) is continuous at the point $x = 0$, while its derivative has a discontinuity of $2p_0$ at this point. From these two conditions we find the reflection and transmission amplitudes, $\tilde{r}$ and $\tilde{t}$, of potential (33):

$$\tilde{r} = \frac{p_0}{ik - p_0}, \quad \tilde{t} = \frac{ik}{ik - p_0}. \tag{34}$$

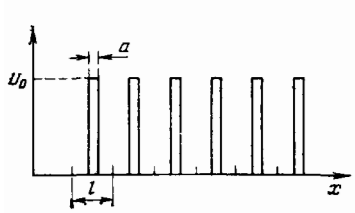

FIG. 3.

The Kronig-Penney potential is the sum of potentials (33) separated from each other by a distance l. How do we identify the period in this potential? For example, the period could be chosen to be asymmetric,

$$u(x) = 2p_0 \delta(x)\, \theta(0 \leqslant x < l),$$

by placing a δ-function at the beginning of the period. In this case we have $\vec{r} = \tilde{r}$ and $\overleftarrow{r} = \tilde{r}\exp(2ikl)$. If the period is to be symmetric, we must place the δ-function at its center:

$$u(x) = 2p_0 \theta(0 \leqslant x \leqslant l)\, \delta(x - l/2).$$

In this case we have

$$\vec{r} = \overleftarrow{r} = r = \tilde{r}\exp(ikl), \quad \vec{t} = \overleftarrow{t} = t = \tilde{t}\exp(ikl). \tag{35}$$

Substituting (35) into (11) and (17), we find

$$R = \frac{(x + p\,\mathrm{tg}\,x)^{1/2} - (x - p\,\mathrm{ctg}\,x)^{1/2}}{(x + p\,\mathrm{tg}\,x)^{1/2} + (x - p\,\mathrm{ctg}\,x)^{1/2}}, \quad x = \frac{kl}{2}, \quad p = p_0 \frac{l}{2}, \tag{36a}$$

$$\exp(iql) = \frac{(x\,\mathrm{ctg}\,x + p)^{1/2} + i(x\,\mathrm{tg}\,x - p)^{1/2}}{(x\,\mathrm{ctg}\,x + p)^{1/2} - i(x\,\mathrm{tg}\,x - p)^{1/2}}. \tag{37a}$$

In the case of monatomic crystals we have $p_0 = u_0 l/2$ and $u_0 = 4\pi N_0 b$, where N_0 is the number of atoms per unit volume, and b is the coherence length of the scattering.

Expressions (36a) and (37a) have branch points at $x = x_n = \pi n/2$ $n = 0,1,2,\ldots$. Near the point x_n it is convenient to introduce a function

$$f_n = \alpha_n \,\mathrm{ctg}\,\alpha_n \approx 1 - \frac{\alpha_n^2}{3} + \ldots, \quad \alpha_n = x - x_n,$$

which is regular at x_n and to rewrite expressions (36a) and (37a) in a simpler form. In the case $\alpha_n \geqslant 0$ we have

$$R = e^{i\pi n} \frac{[x\alpha_n + (p\alpha_n^2/f_n)]^{1/2} - (x\alpha_n - pf_n)^{1/2}}{[x\alpha_n + (p\alpha_n^2/f_n)]^{1/2} + (x\alpha_n - pf_n)^{1/2}}, \tag{36b}$$

$$q = k_n + \frac{2}{l} \arcsin\left[\sin\alpha_n \cdot \left(1 - \frac{pf_n}{x\alpha_n}\right)^{1/2}\right], \tag{37b}$$

where $k_n = \pi n/l$. In the case $\alpha_n \leqslant 0$ we have

$$R = \exp[i\pi(n-1)] \frac{(x\,|\alpha_n| + pf_n)^{1/2} - [x\,|\alpha_n| - (p\alpha_n^2/f_n)]^{1/2}}{(x\,|\alpha_n| + pf_n)^{1/2} + [x\,|\alpha_n| + (p\alpha_n^2/f_n)]^{1/2}}, \tag{36c}$$

$$R = k_{n-1} + \frac{2}{l} \arcsin\left[\sin\alpha_{n-1} \cdot \left(1 + \frac{p\alpha_n}{xf_n}\right)^{1/2}\right]. \tag{37c}$$

