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EVANESCENT WAVES IN POTENTIAL SCATTERING FROM REGULAR LATTICES*

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ABSTRACT

A recently developed approach to scattering by regular structures is applied to an investigation of diffracted evanescent waves. The scattered field is expressed exactly, in the near or far field, by a sum of "plane lattice wave" modes. Attention is directed at the diffraction conditions obeyed by these modes when the scatterer is a finitely thick three dimensional non-orthogonal (triclinic) lattice of individual scattering centers.

I. Introduction

Recent work has shown clearly that the angular spectrum of plane waves and especially the evanescent modes of the angular spectrum can play a helpful role in the study of a wide range of electrodynamic phenomena[1]. Within the past several years, the angular spectrum has been brought to play in new approaches to Cerenkovian effects[2] and inverse scattering[3], for example. In addition, it has figured in a study of source-free fields[4], a formulation of a diffraction theory of holography[5], and the quantization of an electromagnetic wavefield in an infinite space half-filled with dielectric[6].

It is important to realize that there are really two aspects to the use of the evanescent modes of a radiation field. In the first place, there may be no unique set of evanescent modes associated with a given field. This is due simply to the fact that evanescent modes are characterized by exponential decay in one direction and plane-wave propagation in the transverse directions, and the direction in which the exponential decay occurs may be undetermined. Thus one must approach with great caution the task of assigning physical significance to an evanescent wave. This lack of unique or clear physical meaning need not detract, of course, from the power of mathematical mode expansions which include evanescent modes.

On the other hand, there are physical problems for which a given direction is already singled out. It may happen that this quasi-one-dimensionality suggests the introduction of a mode expansion involving evanescent modes in a particular way. Individual evanescent modes, in such situations, may have a very direct physical interpretation. For example, the wave field outside of a totally internally reflecting dielectric decays away from the dielectric surface. Lalor and Wolf[7] have treated the problem of reflection and refraction at such an interface by the use of the physically suggested mode decomposition of the transmitted field; and Carniglia and Mandel[6] have found triads of evanescent and non-evanescent modes at a dielectric interface to be essential for their treatment of a field quantization problem.

In much of the previous work mentioned above, the principal interest has been in the "collective" interaction of a material, usually amorphous (isotropic and spatially homogeneous), with an electromagnetic wave. There are, however, large classes of problems in which the microscopic view is more natural. Among such problems we can include electromagnetic scattering at such short wave lengths (X-rays and gamma rays) that the individual particles in the scatterer act independently, or scattering by media with some regularity or structure such as crystals. In addition, the microscopic viewpoint seems more natural for problems in which particles (electrons or neutrons, for example) comprise the incident wave and in which a particle-particle interaction potential causes the scattering.

Our interest is in this second group of problems. In this paper we extend some earlier work[8] by one of us (JHE) on the quantum mechanical scattering by perfect lattices. In particular, we study the waves scattered by a general triclinic (three-dimensional non-orthogonal) arrangement of identical individual scatterers. We give up the notions of cross section and asymptotic scattering amplitude in order to focus on the distinctions between evanescent and non-evanescent (homogeneous) waves transmitted by the scatterer.

The remainder of the paper is organized as follows. The next section restates the mathematical formalism, especially the Weyl angular spectral decomposition[9] for spherical waves, that will be used throughout the paper. Scattering by a plane orthogonal lattice in two dimensions is treated briefly in order to introduce our notation and summation method. A principal result is the derivation of what we have called a "plane lattice wave" decomposition of the scattered field into discrete modes. Section III then applies the results of Section II to show that a certain familiar critical angle arises naturally in our treatment of scattering.

In Section IV we apply the concepts illustrated in Section II for single-layer rectangular lattices to an arbitrary triclinic multi-layer lattice. In particular, the notion of "plane lattice waves" is valid in this larger context. Section V is concerned with <u>evanescent</u> plane lattice waves, of which there are infinitely many, for arbitrary lattice angles and direction of incident radiation. We find that all integer points outside a certain ellipse define evanescent plane lattice modes. We discuss briefly in Section VI scattering from a three-dimensional lattice each unit cell of which contains two scattering centers of different type. Finally, after a short concluding section which summarizes our results, in two Appendices we comment on the validity of the Born approximation as used throughout the paper, and on the form of the second order terms in the Born scattering series. One sees easily, for example, how first order evanescent waves can be scattered into second order non-evanescent waves.

II. Weyl Expansion and Evanescent Waves in Two Dimensions

In order to introduce our treatment of scattering by three-dimensional, finitely thick, lattices of extended scatterers, we review here our earlier treatment[8] of two-dimensional lattices.

As the simplest case we consider a two-dimensional $(2N + 1) \times (2N + 1)$ orthogonal lattice of identical scattering units - atoms, molecules or other microscopic scatterers - lying in the x-y plane of our coordinate system. The scattering units interact with the incident wave or particle - neutron, electron, etc. - through the single particle potential $(\hbar^2/2m)\, U_0(\underline{r})$, which for convenience we may imagine to have a finite range.

We assume a scalar incident wave field, with the incident wave vector $\underline{k}$ lying in the positive z-direction, as shown in Figure 1. In the first Born approximation (applicable, roughly speaking, when multiple scattering is negligible (see App.A)), the amplitude of the scattered wave is

$$\Psi_s(\underline{r}) = -\frac{1}{4\pi}\int \frac{e^{ik|\underline{r}-\underline{r}'|}}{|\underline{r}-\underline{r}'|}\, U(\underline{r}')\, e^{i\underline{k}\cdot\underline{r}'}\, d^3r' \tag{2.1}$$

We have suppressed the time dependence $\exp\left\{-i\left(\hbar k^2/2m\right)t\right\}$; and have written $(\hbar^2/2m)U(\underline{r}')$ for the total scattering potential at point $\underline{r}'$ due to all the scattering centers in the lattice. That is,

$$(2.2) \qquad U(\underline{r}') = \sum_{\xi,\eta=-N}^{+N} U_0\left(\underline{r}' - \underline{\rho}(\xi,\eta)\right),$$

where $\underline{\rho}(\xi,\eta) = \xi\underline{a} + \eta\underline{b}$. As in Figure 1, $\underline{a}$ and $\underline{b}$ are the primitive vectors of the lattice, parallel to the x and y axes. The symmetry of the sum over integers ξ and η in (2.2) indicates that the origin of coordinates has been put at the central lattice site.

It should be noted that, except for the special form of our potential given in (2.2), our discussion so far does not depart at all from the usual Born Approximation approach to scattering. In optical problems[10] one simply has, in place of $U(\underline{r}')$, some constant times the dielectric susceptibility $\chi(\underline{r}')$. However, the special form of our potential is important and may be exploited significantly in the limit of a lattice with very large N.

We may mention in advance one point of view of our problem, adopted from optics, that might be helpful. Since our potential, in the limit of large N, will be periodic with double period $\underline{a}$ and $\underline{b}$ it will have a double Fourier series representation. Each term in the series for the potential will be a sinusoidal function of x' and y' and will thus affect the scattering as a two-dimensional sinusoidal diffraction grating would. The final scattered wave could therefore be viewed as the superposition with complex coefficients of waves scattered by a discrete collection of sine gratings.

We must keep in mind, however, that there is no limit to the fineness of detail (no smallest structure) in the individual single-particle potential $U_0(\underline{r}')$. Thus the discrete collection of imagined sine gratings would, in general, be infinite in number. We will not pursue this point of view further.

After introducing $\underline{s} = \underline{r}' - \underline{\rho}(\xi, \eta)$ into Eqs. (2.1) and (2.2), and using the temporarily assumed orthogonality of $\underline{k}$ and $\underline{\rho}(\xi, \eta)$, one gets

$$(2.3) \qquad \Psi_s = -\frac{1}{4\pi} \sum_{\xi,\eta} \int \frac{e^{ik|\underline{r} - \underline{\rho}(\xi,\eta) - \underline{s}|}}{|\underline{r} - \underline{\rho}(\xi,\eta) - \underline{s}|} U_0(\underline{s})\, e^{i\underline{k}\cdot\underline{s}}\, d^3s \, .$$

The presence of the spherical wave factor in the integrand indicates, of course, that each scattering center acts as a point source for scattered radiation. We will find it convenient throughout our investigation to use Weyl's angular spectral decomposition of such a factor. Usually one now writes the Weyl decomposition as a double integral:[9]

$$(2.4) \qquad \frac{e^{ik|\underline{R}|}}{ik|\underline{R}|} = \frac{1}{2\pi}\iint \frac{dp\,dq}{m}\, e^{i\underline{P}\cdot\underline{R}} ,$$

where the vector $\underline{P}$ is defined by its Cartesian components

$$(2.5) \qquad \underline{P} = (kp,\ kq,\ km),$$

with the restriction

$$(2.6) \qquad p^2 + q^2 + m^2 = 1 .$$

Both p and q are real and run through all possible real values, and m is defined as $m = (\pm)\sqrt{1-p^2 - q^2}$, with the sign chosen so that, for $z > 0$, m is either positive real (when $p^2 + q^2 \leq 1$) or positive imaginary (when $p^2 + q^2 > 1$). Here, by z, of course, we are denoting the corresponding component of $\underline{R}$. For $z < 0$ the opposite sign convention is to be chosen in each case.

