Band spectrum cutoff in linear and plane crystals

M. I. Faĭngol'd

Institute of Engineering Thermophysics, Academy of Sciences of the Ukrainian SSR

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Models of extremely thin single crystals consisting of an atomic chain and a plane lattice are analyzed. A fundamental upper limit is imposed on the allowed energy bands for any particles (including photons) in such lattices by a characteristic positive value: the "cutoff energy" E_a. The highest allowed band may lie partially in the region $E > 0$ but not above E_a. The cutoff energy E_a is determined entirely by the lattice constant and the mass of the particle. The relationship between the band structure and the nature of the scattering of particles by these lattices is discussed. Expressions are found for the band spectrum in such lattices in terms of the amplitude for the elastic scattering of external particles. The spectrum cutoff is shown to be a general property of linear and plane lattices.

1. INTRODUCTION

The nature of the energy spectra of filamentary and film crystals is assuming an important role in research on various effects which occur in these crystals.[1–3] In the present paper we analyze the nature of the energy spectrum on the basis of models of extremely thin unbounded crystals, i.e., systems of atoms in a regular arrangement in an isolated straight line or plane in the space which surrounds them. We call the corresponding lattices "linear or plane lattices."

As was originally shown by Kagan and Afanas'ev,[4] the resonant nuclear properties in scattering by linear and plane lattices "embedded" in free space may be quite different from their values for an isolated nucleus. A corresponding effect is described in Ref. 5 for the case of coherent scattering of photons by the atoms of a $2D$ crystal. Changes in resonant properties can also occur in $3D$ lattices,[4,6–8] but there the effect is manifested in a different way (in particular, the elastic width is observed to disappear completely under certain conditions).

The reason for this difference is that the boundary conditions are of a substantially different nature.[4] Linear and plane lattices coincide with their boundaries (their $3D$ volume is zero in the point approximation of the lattice sites). The effect of the boundary of a bulk lattice, in contrast, is small or (in the limit of an unbounded lattice) vanishes completely.

In the present paper we show that the resulting physical difference between these types of lattices turns out to be even more profound when we examine bound states. We are using the word "bound" here to refer to the transverse motion; the motion in the direction along the lattice is, in constrast, infinite. The total energy of the motion of a bound particle can therefore be positive. In this energy region, we could expect the appearance of discontinuities in a continuous spectrum, by analogy with bulk lattices. Actually, as we will see below, the effect is far more radical: The band spectrum in "embedded" lattices disappears completely at energies above a characteristic maximum value $E_a > 0$ for a given structure. In other words, the number of allowed energy bands in such lattices is finite, and the upper boundary of the uppermost band cannot be above E_a. The quantity E_a might be called the "cutoff energy" of the band spectrum. This cutoff stems from the coherent scattering of a particle by the lattice sites, which always occurs. Because of this process, the longitudinal motion of the particles in a lattice which coincides with its own boundary transforms into a transverse motion at a sufficiently large value of E, and a particle detaches from the lattice and goes off into free space.

Below we present a general theory for the cutoff effect, in which we make use of only the Bloch nature of the longitudinal motion of a particle in the field of an embedded lattice. We show that under the conditions assumed here the cutoff of the spectrum occurs for any particle, including photons, in a crystal. The conclusions derived below are illustrated through a direct calculation of the asymptotic behavior of the wave function of a particle in a bound state in an isolated atomic plane or chain. We also discuss the relationship between the cutoff of the spectrum and the features of the scattering of external particles by thin crystals. We derive a definite relationship between the poles of the scattering amplitude and the band spectrum of embedded lattices. On this basis we examine a specific model: a neutron in a chain of nuclei. For this model it is possible to derive an exact dispersion relation.

2. UPPER BOUNDARY ON THE SPECTRUM OF EMBEDDED LATTICES

The wave function of a particle in an embedded lattice is

$$\Psi(\mathbf{r}) = \Psi_{\mathbf{k}_\parallel}(\mathbf{r}_\perp, \mathbf{r}_\parallel)\exp(i\mathbf{k}_\parallel\mathbf{r}_\parallel), \tag{2.1}$$

$$\Psi_{\mathbf{k}_\parallel}(\mathbf{r}_\perp, \mathbf{r}_\parallel) = \Psi_{\mathbf{k}_\parallel}(\mathbf{r}_\perp, \mathbf{r}_\parallel + \mathbf{a}_{mn}); \quad m, n = 0, \pm 1, \ldots, \tag{2.2}$$

where $\parallel$ and $\perp$ label the vector components which are respectively parallel and perpendicular to the lattice, and $\mathbf{a}_{mn} = m\mathbf{a}_1 + n\mathbf{a}_2$ are lattice vectors (in the case of a chain we would have $a_1 = a, a_2 = 0$).