It follows from (36b) that under the conditions $p > 0$ and $0 < x\alpha_n < pf_n$ there is a total reflection. Here

$$R = \exp(i\pi n + 2i\chi),$$

$$\chi = -\arccos\left\{\left(\frac{x\alpha_n}{p}\right)^{1/2}\left[\frac{f + (p\alpha_n/x)}{f_n^2 + \alpha_n^2}\right]^{1/2}\right\}, \tag{36d}$$

$$q = k_n + i\Delta_n, \quad \Delta_n = \mathrm{arsh}\left[\sin\alpha_n \cdot \left(\frac{pf_n}{x\alpha_n} - 1\right)^{1/2}\right]. \tag{37d}$$

With increasing k inside the interval of total reflection, χ increases from $-\pi/2$ to 0. In the case $p < 0$, total reflection occurs at $pf_n < x\alpha_n < 0$, as follows from (36c). The corre-

sponding equations can be found from (36d) and (37d) through the substitutions $\alpha_n \to |\alpha_n|$ and $p \to |p|$. The width of the region of total reflection is found from the equation $x\alpha_n = pf_n$. Within $u_0 l^2$ this width is

$$|k^2 - k_n^2| = 2|u_0| \left[1 - \frac{u_0 l^2}{(\pi n)^2}\right]^{1/2}. \tag{38}$$

If we ignore corrections $\sim u_0 l^2$, we can approximate Eqs. (36a) and (37a) near the case of Bragg reflection by

$$R = (-1)^n \frac{(k - k_n^2)^{1/2} - (k^2 - k_n^2 - 2u_0)^{1/2}}{(k^2 - k_n^2)^{1/2} + (k^2 - k_n^2 - 2u_0)^{1/2}}; \tag{36e}$$

$$q \approx [k_n^2 \mp (k^2 - k_n^2)^{1/2} (k^2 - k_n^2 - 2u_0)^{1/2}]^{1/2}, \tag{37e}$$

where the sign inside the radical should be chosen in such a way that in the case $u_0 > 0$ the condition $q < k$ always holds, while at $u_0 < 0$ the condition $q > k$ always holds. The quantity q is determined in a single-valued way by the value of k, not in a double-valued way as follows from many text books.

The region $0 < x \lesssim \pi/2$ should be analyzed separately. In this region expressions (36a) and (37b) are conveniently written

$$R = \frac{x[1 + (p/f)]^{1/2} - (x^2 - pf)^{1/2}}{x[1 + (p/f)]^{1/2} + (x^2 - pf)^{1/2}}, \quad f = x \operatorname{ctg} x, \tag{36f}$$

$$\exp(iql) = \frac{(f^2 + pf)^{1/2} + i(x^2 - pf)^{1/2}}{(f^2 + pf)^{1/2} - i(x^2 - pf)^{1/2}}. \tag{37f}$$

The region of total reflection is determined by the relation $x^2 < pf$; we can then find the characteristic limiting energy for ultracold neutrons:

$$x_{\lim}^2 = pf \to k_{\lim}^2 \approx \frac{u_0}{1 + (u_0 l^2/12)}. \tag{39}$$

From (37f) we find

$$\cos\frac{ql}{2} = \cos x \left(1 + \frac{p}{f}\right)^{1/2},$$

$$\sin ql/2 = \sin x \left(1 - \frac{pf}{x^2}\right)^{1/2}. \tag{37g}$$

We can thus write (36f) as

$$R = \frac{\sin[(k - q)l/2]}{\sin[(k + q)l/2]}. \tag{36g}$$

This expression can be continued in a natural way to the entire domain of k. In particular, inside the interval of Bragg reflection we find from (36g) the approximate result

$$R = (-1)^n \frac{\alpha_n - i\Delta_n}{\alpha_n + i\Delta_n}, \quad \Delta_n \approx \left[\frac{\alpha_n}{2k_n(k^2 - k_n^2 - 2u_0)}\right]^{1/2}, \tag{36h}$$

from which we immediately find expression (36e).

