

Particles in finite and infinite one-dimensional periodic chains

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Abstract. Particle motion in one-dimensional crystal chains is studied with the help of the transfer matrix method. The transition from a finite to an infinite chain is analyzed. In the cases where an analytic solution is impossible, the method allows calculating the energy spectra with reasonable accuracy, based on the known cell potential. It turns out that the structure of allowed and forbidden energy bands arising in an ideal lattice contains some features that are absent in the real world. This means that the model of an ideal lattice should be extended in order to describe reality. We show that accounting for small random perturbations of periodicity may serve as such an extension. Light propagation in a layered medium (including a photonic crystal) is studied using the same method.

Keywords: periodic lattice, finite lattice, transfer matrix, random perturbations, tight binding and weak binding approximations

1. Introduction

Analyzing particle motion in a linear chain of repeating potential centers (in a one-dimensional crystal) is an indis-

pensable element of many courses in quantum mechanics (see, e.g., [1–7]). These problems provide a basis for understanding numerous phenomena in solid state physics or related phenomena.

A traditional presentation of these questions consists of the formulation of certain general statements for an arbitrary periodic lattice, followed by studying a phenomenon using some special example that allows analytic treatment, with the results then extended to the general case. Cell potentials in a simplified form are used in such examples. The respective descriptions only attempt to prove the existence of a band structure and address its main properties. The question remains as to whether the particular features of solutions obtained reflect the general properties of periodic structures or whether they are related to specifics of the models used (rectangular boundaries or δ -functions, sinusoidal lattices, and so on). Finding appropriate dependences for realistic potentials is implicitly assumed to be too complicated a problem; therefore, the research uses their simplified forms or simply the approximation of measurement results.

The well-known transfer matrix method [8] (see Section 2) is used in this study. In work known to the author (see also [5, 11]), this method is applied to some models of infinite lattices, and general conclusions, to a large degree, rely on the analysis of these examples.¹ In contrast, we build descriptions that are applicable for cell potentials of an arbitrary shape. Appendix B collects examples known to the author that permit an analytic solution (and only remotely resemble realistic potentials). For a given cell potential, formulas in Section 2, in particular, give a simple algorithm

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¹ In the method of recurrent relations [12], which is close to the method used here, the properties of forbidden bands (gaps) remain outside the focus of the researcher.

for computing the dispersion law with reasonable accuracy based on the shape of the cell potential and a numerical solution of the Schrödinger equation in the cell.

General properties of states in periodic lattices are discussed in Section 3. Briefly described are the allowed and forbidden energy bands, and the tight-binding approximation is developed, irrespective of the shape of the cell potential. It turns out that forbidden energy bands are preserved for arbitrary cell potentials for high-energy electrons, which contradicts physical expectations. (The author is not aware of discussions of this problem in the literature.) This implies that the model of a purely periodic potential needs to be augmented in order to be applicable to the description of real-world lattices. Such an additional factor can be small random deviations from periodicity, discussed in Section 5. Accounting for such deviations allows us to answer the question why in real materials the band structure with electrons delocalized over the entire crystal is realized only for electrons of the highest energy levels (for example, valence electrons), and remaining electrons can be considered localized close to respective ions.

The analysis of properties of finite lattices is commonly viewed as an introduction to studies of infinite periodic lattices. A standard numerical analysis of a finite lattice for a moderately high number of cells suffers from error accumulation in subsequent transitions through cell boundaries, whereby the resulting final error is not controlled sufficiently well. However, studying the set of levels and (or) transparency bands for finite lattices with more or less appropriate cell potentials is of value on its own. The transfer matrix method allows solving these questions and is free of error accumulation in studies of finite lattices (see Section 4). In particular, it turns out that the change in boundary conditions simply leads to a shift of level positions within its allowed band in the problem of bound states and to a slight shift in boundaries of the forbidden band in the scattering problem. Formulas in Section 4, in particular, give an algorithm to compute the positions of levels and boundaries of forbidden bands given the shape of the cell potential after numerical solution of the Schrödinger equation within the cell.