After applying Weyl's formula to each spherical wave in the integrand of (2.3) and carrying out the sums one finds

$$(2.7) \qquad \Psi_s(\underline{r}) = -\frac{ik}{8\pi^2}\iint \frac{dp\,dq}{m} F_N(pa)\,F_N(qb) \times \int d^3s\, U_0(\underline{s})\, e^{i\underline{k}\cdot\underline{s}}\, e^{i\underline{P}\cdot(\underline{r}-\underline{s})}$$

where

$$(2.8) \qquad F_N(\sigma) = \frac{\sin(N+\frac{1}{2})k\sigma}{\sin\frac{1}{2}k\sigma} .$$

It is clear that, for large N, the diffraction functions F_N become very sharply peaked and behave as delta functions. In fact one has the useful identity:

$$\lim_{N\to\infty} \frac{\sin(N+\frac{1}{2})x}{\sin\frac{1}{2}x} = 2\pi\sum_{\alpha=-\infty}^{\infty}\delta(x-2\pi\alpha)$$

where convergence is in the sense of distributions. Thus the p and q integrations in (2.7) may be exactly performed, and only these values of p and q contribute to the integration which satisfy

$$kpa = 2\pi\alpha$$
$$kqb = 2\pi\beta$$

where α and β are arbitrary integers. Obviously, since $\underline{a}$ and $\underline{b}$ are in the x and y directions, respectively, and since $\underline{k}$ is in the z-direction, these equations can be rewritten as:

$$(2.9a) \qquad \underline{P}\cdot\underline{a} = 2\pi\alpha + \underline{k}\cdot\underline{a}$$

$$(2.9b) \qquad \underline{P}\cdot\underline{b} = 2\pi\beta + \underline{k}\cdot\underline{b}, \qquad \alpha,\beta = 0, \pm 1, \pm 2, \ldots$$

We will use this more elaborate form since we shall show in Sec.IV that this generalization is, in fact, the only change in the restrictions on the vector $\underline{P}$ which will be required in the larger context of non-orthogonal lattices and non-normally oriented incident waves. The vector $\underline{P}$ which satisfies these equations for specific integers α and β will be denoted by $\underline{P}_{\alpha\beta}$. In the present context of an orthogonal lattice and normally incident radiation we may write $\underline{P}_{\alpha\beta} = k(p_{\alpha\beta}, q_{\alpha\beta}, m_{\alpha\beta})$ where

(2.10) $$p_{\alpha\beta} = \alpha\left(\frac{\lambda}{a}\right), \qquad q_{\alpha\beta} = \beta\left(\frac{\lambda}{a}\right) \quad \text{and} \quad m_{\alpha\beta} = (\pm)\sqrt{1 - p_{\alpha\beta}^2 - q_{\alpha\beta}^2},$$

λ being the wavelength of the incident radiation. Using this notation, we may finally write the scattered wave function of Eq. (2.1) very compactly:

(2.11a) $$\Psi_s(\underline{r}) = \sum_{\alpha,\beta=-\infty}^{\infty} \Gamma_{\alpha\beta}\, e^{i\underline{P}_{\alpha\beta}\cdot\underline{r}}$$

where

(2.11b) $$\Gamma_{\alpha\beta} = \frac{-i}{2kab}\cdot\frac{1}{m_{\alpha\beta}}\int d^3s\, U_0(\underline{s})\, e^{i(\underline{k}-\underline{P}_{\alpha\beta})\cdot\underline{s}}$$

This form makes evident the principal utility we find in the Weyl decomposition. It allows us to express the scattered radiation as a sum of elementary scattered waves, which we will call plane lattice waves, with amplitudes $\Gamma_{\alpha\beta}$ and propagation vectors $\underline{P}_{\alpha\beta}$. One important property which these plane lattice waves possess is already evident and may be mentioned. Since $p_{\alpha\beta}^2 + q_{\alpha\beta}^2 + m_{\alpha\beta}^2 = 1$, it follows immediately that each plane lattice wave separately satisfies the homogeneous free space wave equation $(\nabla^2 + k^2)\, e^{i\underline{P}_{\alpha\beta}\cdot\underline{r}} = 0$ for $|z| > 0$. In other words, the scattered radiation has been decomposed into certain special free wave modes, modes which we will see are particularly suited to the geometry of the scatterer.

It is interesting that the mode expansion given in (2.11a) depends on just two discrete parameters α and β. (This remains true for three dimensional scatterers). One may say that the two-discrete-parameter lattice-mode series in (2.11a) stands in the same relation to a three-discrete-parameter Fourier series as the two-continuous-parameter angular spectral integral (2.7) stands to the corresponding conventional three-continuous-parameter Fourier integral.

Note also that if the scattered field itself is known on some plane $z > 0$, then the coefficients $\Gamma_{\alpha\beta}$ may be determined by a Fourier inversion, complicated slightly by the non-orthogonality of the $\underline{a}$ and $\underline{b}$ vectors:

$$(2.12) \qquad \Gamma_{\alpha\beta} = \frac{1}{ab} \int_0^a d r_a \int_0^b d r_b \; e^{-i \underline{P}_{\alpha\beta} \cdot \underline{r}} \; \Psi_s(\underline{r})$$

Here r_a and r_b are components of $\underline{r}$ along the $\underline{a}$ and $\underline{b}$ directions, and the consequent non-orthogonal area element obeys $dr_a \, dr_b = |(\underline{a} \times \underline{b})|^{-1} dxdy$. Knowing the coefficients $\Gamma_{\alpha\beta}$ then allows, of course, the construction of the solution $\Psi_s(\underline{r})$ on <u>any</u> plane $z > 0$, and the whole scattering problem is solved. Such an approach to a solution is more or less in the spirit of classical Kirchhoff diffraction theory, which attempts to construct the entire diffracted field from a knowledge of the field itself either in apertures or on edges, and is, of course, distinct from our present approach in which we attempt to describe the field from a knowledge of a scattering potential. The inverse or reconstruction problem, in which the potential is sought in terms of the scattered waves, has been discussed recently by Wolf[10], using the angular spectrum of plane waves.

It is important to emphasize that the sum of plane lattice waves in (2.11) expresses the scattered field exactly for all points $\underline{r}$ in the half-space $z > 0$. The conventional scattering amplitude (i.e. the coefficient of e^{ikr}/r in Ψ_s) is now rather awkward to isolate. In other words, Ψ_s as expressed by (2.11) correctly describes the "induction" field near the lattice, as well as the asymptotic "radiation" field.

The double sum solution in (2.11) is not in closed form, but it is very useful nevertheless. The scattered wave is a sum of plane lattice waves of two types corresponding to the two types contained in the Weyl decomposition (2.4): evanescent plane lattice waves (for which α and β are such that $p^2_{\alpha\beta} + q^2_{\alpha\beta} > 1$ and $m_{\alpha\beta}$ is imaginary) which are exponentially damped, rather than oscillatory, with increasing $|z|$; and homogeneous plane lattice waves (for which $m_{\alpha b}$ is real), and whose dependence on all three coordinates is oscillatory.

For evanescent plane lattice waves the direction of travel (the direction perpendicular to the surfaces of constant phase) lies in the $z = 0$ lattice plane. There is no component of the propagation vector in the z-direction. One may verify that there is an evanescent wave propagating perpendicular to each lattice diagonal. The homogeneous waves travel into the $z > 0$ half-space. We may observe that since a real $m_{\alpha\beta}$ requires sufficiently small integers α and β, there are only a finite number of such homogeneous plane lattice waves. By the same token there are always <u>infinitely many evanescent plane lattice waves</u> in the scattered field.

A further general remark can be made concerning the scattered wavefield. As (2.10) shows, if we have

$$(2.13) \qquad \left(\alpha \frac{\lambda}{a}\right)^2 + \left(\beta \frac{\lambda}{b}\right)^2 > 1,$$

then $m_{\alpha\beta}$ is certainly imaginary, so we may call (2.12) the <u>evanescence condition</u> for orthogonal lattices and normally incident radiation. It is interesting to note that if either $\lambda > a$ or $\lambda > b$, then <u>all</u> the waves, except the $\alpha = 0$ and $\beta = 0$ waves, are necessarily evanescent. As soon as the radiation wavelength exceeds both lattice spacings, only one homogeneous wave (the forward-travelling 00 wave) is allowed, and all the non-forward scattered waves are evanescent plane lattice waves, which travel in the x-y plane. This is the same as saying that 0° and 90° are the only allowed scattering angles; or, in other terms, that very small details of the scatterer give rise only to evanescent transmitted waves[3,10].

In concluding this section we must point out that we recognize that some of the results presented in it are not new. In particular, up to Eqs. (2.9), which embody much of the traditional Bragg-Laue picture of scattering, our results are standard ones[10]. However, following Eqs. (2.9), we have concentrated on explaining a picture of the scattering in which some of the familiar features, such as the asymptotic amplitude and the scattering cross section, do not appear naturally, in order to focus our attention on aspects of the near field, such as evanescent waves, which are traditionally overlooked altogether.