In approximation (36e) it is a straightforward matter to calculate analytically the total intensity of Bragg reflection:

$$I = \int_{-\infty}^{\infty} |R(E)|^2 \, dE = \int_{-\infty}^{\infty} \left|\frac{y^{1/2} - (y - a)^{1/2}}{y^{1/2} + (y - a)^{1/2}}\right|^2 dy, \tag{40}$$

where $a = 2u_0\hbar^2/2m$, m is the mass of the neutrons, $y = E - E_n$, and $E_n = \hbar^2 k^2/2m$. A calculation can be carried out easily not only for a real potential u_0 but also for a complex potential. We reproduce here only the final result:

$$I = |u_0| f(\varphi), \quad \varphi = \operatorname{arctg}\frac{\operatorname{Im} u_0}{\operatorname{Re} u_0}, \tag{41}$$

$$f(\varphi) = -\pi \sin|\varphi| \cdot \cos 2|\varphi| - \frac{8}{3} + 4\cos^2\varphi + 4\cos|\varphi| \times \sin^2|\varphi| \ln \operatorname{ctg}\frac{|\varphi|}{2}. \tag{42}$$

7. RELATION BETWEEN THE PHASES OF THE AMPLITUDES *r* AND *t*

We have seen in several places that the phase r differs from the phase t by $\pm\pi/2$. We can now prove a general theorem.

Theorem. The following relation holds for an arbitrary real potential (We are talking here about a symmetric potential; the generalization to an asymmetric potential is obvious):

$$\arg(r) - \arg(t) = \pi\left(n + \frac{1}{2}\right). \tag{43}$$

The validity of this relation was proved in Ref. 8. We will prove this theorem in a slightly different way, by means of purely physical arguments. We appeal exclusively to the unitarity condition, which states that in the case of a purely real potential there should be neither a creation nor disappearance of particles.

Let us carry out a gedanken experiment, as illustrated in Fig. 4. Partially reflecting mirrors A and B are represented by the same potential, while mirrors M_1 and M_2 reflect totally. In other words, their reflection amplitude is -1. Two beams interfere at mirror B, and the result of the interference affects the count rates at detectors D_1 and D_2. The phase on one of the paths can be varied in an arbitrary way. As this phase is varied, the count rate of the detectors will change, but the total number of particles detected will always be equal to the number of incident particles. If the intensity of the incident particles is one, the total count rate is also one. Let us assume that the amplitude of the wave incident on mirror A is 1. The amplitude of the wave which propagates along the upper path in the direction of detector D_1 is then $re^{i\varphi}t$, while that which propagates along the lower path is tr. (We are considering only the phase difference on the two paths; we are ignoring the common phase, which is irrelevant.) Analogously, waves which have propagated along the upper and lower paths, with respective amplitudes $te^{i\varphi}t$ and rr, propagate in the direction of D_2 after mirror B. the total intensity detected by the two detectors is

$$I = |tre^{i\varphi} + tr|^2 + |t^2 e^{i\varphi} + r^2|^2 = 1. \tag{44}$$

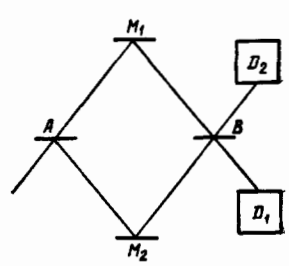

FIG. 4.