In Appendix C, the transfer matrix method is applied to the description of light propagation in a layered structure — a stack composed of a large number of planar plates, where the notion of a photonic crystal emerges in a natural way (see, e.g., [9]).

2. Transfer matrix

We consider electron states in a system of N equivalent cells of length a (*lattice constant*) with a potential of an arbitrary form within each of them. Lattices with large but finite N are considered. It is common to think that as $N \rightarrow \infty$, we pass to a *periodic lattice*, as is discussed in many textbooks.

The sets of states in a periodic lattice and a finite lattice are different. Stationary states of particles in a finite-size lattice are standing waves with phase relations that depend on details of the boundary conditions. States resembling traveling waves in unbounded space occur in a periodic lattice. Similarly to infinite space, standing waves can be considered a superposition of traveling waves and vice versa. Nevertheless, the results obtained for periodic lattices can be applied (and successfully so) to the description of real-world

lattices. This means that for large N , the details of boundary conditions influence the results only slightly. In Section 4, we discuss how this happens.

The system Hamiltonian is written as

$$\hat{H} = \frac{\hat{p}^2}{2m} + \sum_{n=0}^{N-1} U(x - na), \quad (1)$$

where $U(y) = 0$ for $y \leq 0$ and $y > a$. No assumption is made about the shape of $U(x)$ within the cell.

We let E denote the electron energy; for $E > 0$ or $E < 0$, respectively,

$$k = \frac{\sqrt{2mE}}{\hbar}, \quad \kappa = \frac{\sqrt{2m|E|}}{\hbar}. \quad (2)$$

Transfer matrix. For a given electron energy E , the Schrödinger equation in the cell ($0 \leq x < a$) has two linearly independent solutions denoted as $\phi_1(x, E)$ and $\phi_2(x, E)$ in what follows. The general solution for the cell $n + 1$ takes the form

$$\begin{aligned} \psi(x, E)|_{na < x < (n+1)a} = & c_1^{(n+1)} \phi_1(x - na, E) \\ & + c_2^{(n+1)} \phi_2(x - na, E). \end{aligned} \quad (3)$$

The wave function and its derivatives are continuous at the cell boundaries; the matching conditions at the boundary between the first and second cells are

$$\psi(a - 0) = \psi(a + 0), \quad \psi'(a - 0) = \psi'(a + 0). \quad (4)$$

Inserting expressions (3), we rewrite these conditions as a matrix relation:

$$\begin{aligned} \hat{A} \begin{pmatrix} c_1^{(1)} \\ c_2^{(1)} \end{pmatrix} &= \hat{B} \begin{pmatrix} c_1^{(2)} \\ c_2^{(2)} \end{pmatrix}, \quad \hat{A} = \begin{pmatrix} \phi_1(a) & \phi_2(a) \\ \phi_1'(a) & \phi_2'(a) \end{pmatrix}, \\ \hat{B} &= \begin{pmatrix} \phi_1(0) & \phi_2(0) \\ \phi_1'(0) & \phi_2'(0) \end{pmatrix}. \end{aligned}$$

This relation can be rearranged as

$$\begin{pmatrix} c_1^{(2)} \\ c_2^{(2)} \end{pmatrix} = \hat{T} \begin{pmatrix} c_1^{(1)} \\ c_2^{(1)} \end{pmatrix}, \quad \text{where} \quad \hat{T} = \hat{B}^{-1} \hat{A} \equiv \begin{pmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{pmatrix}. \quad (5)$$

The matrix \hat{T} is called the *transfer matrix*. (This matrix corresponds to the finite translation operator \hat{T}_a in the basis of functions ϕ_1 and ϕ_2 .)²

The determinants of \hat{B} and \hat{A} are the Wronskians $W(x) = \phi_1(x)\phi_2'(x) - \phi_2(x)\phi_1'(x)$ taken at $x = a$ and $x = 0$. The Wronskian of a linear second-order differential equation that does not contain the first derivative is independent of the coordinates, i.e., $W(a) = W(0)$. Hence, $\det \hat{T} = 1$. Because solutions ϕ_1 and ϕ_2 can be taken as real-valued without loss of generality, the trace of the transfer matrix

² From a technical standpoint, it is sometimes convenient to split the cell into separate pieces, find the transfer matrices \hat{T}_z for each of them, and then construct the cell transfer matrix discussed here as the product $\hat{T} = \prod \hat{T}_z$. For example, this procedure is used to construct the transfer matrix for an electromagnetic wave passing through a stack of planar plates (see Appendix C).