III. The Critical Angle of Evanescence

We now apply the results of Section II to show how a critical angle may come to exist. By critical angle we refer to an angle between the incident wave vector $\underline{k}$ and the lattice normal $\underline{a} \times \underline{b}$ beyond which the non-forward scattered wave is almost entirely evanescent.

For our purpose here it is sufficiently general to let $\underline{k}.\underline{b} = 0$ and take the lattice to be one dimensional ($\underline{a}.\underline{b} = 0, |\underline{a}| = a, |\underline{b}| \to \infty$). Then $\underline{k}.\underline{a} = k\, a \sin\theta \cos \phi_k$, where θ is the angle between incident wave vector and lattice normal, and where ϕ_k, the azimuthal angle of the vector $\underline{k}$, is either 0 or π. We are thus considering a slight simplification of the general case sketched in Figure 2.

Now the allowed plane lattice modes are defined by the values of $\underline{P}_{\alpha\beta}$ which are determined by Eqs. (2.9) through the integers α and β. We may solve Eqs. (2.9) for $\underline{P}_{\alpha\beta}$ to find:

$$p^2 + q^2 = \left(\frac{\lambda}{a}\alpha + \sin\theta \cos\phi_k\right)^2 + \left(\frac{\lambda}{b}\beta\right)^2$$

Here, as in Section II, we have used $k = 2\pi/\lambda$ and have defined p and q by

$$(\underline{P}_{\alpha\beta})_x = kp, \tag{3.1a}$$

$$(\underline{P}_{\alpha\beta})_y = kq, \tag{3.1b}$$

and we recall that all modes for which $p^2 + q^2 > 1$ are purely evanescent.

Now we take account of the one-dimensionality we have assumed in this section by setting b = ∞ , thereby obtaining

$$p^2 + q^2 = \left(\alpha \frac{\lambda}{a} \pm \sin\theta\right)^2, \tag{3.2}$$

where the sign ambiguity carried by the factor $\cos\phi_k$ is given explicitly. The resulting expression (3.2) can be cast into familiar form by recognizing that

$$p^2 + q^2 = \sin^2\theta_t$$

where θ_t is the angle of the outgoing wave <u>transmitted</u> through the lattice. This relation follows from the fact that $\underline{P}$ is the outgoing wave vector, from $\underline{P}^2 = k^2$, and from Eqs. (3.1).

At this point we see it is most natural to rewrite (3.2) in the form:

$$\sin\theta_t \pm \sin\theta = \alpha\left(\frac{\lambda}{a}\right) \tag{3.3}$$

which is the familiar expression[11] for the transmission maxima of a one-dimensional diffraction grating. The occurrence of a critical angle is now obvious, since for a given diffractive order α and ratio λ/a there may well be angles of incidence θ for which (3.3) requires an unphysical transmission angle such that $|\sin\theta_t| > 1$. That is, that value of θ for which the condition

$$|\sin\theta \pm \alpha\frac{\lambda}{a}| > 1 \tag{3.4}$$

is first satisfied may be called the critical angle for order α. Since (3.4) corresponds exactly to the condition $p^2 + q^2 > 1$, it signals the appearance of evanescent waves.

It is more interesting, in the context of Section II, to take a less conventional converse view of (3.4). That is, we already recognize (3.3) as a well-known statement defining the <u>possible transmission angles</u> θ_t in the αth order of diffraction. On the other hand, we can turn (3.3) or (3.4) around and determine <u>which orders of diffraction are evanescent</u> for given angle of incidence θ. Then Eq. (2.11b) gives correctly the complex amplitudes of the corresponding transmitted waves, even if they are evanescent.

Perhaps it is unnecessary to point out features of the critical angle (3.4) not shared by, for example, the familiar critical angle for total internal reflection[11]. For $\lambda < a$, Eq. (3.4) allows <u>at least</u> one non-evanescent wave (in addition to the never-evanescent $\alpha = 0$, $\beta = 0$ wave) for <u>every value</u> of θ. The internal reflection critical angle depends only on the index of refraction of the dielectric:

$$\sin\theta_{\text{int.refl.}} = \frac{1}{n}\,, \tag{3.5}$$

and so provides an absolute cut-off of the homogeneous waves. For all $\theta > \theta_{\text{int. refl.}}$ all transmitted waves are evanescent.

We should, however, make it clear that there is no conflict between (3.4) and (3.5). Eq. (3.5) is derived for radiation impinging on a uniform homogeneous dielectric, an object whose basic periodicity or structure parameter can be regarded as very much smaller than the radiation wavelength. For such an object one cannot hold to our particle-by-particle Born-approximate view of the radiation-scatterer interaction. One has refractive, but not diffractive, effects.

Finally, we might imagine scattering by an object so weakly refractive that the Born approximation may be applied, but with some large scale periodicities in its index of refraction. Our result (3.4) will again apply to the effects of these periodicities, and will make the known prediction that periods smaller than a wave-length will give rise only to evanescent transmitted waves. (See references 5 and 10 for example, for discussions of problems in which these effects are important.)

IV. Plane Lattice Waves and a Three Dimensional Scatterer.

We now generalize our scatterer, and thereby take a step in the direction of physical realism. In this section we treat the case of a non-orthogonal, i.e., simple triclinic, three dimensional lattice. In addition we lift the restriction that the wave vector $\underline{k}$ of the incident radiation lie in the z direction. We require only that k_z be positive, so that the wave is travelling toward the $z > 0$ half space.

The lattice is assumed to be very large in the x and y directions, and N layers deep, so that the total scattering potential is (with the origin of coordinates in the center of the first layer)

$$(4.1) \qquad U(\underline{r}) = \sum_{\xi,\eta=-\infty}^{\infty} \sum_{\gamma=0}^{N-1} U_0(\underline{r} - \underline{\rho}_{\xi\eta\gamma})$$

where the vector $\underline{\rho}_{\xi\eta\gamma}$ is composed of the primitive lattice vectors $\underline{a}$, $\underline{b}$, and $\underline{c}$ and integers ξ, η, and γ:

$$(4.2) \qquad \underline{\rho}_{\xi\eta\gamma} = \xi\underline{a} + \eta\underline{b} + \gamma\underline{c} .$$

We orient the coordinate system so that the plane defined by the non-orthogonal vectors $\underline{a}$ and $\underline{b}$ is the x-y plane. We choose $\underline{a} \times \underline{b}$ to define the positive z direction. One lattice layer is shown in Fig. 2.

The method of reduction of the scattered wave into a sum of plane lattice waves which was explained in Sec. II may be followed here, practically without alteration. The introduction of the more general lattice scattering potential given by (4.1) leads to no very severe problems. The only important changes are these two: the lattice is now assumed finitely thick in the z-direction, giving rise to another lattice sum; and the non-orthogonality of $\underline{a}$ and $\underline{b}$ leads to diffraction functions F_N of the form

$$(4.3) \qquad F_N\left(\frac{\underline{a}_i \cdot \underline{L}}{k}\right) = \frac{\sin\left(N + \frac{1}{2}\right)\underline{a}_i \cdot \underline{L}}{\sin \frac{1}{2}\underline{a}_i \cdot \underline{L}} ,$$

where $\underline{a}_i = \underline{a}$ or $\underline{b}$ and $\underline{L} = \underline{k} - \underline{P}$, instead of the somewhat simpler ones given in Sec. II. This straightforward change in the argument of the diffraction functions (which arise from the sums over ξ and η) gives rise to the more general restrictions on the scattered wave vector $\underline{P}$ given in Eqns. (2.9) which we reproduce here for convenience:

$$(4.4a) \qquad \underline{P} \cdot \underline{a} = 2\pi\alpha + \underline{k} \cdot \underline{a}$$

$$(4.4b) \qquad \underline{P} \cdot \underline{b} = 2\pi\beta + \underline{k} \cdot \underline{b} , \qquad \alpha, \beta = 0, \pm 1, \pm 2, \pm 3, \cdots$$

The scattered wave is, therefore, expressible just as in (2.11a):

$$(4.5) \qquad \Psi_s(\underline{r}) = \sum_{\alpha,\beta=-\infty}^{\infty} \Gamma_{\alpha\beta}\, e^{i \underline{P}_{\alpha\beta} \cdot \underline{r}}$$

where the plane lattice wave amplitude in this more general case, (a three-dimensional non-orthogonal lattice) has the form:

$$(4.6) \qquad \Gamma_{\alpha\beta} = \frac{-i}{2k\Delta} \cdot \frac{1}{m_{\alpha\beta}} \cdot \frac{1-\exp\{-iN\underline{c}\cdot\underline{L}_{\alpha\beta}\}}{1-\exp\{-i\underline{c}\cdot\underline{L}_{\alpha\beta}\}} \int d^3s\, U_0(\underline{s}) e^{i\underline{L}_{\alpha\beta}\cdot\underline{s}}$$

Here we have introduced the abbreviations

$$(4.7) \qquad \Delta = |\underline{a} \times \underline{b}| \quad \text{and} \qquad L_{\alpha\beta} = \underline{k} - \underline{P}_{\alpha\beta}.$$

It is now possible to make an observation about evanescent waves in this general situation in which $\underline{k}\cdot\underline{a}$, $\underline{k}\cdot\underline{b}$, and $\underline{a}\cdot\underline{b}$ may all be non-zero. Note that Eqs. (4.4) are linear inhomogeneous (but coupled, if $\underline{a}\cdot\underline{b} \neq 0$) algebraic equations with real coefficients which determine P_x and P_y, and that P_x and P_y are themselves therefore necessarily real. However, because α, β, $\underline{k}\cdot\underline{a}$ and $\underline{k}\cdot\underline{b}$ are unrestricted in magnitude, either or both of P_x and P_y may be larger than k. Then P_z must be imaginary (recall the plane lattice wave restrictions in Eqs. (2.5) and (2.6)).