We open brackets. We introduce $r = |r|\exp(i\theta_r)$, $t = |t|\exp(i\theta_t)$ and note that we have $|r|^2 + |t|^2 = 1$. We then find

$$I = 1 + 2\,|t|^2\,|r|^2 \times [\cos\varphi + \cos(\varphi + 2\theta_t - 2\theta_r)] = 1. \quad (45)$$

Since the phase φ can be varied in an arbitrary way, and the product $|t||r|$ is generally not zero, we find $2(\theta_t - \theta_r) = (2n+1)\pi$ from the last equality. Q.E.D. (see also Refs. 9 and 10).

In particular, it follows from this theorem that if we introduce the notation $R = \exp(-\alpha)$ for a semi-infinite periodic potential, the quantities α and q are either both real or both imaginary. That this is true can be proved by using the relation

$$|r^2 - t^2| = |r|^2 + |t|^2 = 1. \quad (46)$$

Replacing r and t by R_N and T_N from (20) and (21), we find

$$R_N^2 - T_N^2 = [R^2 - \exp(2iqlN)]\,[1 - R^2\exp(2iqlN)]^{-1}. \quad (47)$$

If the resulting quantity is to have a unit modulus, either q and R are both real, or q and $\ln R$ are imaginary.

The later assertion can be illustrated in an interesting way in the case of a Kronig-Penney potential. This can be done conveniently without appealing to expressions (36) and (37). We write the infinite periodic potential

$$u(x) = 2p_0 \sum_{n=-\infty}^{\infty} \delta\left(x - x_n - \frac{l}{2}\right), \quad x_n = nl. \quad (48)$$

We can seek a solution of the Schrödinger equation with this potential in the form

$$\Psi(x) = \sum_n \exp(iqx_n)\,\psi_n(k, x)\,\theta \quad (x \in I_n), \quad (49)$$

where the interval I_n is the interval between two δ-functions:

$$I_n = \left(x_n - \frac{l}{2},\ x_n + \frac{l}{2}\right), \quad (50)$$

in which the wave function ψ_n consists of two free plane waves,

$$\psi_n(k, x) = \exp[ik(x - x_n)] + R(k)\exp[-ik(x - x_n)]. \quad (51)$$

The reflection amplitude $R(k)$ is given by expression (36), which is unimportant for the matter at hand. The wave functions in two neighboring intervals differ by only a phase $\exp(iql)$, which must not disrupt the continuity of the wave function at the point $x_n + l/2$. It follows from this continuity condition that we have

$$e^{ikl/2} + Re^{-ikl/2} = e^{iql/2}(e^{-ikl/2} + Re^{ikl/2}), \quad (52)$$

or

$$e^{iql/2} = (e^{ikl} + R)(1 + Re^{ikl})^{-1}. \quad (53)$$

It follows immediately that q is real when R is real, and we have $q = \pi n + i\Delta$, where Δ is real in the case $R = \exp(ix)$.

8. EXAMPLE 3. DIATOMIC CRYSTAL

We can use the results of the preceeding section to study more complicated periodic structures. For example, we consider a diatomic crystal. It is a simple matter to generalize the analysis of a diatomic crystal to more-complicated crystals. Polyatomic crystals are characterized by a structure factor. Just how this structure factor is manifested in the reflection amplitude and the Bloch vector can be found easily in the diatomic model.