It follows from property (2.2) that there is a periodicity in the functional dependence of the energy E_δ on the longitudinal quasimomentum $\hbar\mathbf{k}_\parallel$:

$$E_\delta(\mathbf{k}_\parallel) = E_\delta(\mathbf{k}_\parallel + \mathbf{K}_{jl}), \quad j, l = 0, \pm 1, \pm 2, \ldots \tag{2.3}$$

Here δ is a band index, and $\mathbf{K}_{jl}$ are reciprocal lattice vectors. For a chain we would have $\mathbf{K}_{jl} \to K_j = 2\pi j/a$.

By virtue of (2.2), we can expand the function $\Psi(\mathbf{r})$ in a Fourier series:

$$\Psi(\mathbf{r}) = \exp(i\mathbf{k}_\parallel\mathbf{r}_\parallel)\sum_{j,l}\Psi_{jl}(\mathbf{r}_\perp)\exp(i\mathbf{K}_{jl}\mathbf{r}_\parallel). \tag{2.4}$$

Far from the lattice (as $r_\perp \to \infty$) expression (2.4) should

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become the solution of the Schrödinger equation for free space, i.e., a set of waves

$$\Psi(\mathbf{r})\approx\sum_{j,l}\Psi_{jl}\exp[i(\mathbf{k}_{jl\perp}\mathbf{r}_{\perp}+\mathbf{k}_{jl\|}\mathbf{r}_{\|})],\qquad(2.5)$$

where

$$\Psi_{jl}=\text{const},\quad k^2=k_{jl\perp}^2+k_{jl\|}^2=(2M/\hbar^2)E_\delta(k_\|)\qquad(2.6)$$

[in the case of a chain we would have $l=0$, and a factor $(r_\perp)^{-1/2}$, characteristic of axisymmetric systems, would appear in expansion (2.5)].

Comparing (2.4) and (2.5), we find

$$\mathbf{k}_{jl\|}=\mathbf{k}_\|+\mathbf{K}_{jl}.\qquad(2.7)$$

By virtue of (2.6) we then find

$$k_{jl\perp}=[(2M/\hbar^2)E_\delta(\mathbf{k}_\|)-(\mathbf{k}_\|+\mathbf{K}_{jl})^2]^{1/2}.\qquad(2.8)$$

In the situation under consideration here, in which no waves are incident from infinity, real values of $k_{jl\perp}$ would describe only the flux of particles moving away from the lattice. However, such a Ψ function cannot be a solution of the Schrödinger equation for a steady-state problem with real E_δ and $k_\|$. For stationary bound states, the only solution is in the form of a set of waves which are traveling along the lattice, whose amplitudes decay exponentially in the transverse directions. This situation corresponds to purely imaginary values for all $k_{jl\perp}$ from (2.8), i.e., to the condition

$$E_\delta(\mathbf{k}_\|)<(\hbar^2/2M)(\mathbf{k}_\|+\mathbf{K}_{jl})^2.\qquad(2.9)$$

Setting $j=l=0$ here and restricting the analysis (without any loss of generality) to the first Brillouin zone $|\mathbf{k}_\||\leqslant\pi/a$, where a is the smallest of the latice vectors, we find

$$E_\delta(\mathbf{k}_\|)<\hbar^2k_\|^2/2M.\qquad(2.10)$$

Substituting the largest value of the quasimomentum in the zone, $|\mathbf{k}_\||=\pi/a$, into the right side of (2.10), we find an upper limit on the energies which are possible in a bound state:

$$E_\delta<E_a,\quad E_a\equiv\pi^2\hbar^2/2Ma^2.\qquad(2.11)$$

By virtue of periodicity property (2.3), this inequality holds for all $k_\|$.

A corresponding restriction can be derived for the energy of bound photons, $E_\delta=\hbar\omega_\delta$, if we switch to relativistic equations in (2.6) and (2.8), writing $\omega_\delta{}^2/c^2$ in place of $(2M/\hbar^2)E_\delta$. In that case, precisely the same arguments lead to the condition

$$\omega_\delta<\omega_a,\quad \omega_a\equiv\pi c/a.\qquad(2.12)$$

This condition may be thought of as an extension to the case of atomic chains or "grids" with known limitation[9] on the frequencies which are possible for electromagnetic waves propagating in discrete lossless waveguides ("ladder filters").