Just as in Eq.(2.11a) for the two-dimensional monolayer lattice of Sec. II, now Eq. (4.5) makes it clear that exponentially damped lattice waves are the consequence. These are of course the evanescent waves of our general triclinic lattice.

V. Diffracted Evanescent Waves

In the classical Laue theory of diffraction of X-rays by simple space-lattices,[12] one finds the condition for a diffraction maximum to be most concisely expressed by the following equation

$$\hat{n} - \hat{n}_o = \lambda \left[\alpha \underline{a}^* + \beta \underline{b}^* + \gamma \underline{c}^* \right] . \tag{5.1}$$

Here $\hat{n}_o$ and $\hat{n}$ are the unit vectors in the directions of the incident and scattered waves respectively, α, β, γ are any three integers, and $\underline{a}^*$, $\underline{b}^*$, $\underline{c}^*$ the primitive translations of the reciprocal lattice defined by

$$\underline{a}^* = \frac{\underline{b} \times \underline{c}}{V} , \qquad \underline{b}^* = \frac{\underline{c} \times \underline{a}}{V} , \qquad \underline{c}^* = \frac{\underline{a} \times \underline{b}}{V} , \tag{5.2}$$

where V is the volume of the unit cell: $V = \underline{a} \times \underline{b} \cdot \underline{c}$.

We also note that Eq. (5.1) is valid under conditions that are, in fact, equivalent to the use of the first Born approximation. Multiplying (5.1) with $\underline{a}$, $\underline{b}$ and $\underline{c}$ one gets

$$2\pi\alpha = k(\hat{n} - \hat{n}_o) \cdot \underline{a} \tag{5.3a}$$

$$2\pi\beta = k(\hat{n} - \hat{n}_o) \cdot \underline{b} \tag{5.3b}$$

$$2\pi\gamma = k(\hat{n} - \hat{n}_o) \cdot \underline{c} \tag{5.3c}$$

where $\underline{a} \cdot \underline{a}^* = 1$, $a \cdot b^* = a \cdot c^* = 0$, etc. have been used. The Laue equations (5.3) must be satisfied simultaneously if diffraction is to occur.

We see immediately that Eqs. (2.9) and (4.4) are exactly equivalent to the conditions (5.3a) and (5.3b), while (5.3c) corresponds to the condition that the factor

$$\frac{1 - \exp\{-iN\underline{c}\cdot\underline{L}_{\alpha\beta}\}}{1 - \exp\{-i\underline{c}\cdot\underline{L}_{\alpha\beta}\}}$$

in Eq. (4.6) have a maximum.

This agreement between Eq. (5.1), or its component equations, (5.3a) - (5.3c), and our relations (4.4) and (4.6) is to be expected, of course. All of these equivalent expressions merely state momentum conservation for each bombarding particle in its interaction with the regular scatterer. To be explicit, when (5.1) is multiplied by $2\pi\hbar/\lambda$ it may be rewritten as the momentum equation:

$$\hbar(\underline{k}-\underline{k}_0) = \alpha\underline{A}^* + \beta\underline{B}^* + \gamma\underline{C}^*,$$

where A*, B*, and C* are the basic units of crystal momentum transferrable by the scatterer in the directions of the reciprocal lattice:

$$\underline{A}^* = 2\pi\hbar\underline{a}^*$$

$$\underline{B}^* = 2\pi\hbar\underline{b}^*$$

$$\underline{C}^* = 2\pi\hbar\underline{c}^*$$

However this conventional view of (5.1) (or of (4.4) and (4.6)) tends to obscure the possibility that there may be meaningful situations in which the transmitted momentum is required to be complex. The wave associated with an imaginary k_z is not unphysical, merely evanescent, and its complex amplitude is given by (4.6)

We now look in detail at the conditions imposed by the scatterer on these complex-momentum particles. Accordingly, we look for the condition under which P_z is imaginary, or $P_x^2 + P_y^2 > k^2$; that is, we look for the generalization of relation (2.12). Since $(\underline{P} \times \hat{z})^2 = P_x^2 + P_y^2$, and since $\hat{z} = (\underline{a} \times \underline{b})/\Delta$, the condition is easily found with the aid of Eqs. (2.9) to be

$$\text{(5.4)} \qquad [\underline{a}\,(2\pi\beta + \underline{k}\cdot\underline{b}) - \underline{b}\,(2\pi\alpha + \underline{k}\cdot\underline{a})]^2 > k^2\Delta^2 .$$

The limiting cases which refer to the simple situation of Sec. II are easily recovered. If $\underline{k}.\underline{a} = \underline{k}.\underline{b} = \underline{a}.\underline{b} = 0$ we find relation (2.12) again, multiplied by $(2\pi\, ab/\lambda)^2$. Note also that the $\alpha = \beta = 0$ wave is <u>never evanescent</u> since then (5.4) reduces (for arbitrary

$\underline{a},\underline{b},\underline{k}$) to $k_z^2 > k^2$, which is never true.

To get a better understanding of condition (5.4) let us first reduce it to

$$[\xi_a \underline{a} - \xi_b \underline{b}]^2 > \left(\frac{\Delta}{\lambda}\right)^2, \tag{5.5}$$

where we have set

$$\begin{aligned} \xi_a &= \beta + \underline{k}\cdot\underline{b}/2\pi \\ \xi_b &= \alpha + \underline{k}\cdot\underline{a}/2\pi \end{aligned} \tag{5.6}$$

If we consider ξ_a and ξ_b as the components of a two-dimensional vector, we may rotate the corresponding coordinate system through an angle ϕ to diagonalize the quadratic form $[\xi_a \underline{a} - \xi_b \underline{b}]^2$. Doing this, we have for (5.5)

$$\frac{\zeta_a^2}{A^2} + \frac{\zeta_b^2}{B^2} > 1, \tag{5.7}$$

where

$$\begin{pmatrix} \zeta_a \\ \zeta_b \end{pmatrix} = \begin{pmatrix} \cos\phi & -\sin\phi \\ \sin\phi & +\cos\phi \end{pmatrix} \begin{pmatrix} \xi_a \\ \xi_b \end{pmatrix} \tag{5.8a}$$

$$\phi = \frac{1}{2}\tan^{-1}\left(\frac{2\,\underline{a}\cdot\underline{b}}{a^2 - b^2}\right) \tag{5.8b}$$

and

$$\begin{aligned} A^2 &= 2\left(\frac{\Delta}{\lambda}\right)^2 \left[a^2 + b^2 + (a^4 + b^4 + 2a^2b^2\cos 2\theta_{ab})^{\frac{1}{2}}\right]^{-1} \\ B^2 &= 2\left(\frac{\Delta}{\lambda}\right)^2 \left[a^2 + b^2 - (a^4 + b^4 + 2a^2b^2\cos 2\theta_{ab})^{\frac{1}{2}}\right]^{-1}, \end{aligned} \tag{5.9}$$

where θ_{ab} is the angle between $\underline{a}$ and $\underline{b}$.

The general relationship, derived here and expressed by Eqs. (5.6) -(5.9), between the lattice spacings and angles and the direction and wavelength of the incident wave is an exceptionally complicated one. It is not possible in any simple way to determine explicitly which $\alpha\beta$ modes are evanescent. Although the 00 mode is always a homogeneous (non-evanescent) wave, the rest of the homogeneous modes are not even symmetrically grouped about 00 in the $\alpha\beta$ plane.

We may clarify some aspects of the situation by a graphical analysis. Clearly Eq. (5.7) states that for values of ζ_a and ζ_b outside a certain ellipse all modes are evanescent. Consider first normal incidence (i.e., $\underline{k}\cdot\underline{a} = \underline{k}\cdot\underline{b} = 0$) and an orthogonal lattice, which implies $\emptyset = 0$. The relation (5.7) then collapses into

$$\frac{\beta^2}{\left(\frac{\Delta}{\lambda a}\right)^2} + \frac{\alpha^2}{\left(\frac{\Delta}{\lambda b}\right)^2} > 1 \qquad (5.10)$$

and all integer pairs $\alpha\beta$ outside the "ellipse" in Fig. 3 define purely evanescent modes of radiation.[13]

Next, keeping the incidence normal but allowing the axes to be non-orthogonal, we see that the homogeneous region becomes the rotated ellipse of Fig. 4. Of course the axes A and B of the new ellipse are no longer $\frac{\Delta}{\lambda a}$ or $\frac{\Delta}{\lambda b}$ either. Finally, the effect of non-normal incidence is to shift the origin of the ellipse of Fig. 4 to the point ($\underline{k}.\underline{b}/2\pi$, $\underline{k}.\underline{a}/2\pi$) as in Fig. 5. The lengths of the axes of this new ellipse are the same as those of the ellipse in Fig. 4.