We consider a periodic potential in which one period contains two reflecting planes:

$$u = \theta\,(0 \leqslant x \leqslant l)\,[2p_1\delta(x - l_1) + 2p_2\delta(x - l_1 - l_2)]. \quad (54)$$

A potential of this sort is explicitly asymmetric. The amplitudes $\vec{r}$, $\overleftarrow{r}$, and t, calculated by a recurrence approach, are

$$\vec{r} = \exp(2ikl_1)\,\{r_1 + r_2t_1^2\exp(2ikl_2)\,[1 - r_1r_2\exp(2ikl_2)]^{-1}\}, \quad (55a)$$

$$\overleftarrow{r} = \exp(2ikl_3)\,\{r_2 + r_1t_2^2\exp(2ikl_2)\,[1 - r_1r_2\exp(2ikl_2)]^{-1}\}, \quad (55b)$$

$$t = \vec{t} = \overleftarrow{t} = \exp(ikl)\,t_1t_2\,[1 - r_1r_2\exp(2ikl_2)], \quad l_3 = l - l_1 - l_2. \quad (55c)$$

Substituting $r_j = p_j/(ik - p_j)$ and $t_j = ik/(ik - p_j)$; using the relation $t_j^2 - r_j^2 = (ik + p_j)/(ik - p_j)$; and introducing $p = p_1 + p_2$, $\Delta = p_2 - p_1$ and $g = p_1p_2/k$, we find

$$\vec{r} = -i\,[p\cos kl_2 + (2g + i\Delta)\sin kl_2) \times \exp[ik(2l_1 + l_2)]Q^{-1}, \quad (56a)$$

$$\overleftarrow{r} = -i\,[p\cos kl_2 + (2g - i\Delta)\sin kl_2] \times \exp[ik(2l_3 + l_2)]\,Q^{-1}, \quad (56b)$$

$$t = k\exp(ikl)\,Q^{-1},\ Q = k + ip + 2ig\sin kl_2\exp(ikl_2). \quad (56c)$$

From (56a) and (56b) we find

$$\overset{\rightleftarrows}{r} = r\exp(\mp i\eta),$$

$$\eta = k(l_1 - l_3) + \arcsin(\Delta\sin kl_2 \cdot A^{-1}), \quad (57a)$$

$$r = -iA\exp(ikl)\,Q^{-1},$$

$$A = (F^2 + 2pg\sin 2kl_2 + 4g^2\sin^2 kl_2)^{1/2} \approx F, \quad (57b)$$

$$F = [F(2k)\,F(-2k)]^{1/2}, \quad F(\varkappa) = p_1 + p_2\cos\varkappa l_2. \quad (57c)$$

The sign of the root in (57b) and (57c) should be chosen such that at small values $k \to 0$ the limiting relation $F = F(0) = p$ holds for either sign of p. The ratio $\mathscr{F}(\varkappa) = F(\varkappa)/p$ is the structure factor of a cell (of a period). Analogously, (57c) is determined by the geometric mean value $\mathscr{F} = [\mathscr{F}(2k)\mathscr{F}(-2k)]^{1/2}$.

Expressions (56b) and (57b) can alternatively be written

$$r = -i\langle r\rangle\exp(i\varphi), \quad t = |t|\exp(i\varphi), \quad \varphi = kl - \chi, \quad (58a)$$

$$\langle r\rangle = \operatorname{sign} F\,|r| = A(A^2 + k^2)^{-1/2} \approx F(F^2 + k^2)^{-1/2}, \quad (58b)$$

$$|t| = k(A^2 + k^2)^{-1/2} \approx k(F^2 + k^2)^{-1/2}, \quad (58c)$$

$$\sin\chi = (p + g\sin 2kl_2)(A^2 + k^2)^{-1/2} \approx p(F^2 + k^2)^{-1/2}, \quad (58d)$$

$$\cos\chi = (k - 2g\sin^2 kl_2)(A^2 + k^2)^{-1/2} \approx k(F^2 + k^2)^{-1/2}. \quad (58e)$$

Substituting (58a) into (11a) and (17), we find

$$R = \frac{(\sin\varphi + \langle r\rangle)^{1/2} - (\sin\varphi - \langle r\rangle)^{1/2}}{(\sin\varphi + \langle r\rangle)^{1/2} + (\sin\varphi - \langle r\rangle)^{1/2}}, \quad (59a)$$

$$\exp(iql) = \frac{(|t| + \cos\varphi)^{1/2} + i(|t| - \cos\varphi)^{1/2}}{(|t| + \cos\varphi)^{1/2} - i(|t| - \cos\varphi)^{1/2}}. \quad (60a)$$