3. WAVE FUNCTION OF A PARTICLE IN A LINEAR OR PLANE LATTICE

Let us examine the wave functions of the bound state of a particle in a linear or plane Bravais lattice. As the basis states we adopt the s states of a particle in the field of an individual atom (or nucleus) of the lattice, which are the states which dominate the interaction in the case of slow particles:

$$\varphi(r)\approx r^{-1}\begin{cases}e^{-ikr}-S_0(k)e^{ikr}, & E>0,\qquad(3.1a)\\ e^{-|k|r}, & E<0.\qquad(3.1b)\end{cases}$$

Here $k=(2ME)^{1/2}/\hbar$, and $S_0(k)$ is a scattering matrix with poles at the points $k_\delta{}^{(0)}$, which correspond to the individual levels $E_\delta{}^{(0)}$ of a particle in the field of an individual site.

By analogy with the strong-coupling method for a bulk lattice,[10] we write the complete Ψ function of the particle as a superposition of basis functions (3.1) taken with Bloch amplitudes $A_{mn}\equiv A\exp i\mathbf{k}_\|\mathbf{a}_{mn}$:

$$\Psi(r)\approx A\exp(i\mathbf{k}_\|\mathbf{r}_\|)\sum_m\sum_n\frac{\exp[i\mathbf{k}_\|(\mathbf{a}_{mn}-\mathbf{r}_\|)]}{|\mathbf{a}_{mn}-\mathbf{r}|}\times\begin{cases}\exp(-ik|\mathbf{a}_{mn}-\mathbf{r}|)-S_0(k)\exp(ik|\mathbf{a}_{mn}-\mathbf{r}|).\qquad(3.2a)\\ \exp(-|k|\,|\mathbf{a}_{mn}-\mathbf{r}|).\qquad(3.2b)\end{cases}$$

Here and below, the upper row in braces corresponds to the case $E>0$, and the lower to $E<0$. We will not be using function (3.2) to calculate the energy $E_\delta(k_\|)$ by perturbation theory, so in introducing functions (3.1) and (3.2) we replace the fixed values $k_\delta(0)$ by simply k. This approach makes it possible to use expression (3.2) to describe weakly bound states also. The incorporation of states with $E>0$ in expansion (3.2) makes it possible to describe a situation in which a particle is not confined by an individual site but is confined by the lattice as a whole. Correspondingly, the incoming waves in (3.2a) correspond to a transition of a particle with $E>0$ to a given site of the lattice from other sites. Outgoing waves describe the departure of a particle from the given site.

We will shown that, despite the isotropic nature of the waves which are coming into and going out of individual sites in the case $E>0$, their Bloch sum in (3.2a) does not give rise in the surrounding space to waves which are going away from the lattice or coming into it, if conditions (2.9)–(2.11) hold.

To prove this basic assertion we use a Fourier expansion (2.4) of function (3.2):

$$\Psi_{jl}(\mathbf{r}_\perp)=\frac{A}{\sigma}\iint_\sigma\sum_m\sum_n\frac{\exp[i\mathbf{k}_\|(\mathbf{a}_{mn}-\mathbf{r}_\|)]}{|\mathbf{a}_{mn}-\mathbf{r}|}\times\begin{Bmatrix}\exp[-ik|\mathbf{a}_{mn}-\mathbf{r}|]-S_0(k)\exp[ik|\mathbf{a}_{mn}-\mathbf{r}|]\\ \exp[-|k|\,|\mathbf{a}_{mn}-\mathbf{r}|]\end{Bmatrix}\times\exp[i\mathbf{K}_{jl}(\mathbf{a}_{mn}-\mathbf{r}_\|)]d\sigma.$$