Any experimental study of evanescent lattices waves will be made less difficult, of course, if one or more such waves are present which decay very slowly with increasing z. Thus it will be helpful to know which $\alpha\beta$ pair leads to the smallest negative value for P_z^2. If the lattice spacing is not too much larger than the wavelength of the incident beam, then the evanescence ellipse is quite small and contains only a few homogeneous mode points within it. The nearest $\alpha\beta$ points outside the ellipse (which define the most slowly decaying evanescent modes) are easily found graphically. For example, in Figs. 4 and 5, we see several points which lie much closer than one unit to the ellipse.

VI Lattice of Two Types of Scatterers.

A practical situation will most probably involve a three-dimensional lattice composed of more than one type of scattering centre. We now consider a more general case of a lattice infinite in two directions, finite in the third, and having a unit cell consisting of two different scattering sites characterized by scattering potentials U_0 and U_1, as shown in Fig. 6.

If d is the lattice diagonal

$$(6.1) \qquad \underline{d} = \underline{a} + \underline{b} + \underline{c}$$

and $\underline{\rho}_{\alpha\beta\gamma}$ is defined as in Eq.(3.2) then the total potential for our present case is

$$(6.2) \qquad U(\underline{r}) = \sum_{\alpha,\beta=-\infty}^{\infty} \sum_{\gamma=0}^{N-1} \left[U_0(\underline{r} - \underline{\rho}_{\alpha\beta\gamma}) + U_1(\underline{r} - \underline{\rho}_{\alpha\beta\gamma} - \frac{\underline{d}}{2}) \right]$$

where again the lattice is taken to be N layers deep. The origin of coordinates is taken in the first layer of scatterers and centered on a U_0. Once again the forward z-direction is given by $\underline{a} \times \underline{b}$.

Let us rewrite the potential more compactly as:

$$(6.3) \qquad U(\underline{r}) = \sum_{j=0,1} \sum_{\alpha,\beta,\gamma} U_j(\underline{r} - \underline{\rho}_{\alpha\beta\gamma} - \frac{j}{2}\underline{d}).$$

It is now clear that one can proceed exactly as in Sections II and IV, obtaining the scattered wave amplitude $\Psi_s(r)$ in a form analogous to that in Eqs. (4.5) and (4.6)

(6.4) $$\Psi_s(\underline{r}) = \frac{-i}{2k\Delta} \sum_{j=0}^{1} \sum_{\alpha,\beta=-\infty}^{\infty} e^{i\underline{L}_{\alpha\beta}\cdot\frac{j}{2}\underline{d}} \cdot \frac{1-\exp\{-iN\underline{c}\cdot\underline{L}_{\alpha\beta}\}}{1-\exp\{-i\underline{c}\cdot\underline{L}_{\alpha\beta}\}} \times \frac{e^{i\underline{P}_{\alpha\beta}\cdot\underline{r}}}{m_{\alpha\beta}} \int d^3s\, U_j(\underline{s})\, e^{i\underline{L}_{\alpha\beta}\cdot\underline{s}}$$

where the notation is unchanged.

Equation (6.4) points up an experimentally interesting situation where it is possible that there be no first order scattering at all. Here by scattered waves we mean those that are capable of reaching a measuring instrument far from the z = 0 plane, namely, homogeneous waves. To envisage such a situation, consider the case where $U_1 = -U_o$. For the particular outgoing homogeneous wave which satisfies $\underline{L}_{\alpha\beta} = 0$, i.e., $\underline{P}_{\alpha\beta} = \underline{k}$, $\Psi_s(r)$ has zero partial amplitude. Hence there is no scattering in this direction, and since we noted before in Sec. II that for $\lambda >$ a or b, there is only one homogeneous wave, – viz the one going out in the same direction as the incident wave - there is no scattering at all in the usual sense, in this particular case. A second possibility for a partial amplitude to vanish is that the corresponding $\underline{L}_{\alpha\beta}$ be perpendicular to the lattice diagonal $\underline{d}$ and, of course $U_o = -U_1$. In the first case it would be possible to measure experimentally the evanescent components of the field without interference from scattered homogeneous waves. The possibility of actually measuring an evanescent component is dependent upon how far that particular component can be propagated without too severe attentuation. This question has been discussed in Sec. 5.

VII. Summary

We have attempted to outline an unusual approach to potential scattering by regular but non-orthogonal lattices. Our center of attention has been on the near field of the scatterer, and we have shown how the Weyl angular spectral decomposition of a spherical wave can be used to sum all of the contributions to the scattered field. Asymptotic expansions have been avoided deliberately, and the usual scattering amplitude plays no role in our analysis.

We have derived a two-parameter discrete set of waves, our so-called plane lattice waves, in terms of which the scattered waves are expressed exactly. The discrete parameterization afforded by the plane lattice waves has been used particularly to identify the most important evanescent components of the scattered near field.

The general criterion, for arbitrary lattice spacings and incidence angle, governing the appearance of transmitted evanescent waves has been derived in Eqs. (5.5) to (5.9). The complexity of these relations makes it practically necessary to proceed graphically; and several simplified examples are given.

Questions having to do with more general scatterers such as slightly irregular lattices or assemblies of random scattering sites have not been investigated here. The appearance of evanescent waves due to the <u>collective</u> behavior of scatterers in regular, finitely thick crystals can be inferred but not derived from our work. Some of these, and other related topics, are under investigation. We hope to report the results at a later time.

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APPENDIX A

We discuss in the present section the validity of the first order Born approximation, in which we have worked so far. This approximation is meaningful only if $\Psi_s(\underline{r})$ in Eqs. (2.1) is small compared to the incident wave $e^{i\,\underline{k}\cdot\underline{r}}$ in the region of the potential, i.e., if

$$\text{(A1)}\qquad \left|\frac{\Psi_s(\underline{r})}{e^{i\underline{k}\cdot\underline{r}}}\right|_{z=0} \ll 1 .$$

Because our scattered wave is a coherent sum of waves scattered from the whole lattice, we may expect a validity criterion somewhat different from the usual one.

For simplicity, let us again assume a two-dimensional orthogonal lattice with $a \simeq b$. We will consider normal incidence, and, to facilitate calculations, take for the potential $U_0(\underline{r})$ a "rectangular well" of the form

$$\text{(A2)}\qquad \begin{aligned} U_0(\underline{r}) &= -U_0 \quad (= \text{const}), \text{ for } \quad -\tfrac{w}{2} \le x, y, z \le \tfrac{w}{2}, \\ &= 0, \quad \text{otherwise} \end{aligned}$$

Here w of course is the width of the potential well and U_0 its depth. We assume that the individual potentials overlap extensively, so that $w \gg a$. With these assumptions we find

$$\text{(A3)}\qquad \left|\frac{\Psi_s(\underline{r})}{e^{i\underline{k}\cdot\underline{r}}}\right|_{z=0} = \frac{1}{2kab}\left|\sum_{\alpha,\beta=-\infty}^{\infty} \frac{e^{i\underline{L}_{\alpha\beta}\cdot\underline{r}}}{m_{\alpha\beta}} \int d^3s\, U_0(\underline{s})\, e^{-i\underline{L}_{\alpha\beta}\cdot\underline{s}}\right|_{z=0}$$

$$\simeq \left| U_0 w^3 + {\sum_{\alpha,\beta}}' \frac{U_0\, a\, e^{i\frac{2\pi}{a}(\alpha x+\beta y)}}{\lambda\sqrt{\alpha^2+\beta^2-a^2/\lambda^2}} \int_{-\frac{w}{2}}^{\frac{w}{2}} ds_x\, e^{-i\frac{2\pi}{a}\alpha s_x} \right.$$

$$\left. \times \int_{-\frac{w}{2}}^{\frac{w}{2}} ds_y\, e^{-i\frac{2\pi}{a}\beta s_y} \int_{-\frac{w}{2}}^{\frac{w}{2}} ds_z\, e^{-i\frac{2\pi}{\lambda}s_z}\, e^{\frac{2\pi}{a}\sqrt{\alpha^2+\beta^2-a^2/\lambda^2}\,|s_z|} \right| .$$

The first term within the braces is the contribution from the single homogeneous wave $\alpha = \beta = 0$ (we are assuming $\lambda > a$) and the prime over the summation indicates that this term has been removed. A straightforward calculation leads to

$$\left|\frac{\Psi_s(\underline{r})}{e^{i\underline{k}\cdot\underline{r}}}\right|_{z=0} \simeq \frac{\lambda}{4\pi a^2}\left| U_0 w^3 + \frac{2U_0 w a^3}{\pi^2\lambda}\sum_{\substack{\alpha=-\infty\\ \alpha\neq 0}}^{\infty} e^{i\frac{2\pi}{a}\alpha x}\right.$$