It follows from (59a) that total reflection occurs in the region $|\varphi - \pi n| < |r|$. Near $\varphi \approx \pi n$, $n \neq 0$, expression (59a) can be written approximately as

$$R = (-1)^n \frac{[k^2 - k_n^2 - u_0(1 - \mathscr{F})]^{1/2} - [k^2 - k_n^2 - u_0(1 + \mathscr{F})]^{1/2}}{[k^2 - k_n^2 - u_0(1 - \mathscr{F})]^{1/2} + [k^2 - k_n^2 - u_0(1 + \mathscr{F})]^{1/2}}, \quad (59b)$$

where $k_n = \pi n/l$, and $u_0 = 2pl$. We thus see that total reflection occurs in the case $|k^2 - k_n^2 - u_0| < |u_0\mathscr{F}|$, $n \neq 0$. Near $\varphi \approx 0$ expression (59a) takes the form

$$R = \frac{k - (k^2 - u_0)^{1/2}}{k + (k^2 - u_0)^{1/2}}. \quad (59c)$$

Approximate values of q near $\varphi \approx \pi n$ can be found from expression (60a), from which we find, in particular

$$\cos ql = \cos\varphi \cdot |t|^{-1} \approx \cos\varphi \cdot (1 + F^2k^{-2})^{1/2}, \quad (60b)$$

$$\sin ql \approx (\sin^2\varphi - \cos^2\varphi \cdot F^2k^2)^{1/2}, \quad (60c)$$

so that under the condition $\varphi \approx \varphi_n = \pi n$ we have

$$q \approx [k_n^2 + \{[k^2 - k_n^2 - u_0(1 - \mathscr{F})] \times [k^2 - k_n^2 - u_0(1 + \mathscr{F})]\}^{1/2}]^{1/2}. \quad (60d)$$

In the case $\varphi \approx 0$ we have the simpler expression $q \approx (k^2 - u_0)^{1/2}$.

It follows from (57a) that when p_1 and p_2 have imaginary parts the intensities of the reflection from the potential from the right and from the left differ by an amount

$$\delta I = 2I_0 |R|^2 \frac{\Delta}{p} \operatorname{tg} kl_2 \left(\frac{\operatorname{Im}\Delta}{\Delta} - \frac{\operatorname{Im}F}{F}\right), \quad (61)$$

where F is given by expression (57c), and I_0 is the incident intensity. In principle, this difference makes it possible to solve the phase problem in deciphering of diffraction patterns.

Reflection from a crystal of finite thickness should be calculated from expression (21a), which we rewrite as

$$R_N = [R(1 - R^2)^{-1}](1 - e^{2iqlN}) \times [1 + R^2(1 - e^{2iqlN})(1 - R^2)^{-1}]^{-1}. \quad (62)$$

Using expression (59b), we find

$$\frac{R}{1 - R^2} = \frac{2\langle r\rangle}{4(\sin^2\varphi - |r|^2)^{1/2}}. \quad (63)$$

Near the Bragg reflection we assume $ql = \pi n + \alpha$. We consider a thin crystal, for which the condition $2N\alpha < 1$ holds. In this case we can use the expression

$$(1 - e^{2iqlN}) = (1 - e^{2iql})(1 + e^{2iql} + \ldots + e^{2iql(N-1)}) \approx N(1 - e^{iql})(1 + e^{iql}) = -4i(|t|^2 - \cos^2\varphi)^{1/2} N[(|t| + \cos\varphi)^{1/2} - i(|t| - \cos\varphi)^{1/2}]^{-2} \quad (64)$$

where the last equation was found by substituting in (60a). Substituting (63) and (64) into (62) for the case of a thin crystal, we find

$$|R_N|^2 = \left|\frac{NR}{1 - R^2}(1 - e^{2iql})\right|^2 = N^2 \frac{|r|^2(|t|^2 - \cos^2\varphi)}{|t|^2(\sin^2\varphi - |r|^2)}. \quad (65)$$