Here σ is the area of a unit cell, and we have made use of the property $\mathbf{a}_{mn}\mathbf{K}_{jl}=(mj+nl)2\pi$ of the vectors of the direct and reciprocal lattices in the calculation. An integration of a lattice series of the type in (3.2) over the area of a cell, however, yields an integral of one general term of the series [e.g., $(m,n)=(0,0)$] over the entire plane. Accordingly, by introducing polar coordinates in the plane, $r_\|,\vartheta$ (ϑ is the angle between $\mathbf{k}_{jl\|}$ and $\rho_{mn}\equiv\mathbf{a}_{mn}-\mathbf{r}_\|$), integrating over ϑ, and using (2.7), we find

$$\Psi_{jl}(r_\perp)=2\pi\frac{A}{\sigma}\int_0^\infty J_0(k_{jl\|}r_\|)\begin{Bmatrix}e^{-ikr}-S_0(k)e^{ikr}\\ e^{-|k|r}\end{Bmatrix}\frac{r_\|}{r}dr_\|,$$

where $J_0(\xi)$ is a Bessel function of index zero, and $r=(r_{\parallel}^2+r_{\perp}^2)^{1/2}$. The integral which remains can be expressed in terms of elementary functions[11]:

$$\Psi_{jl}(r_\perp)$$

$$=2\pi\frac{A}{\sigma}\begin{cases}[1-S_0(k)]\,(k_{jl\parallel}^2-k^2)^{-1/2}\exp[-(k_{jl\parallel}^2-k^2)^{1/2}r_\perp] & (3.3\text{a})\\ (k_{jl\parallel}^2+|k|^2)^{-1/2}\exp[-(k_{jl\parallel}^2-k^2)^{1/2}r_\perp] & (3.3\text{b})\end{cases}$$

A similar procedure for a chain yields

$$\Psi_j(r_\perp)=2\frac{A}{a}\begin{cases}[1-S_0(k)]K_0((k_{j\parallel}^2-k^2)^{1/2}r_\perp) & (3.4\text{a})\\ K_0((k_{j\parallel}^2+|k|^2)^{1/2}r_\perp) & (3.4\text{b})\end{cases},$$

where $K_0(\xi)$ is a modified Bessel function of index zero.[11] Using the asymptotic expressions for these functions as $r_\perp\to\infty$, we find

$$\Psi_j(r_\perp)$$

$$=(2\pi)^{1/2}\frac{A}{ar_\perp^{1/2}}\begin{cases}[1-S_0(k)]\,(k_{j\parallel}^2-k^2)^{-1/4}\\ \times\exp[-(k_{j\parallel}^2-k^2)^{1/2}r_\perp] & (3.5\text{a})\\ (k_{j\parallel}^2+|k|^2)^{-1/4}\\ \times\exp[-(k_{j\parallel}^2+|k|^2)^{1/2}r_\perp] & (3.5\text{b})\end{cases}.$$

It can be seen from (2.4) and (3.3), (3.5) that in the case $k^2<k^2_{jl\parallel}$ the Ψ function given by (3.2) describes the state of a particle in the form of waves which are traveling along the lattice and whose amplitudes decay exponentially outside the lattice. For values $k^2<0$ ($E<0$), a state of this sort forms from individual bound states (3.1b), and the motion along the lattice occurs through site-to-site tunneling. In the region $0<k^2<k^2_{jl\parallel}$ $(0<E<(\hbar^2/2M)\,k^2_{jl\parallel})$, in contrast, where a particle cannot be confined by an individual site, a bound state arises from the individual scattering states in (3.1a). In this case the waves which are coming into and going out of the individual sites interfere in such a way that far from the lattice we are left with only the decaying components, and among all possible scattering directions the ones which are realized are those along the vectors $k_{jl\parallel}$. The conditions of such an interference are the same as conditions (2.10) and (2.11).

If $E>E_a$, on the other hand, then we have $k^2>k_{\parallel}^2$ throughout the reduced Brillouin zone, and the corresponding amplitudes Ψ_{jl} [for which the sites (j,l) of the reciprocal lattice lie within a circle of radius k] describe outgoing plane waves or (for a chain) conical waves, i.e., a scattering involving the escape of a particle from the lattice. Consequently, in the region $E>E_a$ there are no bound staes in linear or plane lattices. For this reason it is legitimate to call E_a the "cutoff energy" of the band spectrum.