$\text{Tr}(\hat{T}) \equiv 2A(E)$ is also a real quantity:³

$$A(E) = \frac{\phi_1(0)\phi_2'(a) + \phi_1(a)\phi_2'(0) - \phi_2(0)\phi_1'(a) - \phi_2(a)\phi_1'(0)}{4W(0)}. \quad (6)$$

The transfer matrix eigenvalues $\lambda_{1,2}$ depend on the shape of the cell potential and the energy E , and are to be found from the quadratic equation

$$\lambda^2 - \text{Tr}(\hat{T})\lambda + \det \hat{T} \equiv \lambda^2 - 2A(E)\lambda + 1 = 0 \Rightarrow \lambda_1\lambda_2 = 1, \quad (7)$$

$$\lambda_1 + \lambda_2 = 2A(E).$$

Diagonalizing the matrix \hat{T} , we obtain

$$\hat{T} = \hat{R}^{-1} \hat{V} \hat{R}, \quad \text{where} \quad \hat{V} = \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix}. \quad (8)$$

For a chain of N cells, the transfer matrix for the entire chain \hat{T}^{tot} is then

$$\begin{pmatrix} c_1^{(N+1)} \\ c_2^{(N+1)} \end{pmatrix} = \hat{T}^{\text{tot}} \begin{pmatrix} c_1^{(1)} \\ c_2^{(1)} \end{pmatrix}, \quad \text{where} \quad \hat{T}^{\text{tot}} = \hat{T}^N \equiv \hat{R}^{-1} \hat{V}^N \hat{R}. \quad (9)$$

• If $|A(E)| \leq 1$, the eigenvalues λ_i are complex and equal to unity in absolute value (because $\lambda_1\lambda_2 = 1$); we can write $\lambda_1 = \exp(iqa)$; then $\lambda_2 = \exp(-iqa)$. The quantity $\hbar q$ (and not infrequently, also q) is called a *quasimomentum*.⁴ We have

$$\lambda_1 = \exp(iqa), \quad \lambda_2 = \exp(-iqa), \quad (10)$$

$$\lambda_1 + \lambda_2 = 2 \cos(qa) = 2A(E).$$

The change of q by an integer multiple of $2\pi/a$ does not change the eigenvalue λ . For this reason, a physically relevant range of quasimomentum values has the length $2\pi\hbar/a$. It is customary to define the quasimomentum to lie in the interval (the first Brillouin zone)

$$q \in \left(-\frac{\pi}{a}, \frac{\pi}{a}\right). \quad (11)$$

The admissible values of quasimomentum are defined by boundary conditions. In particular, for a finite periodic lattice, $q = \pi r/(Na)$ with integer r such that $|r| \leq N/2$, i.e., the number of states in the respective band equals the number of cells.

• If $|A(E)| > 1$, the eigenvalues are real,

$$\lambda_i \equiv A \pm \sqrt{A^2 - 1}:$$

$$\lambda_1 = \frac{A(E)}{|A(E)|} \exp(\beta a), \quad \lambda_2 = \frac{A(E)}{|A(E)|} \exp(-\beta a),$$

$$|\lambda_1 + \lambda_2| = 2 \cosh(\beta a) = 2|A(E)|, \quad \beta > 0. \quad (12)$$

The quantity β is called the *decay exponent*; it can also be understood as an imaginary quasimomentum. Boundary conditions do not limit possible values of β .