(A4)

$$\times \frac{\sin\left(\frac{\pi w}{a}\alpha\right)}{\alpha^3}\left[\frac{a}{\lambda}\sin\left(\frac{\pi w}{\lambda}\right)\frac{e^{-\frac{\pi w}{a}\sqrt{\alpha^2-a^2/\lambda^2}}}{\sqrt{\alpha^2-a^2/\lambda^2}}\right.$$

$$\left. - \cos\left(\frac{\pi w}{\lambda}\right)e^{-\frac{\pi w}{a}\sqrt{\alpha^2-a^2/\lambda^2}} + 1\right]$$

$$+ \frac{U_0 a^4}{\pi^3\lambda}\sum_{\alpha,\beta}{}' e^{i\frac{2\pi}{a}(\alpha x+\beta y)}\frac{\sin\left(\frac{\pi w}{a}\alpha\right)\sin\left(\frac{\pi w}{a}\beta\right)}{\alpha\beta(\alpha^2+\beta^2)}$$

$$\times\left[\frac{a}{\lambda}\sin\left(\frac{\pi w}{a}\right)\frac{e^{-\frac{\pi w}{a}\sqrt{\alpha^2+\beta^2-a^2/\lambda^2}}}{\sqrt{\alpha^2+\beta^2-a^2/\lambda^2}}\right.$$

$$\left.\left. - \cos\left(\frac{\pi w}{\lambda}\right)e^{-\frac{\pi w}{a}\sqrt{\alpha^2+\beta^2-a^2/\lambda^2}} + 1\right]\right|$$

Since for any complex numbers ξ, η we have $|\xi - \eta| \leq |\xi| + |\eta|$, we may rewrite (A.4), replacing all sines and cosines by their maximum values, as

(A5)

$$\left|\frac{\Psi_s(\underline{r})}{e^{i\underline{k}\cdot\underline{r}}}\right|_{z=0} \leq \frac{\lambda}{4\pi a^2}\left\{ \left|U_0 w^3\right| + \frac{2U_0 w a^3}{\pi^2\lambda}\sum_{\substack{\alpha=-\infty\\ \alpha\neq 0}}^{\infty}\left|\frac{1}{\alpha^3}\right|\right.$$

$$\times\left|\left[\frac{a}{\lambda}\cdot\frac{e^{-\frac{\pi w}{a}\sqrt{\alpha^2-a^2/\lambda^2}}}{\sqrt{\alpha^2-a^2/\lambda^2}} + e^{-\frac{\pi w}{a}\sqrt{\alpha^2-a^2/\lambda^2}}\right.\right.$$

$$\left.\left. + 1\right]\right|$$

$$+ \frac{U_o a^4}{\pi^3 \lambda} \sum_{\alpha,\beta}{}' \left| \frac{1}{\alpha\beta(\alpha^2+\beta^2)} \right| \left| \left[\frac{a}{\lambda} \cdot \frac{e^{-\frac{\pi w}{a}\sqrt{\alpha^2+\beta^2-a^2/\lambda^2}}}{\sqrt{\alpha^2+\beta^2-a^2/\lambda^2}} + e^{-\frac{\pi w}{a}\sqrt{\alpha^2+\beta^2-a^2/\lambda^2}} + 1 \right] \right| \Bigg\}$$

In the first summation both $\frac{a}{\lambda} \cdot \frac{e^{-\frac{\pi w}{a}\sqrt{\alpha^2 - a^2/\lambda^2}}}{\sqrt{\alpha^2 - a^2/\lambda^2}}$ and $e^{-\frac{\pi w}{a}\sqrt{\alpha^2 - a^2/\lambda^2}}$ are ≤ 1 for $\alpha = \pm 2, \pm 3, \ldots$. When $\alpha = \pm 1$ the first exponential term might exceed unity. In the second sum, for all allowed values of α,β, the first two quantities within the square brackets are less than unity. Further we have that

(A6) $$\frac{1}{\alpha\beta(\alpha^2+\beta^2)} < \frac{1}{\alpha^2\beta^2} \qquad \text{for all } \alpha\beta \neq 0 .$$

Hence we are able to obtain the estimate,

(A7) $$\left| \frac{\Psi_s(\underline{r})}{e^{i\underline{k}\cdot\underline{r}}} \right|_{z=0} \leq \frac{\lambda U_o w^3}{4\pi a^2} \left[1 + \left(2 + \frac{a}{\lambda} \cdot \frac{1}{\sqrt{1-a^2/\lambda^2}} \right) \frac{4a^3}{\pi^2 \lambda w^2} + \left(2 + \frac{a}{\lambda}\right)\left(\frac{a^3}{2\pi^2\lambda w^2} + \frac{4a^4}{\pi^3\lambda w^3}\right) \right] .$$

The quantities within the square bracket are all ~ 1 (except when λ is <u>very</u> close to a) since $\lambda \sim$ w and $\lambda >$ a. Thus a sufficient condition for the validity of the first Born approximation reads

(A8) $$U_o w^2 \ll \frac{4\pi a^2}{\lambda w} .$$

The criterion given in (A8) may be contrasted with the familiar criterion (for low energies and weak potentials) for the validity of the Born approximation[14]:

(A9) $$U_o w^2 \ll 1 .$$

Thus we see that for those evanescent waves for which $\lambda > a$, and for lattices comprised of relatively long range potential centers such that $w \sim \lambda$, the criterion (A8) is somewhat less lenient than the usual one.

It is amusing to notice that, under the conditions stated, the validity criterion (A8) may be phrased as follows: "The number of bound states of the potential U_o must be much smaller than the Fresnel number of the aperture formed by a unit cell of the lattice, viewed from a distance w (i.e., from the "edge" of the potential)".

APPENDIX B

As a last remark we indicate the form of the second order correction $\Psi_s^{(2)}(\underline{r})$ to the scattered wave function $\Psi_s(\underline{r})$. We again consider the infinite, plane, orthogonal lattice of Section 2. We easily find

$$\text{(B1)} \quad \Psi_s^{(2)}(\underline{r}) = \sum_{\alpha,\beta=-\infty}^{\infty} \sum_{\alpha',\beta'=-\infty}^{\infty} \Gamma_{\alpha\beta}\, \Gamma_{\alpha'\beta'}^{(\alpha\beta)}\, e^{i\,\underline{p}_{\alpha\beta}\cdot\underline{\rho}_{\alpha\beta}}\, e^{i\,\underline{p}_{\alpha'\beta'}\cdot\underline{r}}$$

where $\Gamma_{\alpha\beta}$ is as defined in (2.11), $\underline{\rho}_{\alpha\beta}$ is the same as in Section 2 and

$$\text{(B2)} \quad \Gamma_{\alpha'\beta'}^{(\alpha\beta)} = \frac{-i}{2kab}\cdot\frac{1}{m_{\alpha'\beta'}} \int d^3s\; e^{i(\underline{p}_{\alpha\beta} - \underline{p}_{\alpha'\beta'})\cdot\underline{s}}\; U_0(\underline{s}).$$

This result is interesting because it gives us information on the physical behavior of evanescent waves. Interpreting (B1) with the aid of the usual multiple scattering theory[15], we see that the incident homogeneous wave transformed into evanescent waves ($\alpha,\beta \neq 0$) can be again scattered into, say, a homogeneous wave (α', $\beta' = 0$) travelling in the positive z-direction. The first half of this transformation - from homogeneous to evanescent via diffraction - has been shown to play a role in image elimination in holography[5]. We see here that if multiple scattering were important, the second half of the transformation would lead to image formation.

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13. The message conveyed by (5.10) is equivalent, in the inverse "reconstruction" problem (see, e.g., Ref. 10), to the following "inverse" message: if only non-evanescent waves are detected, then details of the scattering potential of dimensions $\Delta x, \Delta y$, and Δz may be reconstructed so long as

$$(\Delta x)^{-2} + (\Delta y)^{-2} + (\Delta z)^{-2} \leq 4\lambda^{-2} .$$

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Figure Captions

Fig. 1 A rectangular two-dimensional lattice of scatterers. $\underset{\sim}{a}$ and $\underset{\sim}{b}$ are the primitive lattice vectors, and the incident wave vector $\underset{\sim}{k}$ is shown perpendicular to the lattice plane.

Fig. 2 One layer of a non-rectangular three-dimensional lattice. The z-axis has been chosen perpendicular to the plane defined by the primitive lattice vectors $\underset{\sim}{a}$ and $\underset{\sim}{b}$ which make angle θ_{ab} with each other. The incident wave vector $\underset{\sim}{k}$ is directed at an angle θ from the z-axis.

Fig. 3 The evanescence ellipse in the α-β plane which separates the regions of evanescent and homogeneous mode index pairs $\alpha\beta$. In this example we have chosen the physical scattering lattice to be square with $|\underset{\sim}{a}| = |\underset{\sim}{b}| = 2\sqrt{2}\,\lambda$, and the incident wave to be directed normal to the lattice. The consequence is that the evanescence ellipse is a circle. Only a small number of homogeneous modes, corresponding to the index pairs within or on the circle, will propagate beyond the scatterer into the $z > 0$ half-space.

Fig. 4 The evanescence ellipse for the same conditions as in Fig. 3, except that $\theta_{ab} = 45^{\circ}$ instead of 90°.

Fig. 5 The evanescence ellipse for the same conditions as in Fig. 4, except that the incident wave is not directed normal to the lattice, but such that $\underline{k}$ is still normal to the lattice vector $\underline{a}$ and makes an angle 60° with $\underline{b}$. The angle θ (see Fig. 2) is then 45°.

Fig. 6 Schematic diagram of a two-dimensional lattice with two different types of scattering sites.