4. DISPERSION RELATIONS FOR A NEUTRON IN A CHAIN AND IN A PLANE LATTICE

We now consider an exactly solvable model: a neutron in a simple chain of nuclei. Kagan and Afanas'ev[4] have derived an expression for the amplitude (A) for the elastic scattering of a neutron by a chain of identical nuclei

$$A(k,\,k_\parallel)=(f^{-1}-\xi(k,\,k_\parallel))^{-1}. \tag{4.1}$$

Here f is the amplitude for elastic scattering by an isolated nucleus, and

$$\xi(k,\,k_\parallel)=\frac{2}{a}\sum_{m=1}^{\infty}\frac{e^{iakm}}{m}\cos(ak_\parallel m). \tag{4.2}$$

In the case of scattering near a resonance, a short-lived excited nucleus-plus-neutron complex arises, which is completely delocalized (a collective compound nucleus). In a similar way we could treat a completely delocalized (in the longitudinal direction) stable state of a neutron which has "attached itself" to a chain. The characteristics of such a state can be found by examining the wave function of a neutron which does not contain incident waves.[12,13] In the present paper, however, we will use a new and simpler method, which is based on an analysis of expression (4.1). For this purpose we make use of the general principle according to which the bound states of any system correspond to poles in its scattering amplitude continued analytically to the complex E plane. A new point here will be the circumstance that, because of the spatial extension of the scatterer, the poles of amplitude A which describe delocalized bound states lie not at isolated points $E=E_\delta^{(0)}$ but in continuous sets $E_\delta(k_\parallel)$, which form arcs of curves in the E plane. Each point of such an arc corresponds to a certain value of $k_\parallel$ (more precisely, to the set $k_\parallel+2\pi j/a$). In the case of stationary states, these arcs lie on the real axis, $E_\delta(k_\parallel)=E^*_\delta(k_\parallel)$, and describe allowed energy bands (Fig. 1).

For a chain with amplitude (3.1) the positions of the poles and thus the energy bands $E_\delta(k_\parallel)$ are determined by the equation

$$f^{-1}-\xi(k,\,k_\parallel)=0. \tag{4.3}$$

We are interested in only stationary stats, i.e., in the case in which the total width of the seed level $E_\delta^{(0)}$ of an isolated nucleus in the expression for f is the same as the elastic width: $\Gamma=\Gamma_1$ (a chain of nonabsorbing nuclei). In this case the most general expression for f is known to be

$$f^{-1}=g(k)-ik, \tag{4.4}$$

where $g(k)$ takes on real values for all real E. The series

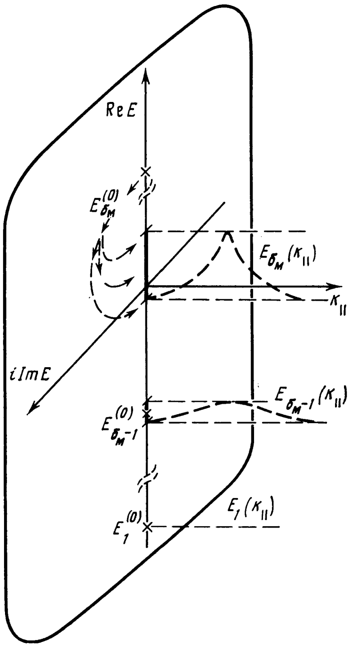

FIG. 1. Transformation of isolated point poles in the scattering amplitude (shown by the crosses) into continuous features (shown by the line segments) in the complex E plane. This diagram describes the conversion of discrete levels $E_\delta^{(0)}$ into bands $E_\delta(k_\parallel)$ during the formation of a chain.

(4.2) can be summed in terms of elementary functions[11]:

$$\xi(k, k_\parallel) = \begin{cases} -(1/a)\ln(2|\cos ak - \cos ak_\parallel|) + (i/a)(j+j'+1) - ik, & (4.5a) \\ -(1/a)\ln[2(\mathrm{ch}\, a|k| - \cos ak_\parallel)] + |k|, & (4.5b) \end{cases}$$

where

$$j = \left[\frac{a(k+k_\parallel)}{2\pi}\right], \quad j' = \left[\frac{a(k+k_\parallel)}{2\pi}\right], \qquad (4.6)$$

and $[x]$ means the greatest interger in x (see also Ref. 4).

Substituting this result into (4.3), we find

$$\ln(2|\cos ak - \cos ak_\parallel|) + ag(k) = i(j+j'+1), \; E>0, \qquad (4.7a)$$

$$\ln[2(\mathrm{ch}\, a|k| - \cos ak_\parallel)] + ag(k) = 0, \quad E<0. \qquad (4.7b)$$

A solution with real k and $k_\parallel$ in (4.7a) is possible only under the condition

$$j+j'+1=0 \qquad (4.8)$$

or, by virtue of (4.6),

$$1 + \frac{ak}{\pi} = \left\{\frac{a(k+k_\parallel)}{2\pi}\right\} + \left\{\frac{a(k-k_\parallel)}{2\pi}\right\}, \qquad (4.9)$$

where $\{x\}$ is the fractional part of x. This condition can be satisfied only for

$$k^2 < k_\parallel^2, \qquad ak/\pi < 1. \qquad (4.10)$$

The latter inequalities are the same as conditions (2.10) and (2.11).