Since in the absence of absorption the relation $|t|^2 + |r|^2 = 1$ holds, we have $|t|^2 - \cos^2\varphi = \sin^2\varphi - |r|^2$. Consequently, the intensity of the reflection from a thin crystal is given by

$$|R_N|^2 = N^2|r|^2|t|^{-2} \approx N^2F^2k^{-2} = L^2u_0^2\mathscr{F}^2(4k^2)^{-1}, \quad (66)$$

where $L = Nl$.

This limiting expression for a thin crystal is the same as that found by perturbation theory, i.e., in a kinematic theory of diffraction.

9. LAUE DIFFRACTION

Laue diffraction can also be analyzed in the one-dimensional approximation. Essentially the only place where we have to go beyond one dimension is in satisfying the boundary conditions at the entrance and exit surfaces. We consider the potential

$$u = 2p_0\theta(0 \leqslant z \leqslant a) \sum_{n=-\infty}^{\infty} \delta\left(x - x_n - \frac{l}{2}\right), \quad x_n = nl. \quad (67)$$

This potential represents a crystal which has an infinite dimension along the x axis and which has crystal planes perpendicular to x and parallel to the z axis. The width of the crystal along the z axis is a. The entrance surface can be stopped down by a slit of finite width. For simplicity we assume that this slit is wide enough that we can ignore diffraction effects associated with the finite dimensions of the slit.

We assume that a plane wave $\exp(i\mathbf{kr})$ with wave-vector components $k_\parallel$ and $k_\perp$ along the x and z axes, respectively, is incident from the region $z < 0$. Waves are excited in the crystal; these waves are normal modes for the given medium, just as only normal modes are excited in a waveguide. In our case, these normal modes are Bloch waves

$$\Psi = e^{ik_z z} \sum_{n=-\infty}^{\infty} e^{iqx_n} \psi_n(k_x, x)\,\theta(x \in I_n), \quad (68)$$

where the functions $\psi_n(k_x, x)$ within intervals (50) are given by expression (51), where k should be replaced by k_x. We note that k_x and k_z differ from $k_\parallel$ and $k_\perp$, but we have

$$k_x^2 + k_z^2 = k_\parallel^2 + k_\perp^2 = k^2. \quad (69)$$

The incident plane wave must convert in a continuous way into a set of waves (68) at the entrance surface. It follows that continuity must prevail strictly at least one point inside the intervals I_n. Since many intervals I_n can fit in a sufficiently wide slit, the wave vector q must either be the same as

$k_\parallel$ or differ from $k_\parallel$ only by $2\pi n/l$. In other words, we must have

$$q_n = k_\parallel + \frac{2\pi n}{l}. \tag{70}$$

Knowing the Block vector q, we can solve expression (37) for k; i.e., we can find k_x. We can then use (69) to find $k_z = k^2 - k_x^2$. The number of Bloch waves in the crystal is limited by the condition $k_z^2 > 0$. To determine k_x we use approximation (37e). Under the conditions $u_0 > 0$ and $q < k_n$, we find from this approximation

$$q < k_x = \{k_n^2 + u_0[1-(1+y^2)^{1/2}]\}^{1/2} < k_n, \tag{71a}$$

where $y = (k_n^2 - q^2)/u_0$. Under the condition $q > k_n$ we find

$$k_n < q < k_x = \{k_n^2 + u_0[1+(1+y^2)^{1/2}]\}^{1/2}, \quad k_x^2 > k_n^2 + 2u_0. \tag{71b}$$

Expressions (71) for k_x also holds at $u_0 < 0$; the only change is that the signs of the inequalities in (71) are reversed.