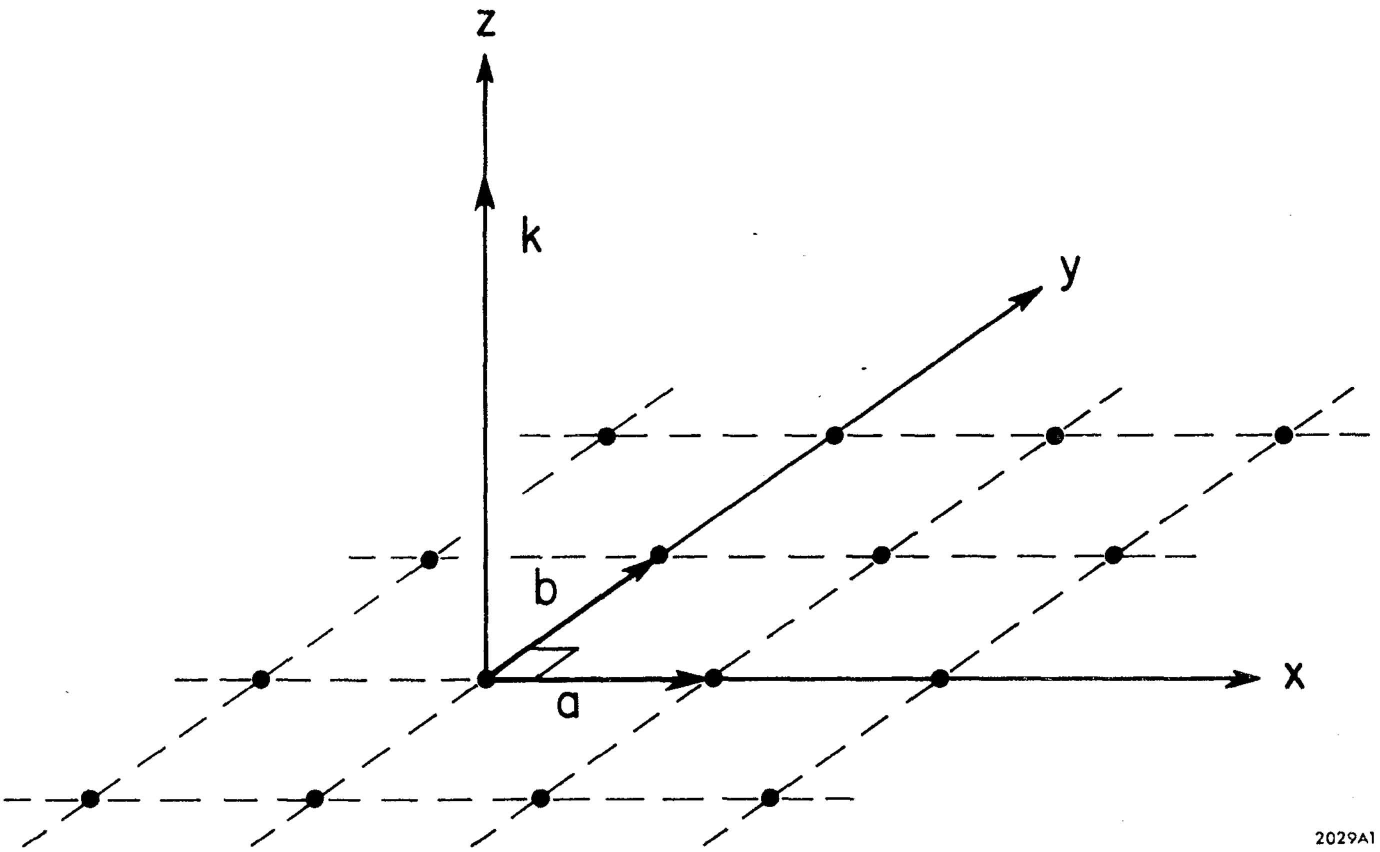

Figure 1

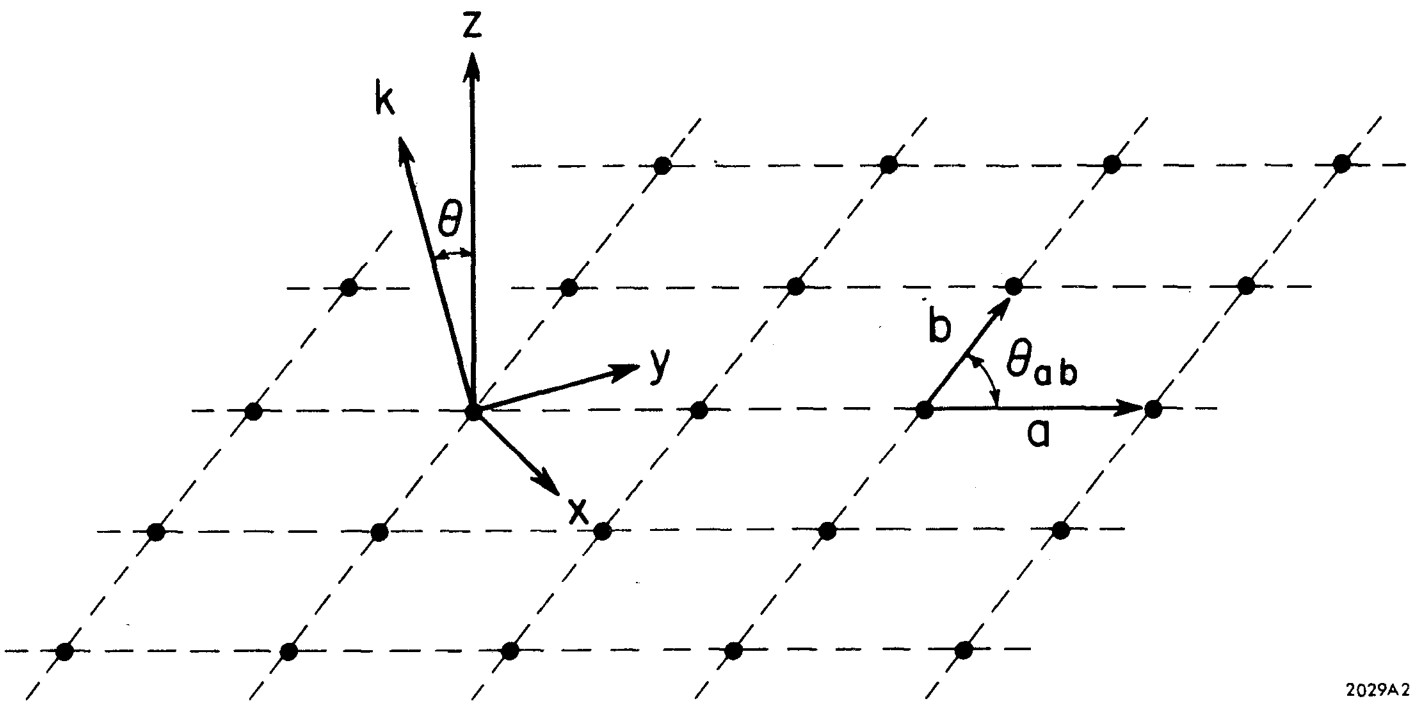

Figure 2

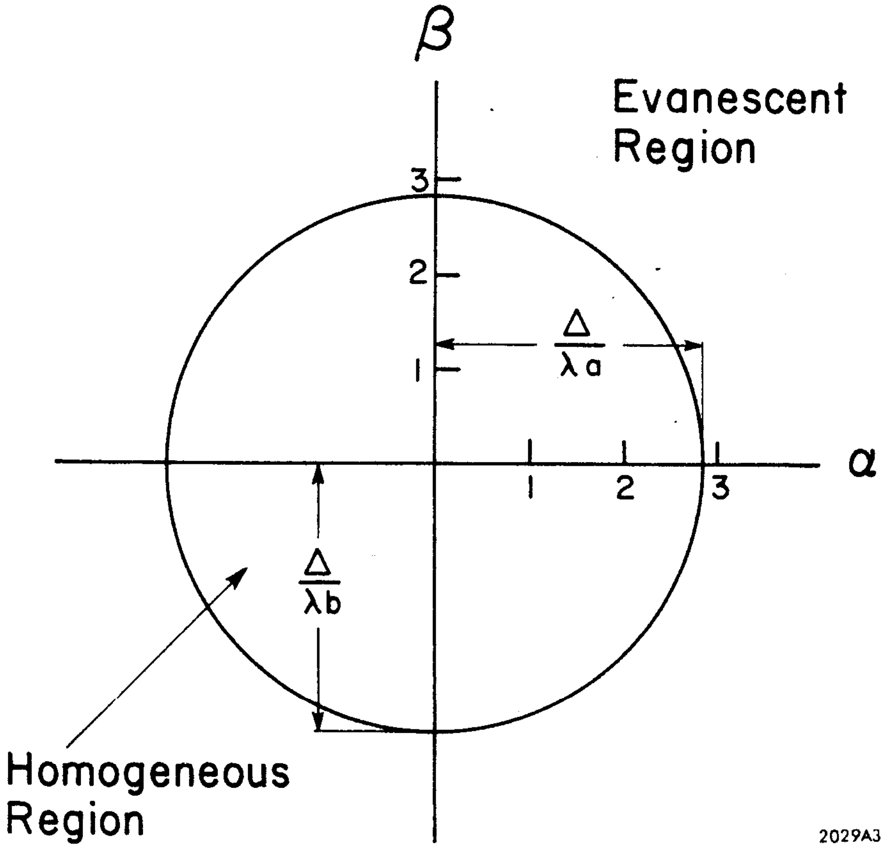
β
Evanescent
Region
3
2
1
$\frac{\Delta}{\lambda a}$
α
1
2
3
$\frac{\Delta}{\lambda b}$
Homogeneous
Region
2029A3