3. States in bands of infinite lattices

The dependence of A on the energy E is a continuous function. A small change in E entails a small change in $A(E)$. For an infinite lattice, the values of E such that $|A(E)| \leq 1$ fill continuous regions—the *allowed energy bands* \mathcal{T}_p . The allowed bands alternate with the bands where $|A(E)| > 1$ —the *forbidden bands* \mathcal{S}_p (p is the band number in the order of increasing energy beginning with $p = 1$).

3.1 Allowed bands

For $|A(E)| \leq 1$, relation (10) can be treated as an equation for the dependence of energy on the quasimomentum q —the *dispersion law* $E(q)$. It is apparent that for each value of energy, there are two solutions with quasimomenta q and $-q$, i.e., the eigenstates of the Hamiltonian are doubly degenerate (just as for free motion), which is the statement of the *Kramers theorem*:

$$E(-q) = E(q). \quad (13)$$

Inserting the wave function (3) into the known expression for the probability density flux [13], we can readily see that solutions with definite quasimomentum describe particles propagating along the lattice without damping. In other words, the eigenvectors of \hat{T} are common eigenvectors of the Hamiltonian and the finite translation operator with the same energy and different signs of the quasimomentum (electron motion in a positive or negative direction of the lattice).

• By virtue of (13), the value $q = 0$ corresponds to an extremum, and for $qa \ll 1$ we can write

$$E(q) = E_0 + \frac{\hbar^2 q^2}{2m^*}. \quad (14)$$

The coefficient m^* is called an *effective mass*. If $m^* < 0$, we are talking about negative masses. In most cases, the quantity $|m^*|$ is close to the electron mass m_e ; in various crystals, $0.05m_e \lesssim |m^*| \lesssim 100m_e$. The effective mass is positive in bands \mathcal{T}_p for odd p and negative in bands \mathcal{T}_p with even p .

• It can be readily seen that a relation like (13) is also obtained close to the upper boundary of the quasimomentum range (at the boundary of the Brillouin zone),

$$E\left(\frac{\pi}{a} - q\right) = E\left(\frac{\pi}{a} + q\right). \quad (15)$$

Hence, it follows that $dE/dq|_{(q=\pi/a)} = 0$ and, by analogy with (14), the notion of effective mass can also be introduced for small deviations of quasimomentum from π/a .

• Eigenfunctions of the transfer matrix—common eigenfunctions of the operator of finite translation and energy—are often written in the form $\psi = \exp(iqx)u_q(x)$, where the *Bloch amplitude* $u_q(x)$ is a periodic function:

$$\psi = \exp(iqx)u_q(x), \quad u_q(x+a) = u_q(x). \quad (16)$$

The set of Bloch functions $\exp(iqx)u_q(x)$ is complete.

3.2 Forbidden bands. A semi-infinite chain. Surface levels

For $|A(E)| > 1$, the probability of an electron staying in a cell increases for an increasing or decreasing cell number as $\exp(2\beta n)$ or $\exp(-2\beta n)$ (12), becoming infinitely large as $n \rightarrow \infty$ or $n \rightarrow -\infty$, which is not allowed. Such solutions are

³ The determinant and trace of a matrix are invariant under a change of basis. For this reason, specific computations can be carried out for complex-valued ϕ_i , which can be more convenient in some problems.

⁴ Attention should be paid to the fact that the notion of quasimomentum is introduced for a finite lattice.

not realizable in an infinite chain, and this is why such a band is called *forbidden*. In a forbidden band, the dependence of $|A|$ on E has the form of a hump growing from the boundaries, where this quantity equals unity, to some maximum value, and the decay exponent β varies from zero to some maximum value.

For a *semi-infinite lattice* ($x \geq 0$), a solution that corresponds to the eigenvalue $\lambda_2 = \pm \exp(-\beta a)$ in (12) can be realized.

In the vicinity of the flat surface of a three-dimensional crystal, it is appropriate to consider displacements parallel and perpendicular to the boundary ℓ . The states correspond to waves propagating along the surface (with a quasimomentum \mathbf{q}_ℓ) and decaying away from the boundary (with the decrement β). The respective *surface levels* were discovered by I E Tamm in 1932.