Although the result which has been found here on the basis of this model has been derived rigorously, it does not depend on the form of $g(k)$, i.e., on the particular parameters of the model, since it is (as we emphasized above) a general property of embedded lattices.

It is also a straightforward matter to derive the explicit functional dependence $E_\delta(k_\parallel)$ from (4.7). We know that in the approximation of a singular interaction we can write

$$g(k) = \frac{(2M)^{1/2}}{\hbar} \begin{cases} -(E_\delta^{(0)})^{1/2}, & \delta = \delta_M, \quad (4.11a) \\ |E_\delta|^{1/2}, & \delta = 1, 2, \ldots, \delta_M - 1, \quad (4.11b) \end{cases}$$

where the upper row corresponds to a virtual level, and the lower row to a real level, of an isolated nucleus.[14] Adopting the case of the virtual level for definiteness, we find

$$E_{\delta_M}(k_\parallel) = \frac{E_a}{\pi^2} \begin{cases} \mathrm{Arccos}^2(\cos ak_\parallel + {}^1/_2 \exp[-(a/\hbar)(2ME_{\delta_M}^{(0)})^{1/2}]) & (4.12a) \\ -\mathrm{arch}^2(\cos ak_\parallel + {}^1/_2 \exp[-(a/\hbar)(2ME_{\delta_M}^{(0)})^{1/2}]) & (4.12b) \end{cases};$$

only the principal branch, $(\mathrm{Arccos}\, x) \in [0, \pi]$, is used in (4.12a).

We know that an isolated pole corresponding to a virtual level lies on an unphysical sheet of a Riemann surface.[14] The existence of solution (4.12) means that as a chain is formed the pole point not only deforms into a line segment but also moves onto the physical sheet. This result agrees with the circumstance that a bound state can arise in a system of potential wells even if there are no such states in an isolated well.[15]

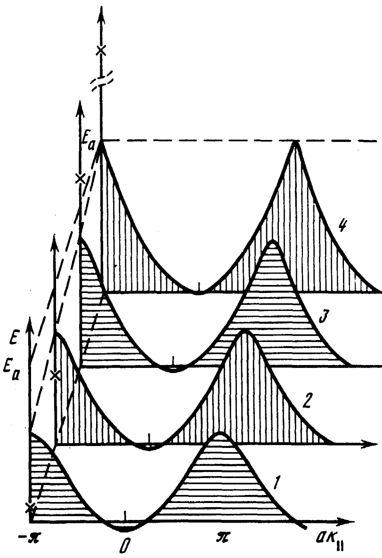

FIG. 2. Dispersion curves of the highest-lying allowed band in a linear chain for four different energies of the seed virtual level $E_{\delta_M}^{(0)}$ (shown by the crosses): 1—$5\times10^{-2}\,E_a$; 2—$0.45\,E_a$; 3—$1.25\,E_a$; 4—$10\,E_a$.

Figure 2 shows several dispersion curves plotted from (4.12) for various values of $E_{\delta_M}^{(0)}$. We see that no matter how high the seed virtual level $E_{\delta_M}^{(0)}$ lies the energies of the real bound states which arise from it are always lower than E_a. Near the point $k_\parallel = 0$ the energy is always negative and is described by branch (4.12b), which can be written in the following form at sufficiently small values of $k_\parallel$:

$$E_{\delta_M}(k_\parallel) = E_{\delta_M}(0) + \hbar^2 k_\parallel^2 / 2M^*. \qquad (4.13)$$

Here

$$E_{\delta_M}(0) = -\frac{E_a}{\pi^2}\mathrm{arch}^2\left(1 + \frac{1}{2}\exp\left[-\frac{a}{\hbar}(2ME_{\delta_M})^{1/2}\right]\right) \qquad (4.14)$$

is the energy at $k_\parallel = 0$ (the binding energy of the neutron with the chain), and

$$M^* = \frac{1}{\hbar^2}\left(\frac{d^2E}{dk_\parallel^2}\right)^{-1}_{k_\parallel=0} = M \frac{\{1 + {}^1/_2 \exp[-(a/\hbar)(2ME_{\delta_M}^{(0)})^{1/2}]\}^{1/2}}{\mathrm{arch}(1 + {}^1/_2 \exp[-a/\hbar\,(2ME_{\delta_M}^{(0)})^{1/2}])} \qquad (4.15)$$

is the effective mass of a neutron in a linear crystal.