Figure 3

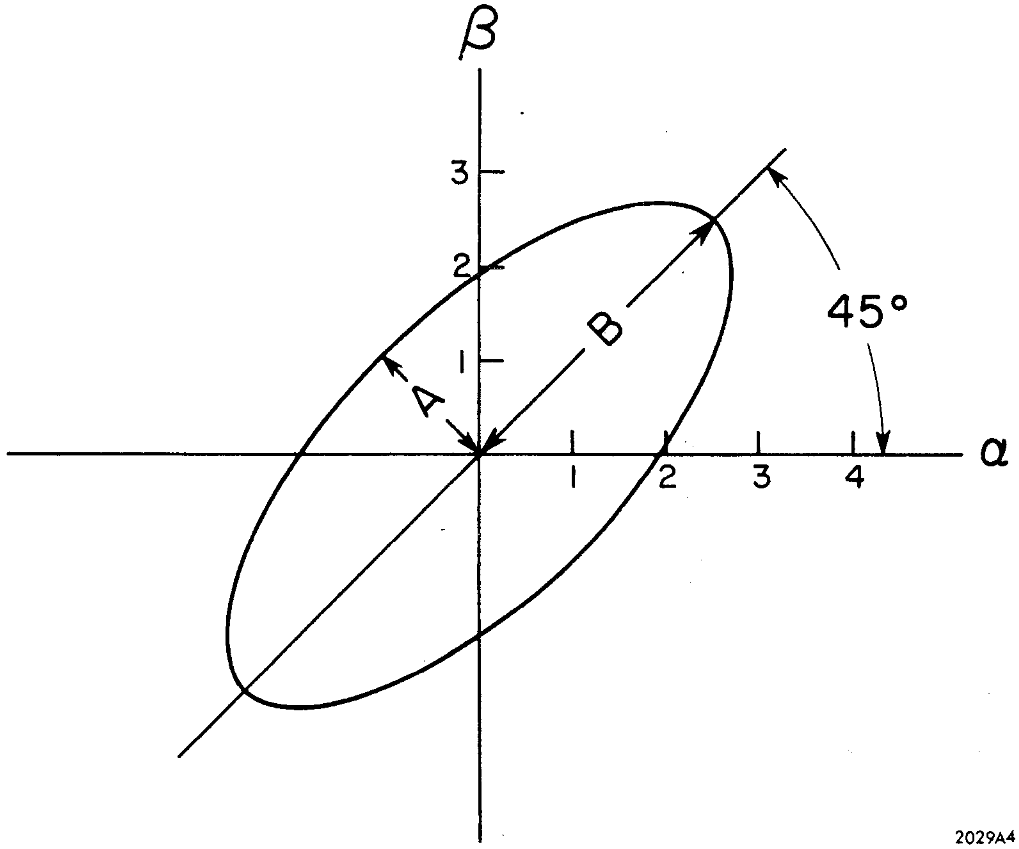

Figure 4.

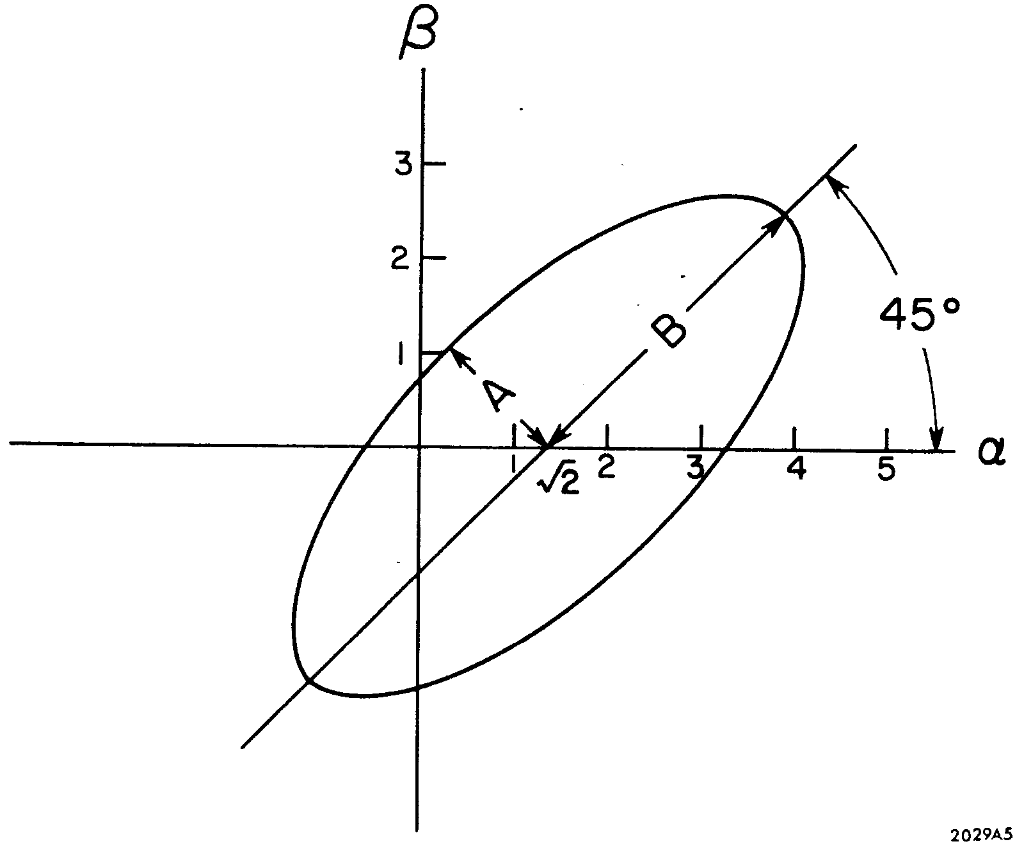

Figure 5

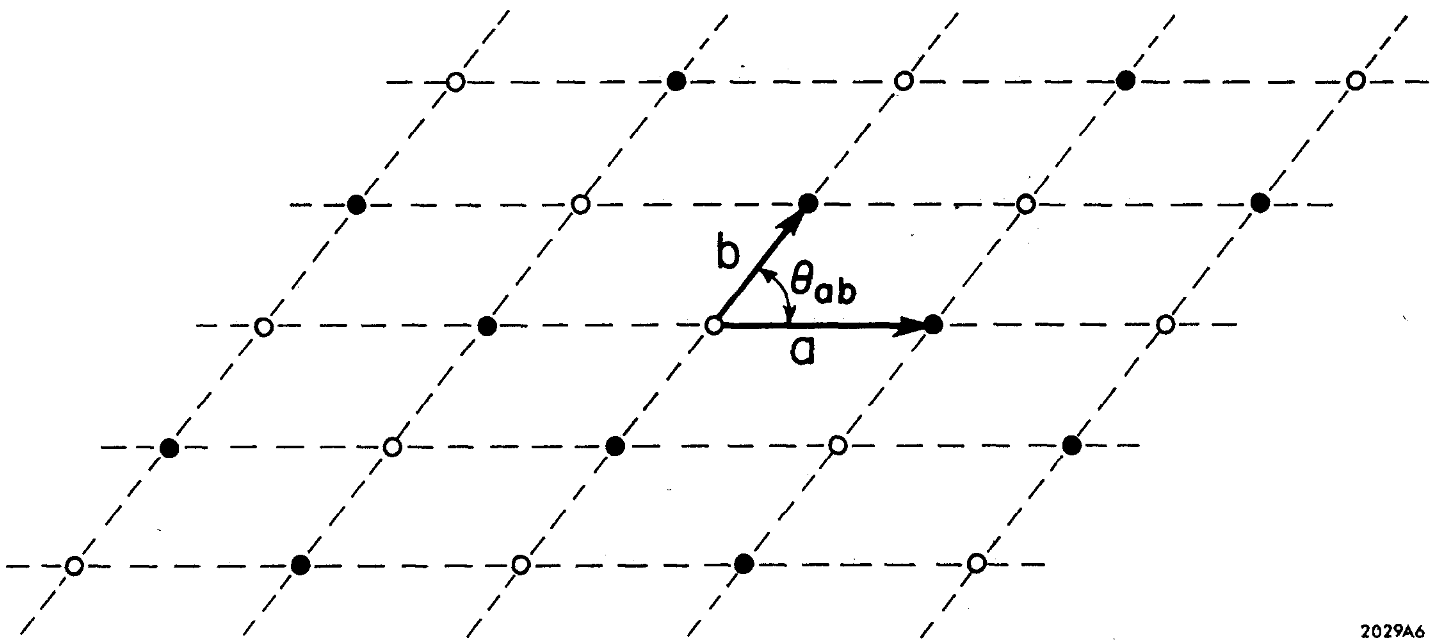

Figure 6