3.3 General picture

Appendix B collects solutions for some infinite lattices that are known to the author. They can be considered illustrations of the general picture, discussed for an arbitrary cell potential.

In particular, alternating allowed and forbidden energy bands occur in the system, and signs of their effective masses also alternate. For the lowest band, the effective mass is positive. If the problem of motion in the field of an isolated cell with free ends has discrete energy levels, then these levels turn out to be inside the allowed bands, and the lowest energy values in these bands are lower than the ‘mother’ levels. With increasing E , the width of forbidden zones decreases.

For low energies, details of the dependence $A(E)$ cannot be described in a general way because they are determined by the shape of the cell potential. With increasing E , the effect of the details in the shape of the cell potential on particle motion weakens.

3.4 High electron energy.

The case of weak binding (nearly free electron)

The case where the electron energy noticeably exceeds the characteristic values of the cell potential offers a description that is only weakly sensitive to the form of this potential. It is *convenient* to fix the energy reference level by the requirement that the cell mean value of the potential is zero,

$$\int_0^a U(x) dx = 0. \quad (17)$$

For any ideal lattice and for electrons with a high energy E , we enter into the domain of *weak binding* described by the smallness of the parameter μ ,

$$\mu = k \int_0^a \frac{U^2(x) dx}{8E^2} \ll 1. \quad (18)$$

If this condition is valid, weak perturbations caused by the potential relief only slightly disturb free motion and the semiclassical approximation can be used for basis functions (3) (‘nearly free motion’), $\phi_{1,2} = \exp[\pm i\sqrt{2m(E - U(x))}/\hbar]$. Inserting this into (6), we obtain

$$A_{\text{weak}}(E) = \cos \left(\int_0^a \sqrt{\frac{2m(E - U(x))}{\hbar^2}} dx \right) \approx \cos[(ka) - \mu] \approx \cos(ka) + \mu \sin(ka), \quad (19)$$

and hence dispersion law (10) takes the form

$$\cos(ka) + \mu \sin(ka) = \cos(qa). \quad (20)$$

If k is not very close to πn , the term proportional to μ can be omitted, and we are dealing with allowed bands where the dispersion law differs only slightly from that for free particles (with a natural replacement $q \rightarrow k - 2n\pi/a$ or $q = \pi(2n+1)/a - k$).

When ka is close to πn , the account for the term proportional to μ in the left-hand side of the dispersion law can take $A(E)$ outside the allowed region $(-1, 1)$, and then *forbidden bands* would form.⁵ To characterize these bands, we write $ka = \pi n + \varepsilon$. The trace of the transfer matrix goes outside the allowed band $(+1, -1)$ for $-\varepsilon^2/2 + \varepsilon\mu \geq 0$. Thus, close to each $k = \pi n/a$, there is a narrow forbidden band with the following properties (cf. (12)):

$$\begin{aligned} \text{band boundaries:} \quad & \frac{\pi n}{a} \leq k \leq \frac{\pi n}{a} + \frac{2\mu}{a}; \\ \text{decay exponent:} \quad & \beta \leq \frac{\mu}{a}. \end{aligned} \quad (21)$$

As the energy increases, the forbidden bands become narrower and possible values of the damping coefficient become smaller, but the bands do not disappear, in contrast to the physical understanding of this phenomenon. This points to the inapplicability of the model with a purely periodic potential to describe reality at large E . Necessary modifications are discussed in Section 5.

Some authors also extend the weak binding case to situations with slow particles when the characteristic field energy \tilde{U} is small compared with the energy of electron localization in the cell $E_{\text{loc}} \approx \hbar^2/2ma^2$ (see, e.g., [11]). For such a problem, the algorithm of computing the transfer matrix in an analytic form and analysis of behavior in a lattice with a cell potential of an arbitrary form are unknown to the author. A solution for a sinusoidal potential, obtained perturbatively, can be found, for example, in [4, 11].