In a corresponding way, we can derive a dispersion relation for a plane lattice (a $2D$ crystal). We make use of an expression which was derived in Ref. 5 for the amplitude for the scattering by a $2D$ crystal:

$$q_0 = \frac{i\eta}{f^{-1} + i(\Phi k - \tilde{\Phi}\eta) - \xi_i}. \qquad (4.16)$$

Here

$$\eta = \frac{\lambda N_\sigma}{\sin\theta} = 2\pi\frac{N_\sigma}{k_\perp} = \frac{2\pi N_\sigma}{(k^2 - k_\parallel^2)^{1/2}}, \qquad (4.17)$$

N_σ is the surface density of sites, Φ is a dimensionless potential, which is equal to unity for s-wave scattering, and

$\tilde{\Phi}(k,k_{\parallel})$ and $\xi_i(k,k_{\parallel})$ are real functions which depend on the geometry of the lattice.

Corresponding to the poles of the amplitude q_0 are the roots of the dispersion relation

$$f^{-1}+ik-i\tilde{\Phi}(k,k_{\parallel})\eta-\xi_i(k,k_{\parallel})=0$$

or, if we use (4.4) and (4.17),

$$g(k)-2\pi i\tilde{\Phi}(k,k_{\parallel})N_\sigma/(k^2-k_{\parallel}^2)^{1/2}-\xi_i(k,k_{\parallel})=0. \quad (4.18)$$

Since $g(k)$, $\tilde{\Phi}(k,k_{\parallel})$ and $\xi_i(k,k_{\parallel})$ are real, a necessary condition for the existence of a solution of Eq. (4.18) is that its second term also be real. This requirement automatically leads to a cutoff of the spectrum at the energy E_a given by (2.11), where a is the smallest of the constants of the $2D$ lattice.

5. PHYSICAL MECHANISM FOR THE CUTOFF

At first glance the results derived here would seem to contradict the known fact that E is unbounded in the field of a uniform string or plane (by virtue of the energy of the longitudinal motion, $E_{\parallel}$). The periodicity of the lattice (which makes it impossible to separate a term $E_{\parallel}$ from E) gives rise to discontinuities in the continuous spectrum of E, but is not by itself sufficient to cut off all states with $E>E_a$, since such states exist both in bulk lattices and in regular systems of chains or grids spanning the entire space.

An important feature of this problem is the fact that there is only a single embedded lattice (or a finite number of them). It is this circumstance, combined with the discrete nature of the problem, which leads to the cutoff of the spectrum. The disappearance of bound states with $E>E_a$ is a rather nontrivial effect, which is possible only in lattices which are bounded in one or two directions.[1)]

The physical mechanism for the effect involves a scattering by sites, which leads to an entanglement of the longitudinal and transverse modes. At large E, the result is the appearance of components $k_\perp$ which are sufficient for the escape of the particle from the lattice. Less clear is why this happens at specifically an energy E_a which depends on only the period, and not the field $U(\mathbf{r})$, of the lattice. The answer is that E_a is the upper boundary of the interval of allowed energies for all lattices with a given a; the specific values of the maximum energies for each such lattice are individual characteristics. The a dependence is related to the wave properties of the particles. The particle energy E corresponds to a wavelength $\lambda=\pi\hbar[2/M(E+|\bar{U}|)]^{1/2}$, where $\bar{U}<0$ is the expectation value of $U(\mathbf{r})$. At $E<E_a-|\bar{U}|$, the wavelength is $\lambda>2a$, the particle does not sense the discrete nature of the lattice, and the motion of the particle is analogous to the waveguide propagation of light in a transparent filamentary or film crystal. If $E>E_a-|\bar{U}|$, on the other hand, then we have a wavelength $\lambda<2a$, and the particle is scattered by sites and moves away from the lattice. This scattering is coherent, so in an infinite system of parallel identical lattices separated by a distance b, even under the conditions $b\gg a_1$, a_2, the system of waves scattered from the various lattices can combine again into self-consistent stationary states which form allowed bands with $E>E_a-|\bar{U}|$. In the case of a single such lattice (or a finite number of them), the scattered waves go off into the surrounding space, and a stationary state with $E>E_a-|\bar{U}|$ is impossible. In the limit $|\bar{U}|\to 0$ the upper boundary of the spectrum approaches E_a.