From (71) and (69) we find

$$k_z = \{k_\perp^2 - u_0[1-(1+y^2)^{1/2} + y]\}^{1/2}, \tag{72a}$$

$$k_z = \{k_\perp^2 - u_0[1+y+(1+y^2)^{1/2}]\}^{1/2}. \tag{72b}$$

If k is not too large, only two Bloch waves can appear in the crystal. The wave function inside the crystal can then be written

$$\Psi = A_1 e^{ik_{z1}z} \sum_n e^{ik_\parallel x_n} \psi_n(k_{x1}, x)\,\theta(x \in I_n) + A_2 e^{ik_{z2}z} \sum_n e^{-i(2k_1 - k_\parallel)x_n} \psi_n(k_{x2}, x)\,\theta(x \in I_n),$$

$$k_1 = \frac{\pi}{l}. \tag{73}$$

If $k_\parallel < k_1$, then we have $2k_1 - k_\parallel > k_1$, so that we can determine k_{x1} and k_{z1} from (71a) and (72a), while we can determine k_{x2} and k_{z2} from (71b) and (72b). Furthermore, we have $k_{x1} \approx k_\parallel$ and $k_{x2} \approx 2k_1 - k_\parallel$. The continuity condition at the entrance surface can be satisfied approximately if the following relations hold:

$$A_1 + R_2 A_2 = 1, \quad A_2 + R_1 A_1 = 0. \tag{74}$$

The reflection amplitudes $R_i(k_{xi})$ can be conveniently written in the form in (36e) near the case of Bragg reflection. Replacing k by expression (71) in those amplitudes, we find, respectively,

$$R_1 = \frac{1}{y + (1+y^2)^{1/2}}, \tag{75a}$$

$$R_2 = -R_1. \tag{75b}$$

Substituting (75) into (74), and solving equations (74) for A_i, we find

$$A_1 = \frac{[y + (1+y^2)^{1/2}]}{2(1+y^2)^{1/2}}, \tag{76a}$$

$$A_2 = \frac{-1}{2(1+y^2)^{1/2}}. \tag{76b}$$

We have thus derived all the formulas pertinent to the dynamic theory of diffraction.

It follows, in particular, from this analysis that if the crystal is sufficiently thick two Bloch waves will propagate rather far apart at the exit surface, and at the exit surface one will observe what appears to be two bright spots, with widths determined by the width of the entrance slit. Each of these spots will give the direct and diffracted waves. If the two waves from the two spots are brought together, as is done in a two-crystal interferometer,[11] one can observe an interference pattern. If k is large, then several Bloch waves may appear in the crystal. If the crystal is sufficiently thick, they may produce several bright spots at the exit surface, and each of these spots will give the entire set of diffracted waves. If a slit is used to single out one of the spots, it becomes possible to separate the various orders of diffraction without resorting to the time-of-flight method.

In the case of a thin crystal, the different Bloch waves do not have room to move far apart; the bright spots at the exit surface overlap and interfere, giving rise to the well-known pattern of pendulum oscillations of the intensity. In the case of multiwave diffraction, the pendulum oscillations occur at different frequencies, and these frequencies combine with each other.

10. CONCLUSION

A simple recurrence approach to the periodic potential has proved very informative and has provided a fresh look at many established concepts. We should state that this method is not limited to scalar particles and a scalar potential. Equations (6) and (15) are written in such a way that they can be generalized directly to the nonscalar and multidimensional case, in which case r, t, and q will all be matrices. Unfortunately, in that case I have not been able to find an elegant general solution for the quadratic matrix equation $X^2 + AX + B = 0$ to which Eqs. (6) and (15) lead after some straightforward manipulations. In the case of symmetric or commuting matrices A and B, it is of course a trivial matter to solve this equation, but there is the hope that either the physical problems of interest will lead to precisely this simple case or it will be found possible to solve this equation in some way or other.

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