6. BAND SPECTRUM AND SCATTERING OF EXTERNAL PARTICLES

The spectrum cutoff effect is related to certain observable features of the scattering of particles by filamentary and film crystals. One such feature is the excitation of two-sided surface waves in scattering by a monatomic crystal film.[12,13] Only the higher (nonzero) harmonics of such waves, i.e., modes with j, l which satisfy the condition

$$(\mathbf{k}_{\parallel}+\mathbf{K}_{jl})^2>(2M/\hbar^2)E. \quad (6.1)$$

are excited. This condition becomes the same as (2.9) at $E=E_{\delta M}(k_{\parallel})>0$.

Denoting by θ the glancing angle of the particles incident on the film, we have $k_{\parallel}^2=k^2\cos^2\theta\leqslant(2M/\hbar^2)E$. In the case $j=l=0$, for example, condition (6.1) clearly cannot be satisfied. This conclusion agrees completely with the conclusion [see (2.9) and (2.10)] that there can exist no waves for which the condition $E>(\hbar^2/2M)k_{jl\parallel}^2$ holds and which are associated with the lattice. Consequently, the impossibility of excitation of a two-sided surface wave with $|\mathbf{k}_{jl\parallel}|<k$ during the irradiation of the surface of a plane crystal is intimately related to the spectrum cutoff effect.

On the other hand, a bound state in the allowed region of positive energies, $0<E<E_a$, can be excited during end-on irradiation of linear and plane crystals of finite thickness (because of the boundedness of the longitudinal dimensions of the crystals, this state is actually a quasibound state). For definiteness we consider a monochromatic beam of particles directed parallel to the axis of an acicular crystal. We assume that no inelastic processes occur. If the beam energy satisfies $E<E_a-|\bar{U}|$, the particles incident on the end of the crystal occupy the corresponding allowed state of the crystal with positive energy E. The momentum $\hbar k$, being perpendicular to the end, has a discontinuity and takes on a set of equidistant quasimomentum values $k_{\parallel}+2\pi j/a$, which are equal to the roots of the equation $E_{\delta M}(k_{\parallel})=E$, according to (2.2). The loss of particles from the beam is minimal in this case and results only from scattering by the two "centers"—the ends of the filament, from which two spherical waves move out. Beginning at the threshold value $E=E_{\delta M}(\pi/a)\leqslant E_a$, an additional scattering arises, because the crystal has no allowed energies with $E>E_{\delta M}(\pi/a)$. Under the condition $k^2>k_{\parallel}^2$ this scattering is described [according to (2.4) and (3.5a)] by conical waves which propagate away from the axis of the crystal. As a result, one should observe a substantial decrease in the intensity of the transmitted beam, $J_{\text{out}}(E)$, at the exit end of the crystal at $E=E_\delta(\pi/a)\approx E_a$. The absence of high-lying allowed bands in this crystal is seen in the circumstance that this decrease persists at all $E>E_a$. For an ordinary single crystal, in contrast, whose dimensions in the directions perpendicular to the beam are comparable to or greater than the length of the crystal along the beam, the dip in the energy dependence of the exit intensity $J_{\text{out}}(E)$ at $E\approx E_a$ (accompanied by a Bragg reflection of the beam from the entrance end) will disappear and reappear repeatedly with further increase of E, as we know.

In summary, the distinctive features in the scattering by linear and plane crystals and also the associated cutoff of the spectrum are surface effects: The two types of $J_{\text{out}}(E)$ behavior pointed out here should blend smoothly into each other as the crystal thickness changes. The "decay" of the allowed states with $E > E_a$ which results from the escape of the scattered waves from the lattice will be seen most vividly in crystalline filaments and films of atomic thickness.

The effect described here may play an important role in the realization and study of various regimes of waveguide propagation of particles (e.g., of slow neutrons), in research on transport processes in thin crystals, etc.

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[1)]For any singly connected (topologically) lattice which is bounded in all directions, only states with $E < 0$ are truly bound, as we know. This comment also applies to real filamentary and film crystals, in which states with $0 < E < E_a$ convert into quasibound states. However, the topological connectedness of such crystals can be altered since the Born-Kármán conditions hold for such crystals physically. These conditions make it possible to eliminate a boundary by closing the lattice into a ring or torus. In this case, all the results remain applicable if the radius of the ring is sufficiently large.

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