3.5 The case of tight binding

The tight-binding approximation corresponds to a situation where the field in an individual cell is such that the state of a particle in this cell (if it is not surrounded by other cells) is localized in a domain with a size substantially smaller than the cell parameter a , and the wave function rapidly decays on approaching the cell boundaries. In other words, before the neighbors are introduced, the electron is localized in a narrow vicinity of an ion (a separated cell) — in a ‘subcell’ with a size $a_0 \ll a$ — and its wave function rapidly decays for $x > a_0$, such that the tunneling coefficient (the integral of overlapping with neighbors) D is small. An allowed band is in this case narrow, and all quantities appearing there, except T_{11} , can be considered constant.

We let E_ℓ denote the level energy of a ‘parent’ well giving rise to the band studied. We write the transfer matrix for the transition between the ends of the subcell for an energy E as

$$\hat{T}_V = \begin{pmatrix} \theta_{11}(E) & \theta_{12}(E) \\ \theta_{21}(E) & \theta_{22}(E) \end{pmatrix}.$$

The condition for a level to exist in this well is $\theta_{11}(E_\ell) = 0$ (cf. (29) in Section 4.2). Outside the subcell, the motion is nearly free, and the wave function evolution is described by

⁵ For $ka \approx \pi n$ (for energies $E \approx \pi^2 n^2 \hbar^2 / (2ma^2)$), the cell contains an integer number of half-waves. A signal reflected in the next cell can return in antiphase, such that multiple reflection would result in opacity.

the tunneling coefficient D , such that the auxiliary translation matrix for passing to the cell boundaries takes the form⁶

$$\hat{T}_a = \begin{pmatrix} \frac{1}{\sqrt{D}} & 0 \\ 0 & \sqrt{D} \end{pmatrix}.$$

The full transfer matrix is

$$\hat{T} = \hat{T}_V \hat{T}_a = \begin{pmatrix} \frac{\theta_{11}}{\sqrt{D}} & \theta_{12}\sqrt{D} \\ \frac{\theta_{21}}{\sqrt{D}} & \theta_{22}\sqrt{D} \end{pmatrix}. \quad (22)$$

The trace of this matrix $A = \theta_{11}/\sqrt{D} + \theta_{22}\sqrt{D}$ reduces to the first term for sufficiently small values of D , and dispersion relation (10) then takes the form

$$\frac{\theta_{11}(E)}{\sqrt{D}} = 2 \cos(qa). \quad (23)$$

Because $1/D \gg 1$, the left-hand side is smaller than 2 in absolute value only for small values of the coefficient $\theta_{11}(E)$, i.e., for energies E close to that of the ‘parent’ level E_ℓ . For a rough estimate, we let E_r denote the energy of the level of the ‘parent’ well closest to E_r (or set $E_r = 0$ if such a level is absent). Then, for E close to E_ℓ , we can write $\theta_{11}(E) = C_\ell(E - E_\ell)$ with a coefficient C_ℓ such that $C_\ell(E_r - E_\ell) \sim 1$.⁷ As a result, the dispersion law takes the form that is the same for all shapes of the cell potential,

$$E - E_\ell = \Delta\epsilon_\ell \cos(qa), \quad \Delta\epsilon_\ell \equiv \frac{E_{\max} - E_{\min}}{2} = \left| 2 \frac{\sqrt{D}}{C_\ell} \right|. \quad (24)$$

The band width $2\Delta\epsilon_\ell$ is small and effective mass (14) is large:

$$\Delta\epsilon_\ell \sim \sqrt{D}|E_\ell - E_r|, \quad m^* \sim \frac{\hbar^2}{(E_\ell - E_r)a^2\sqrt{D}}. \quad (25)$$

(The deviation of the band center from the energy of the parent level is due to the omitted small correction $\theta_{22}\sqrt{D}$; this deviation is of the order of $D|E_\ell - E_r|$.)

If the tunneling coefficient is increased (*on leaving the tight-binding domain*), the form of the dispersion law ceases to be universal. Indeed, the second term in the trace of $A(E)$ must then be taken into account. Furthermore, the dependence of the coefficient C_ℓ on energy, individual for each level and cell potential, also has to be accounted for.

4. From infinite to finite lattices

We consider a lattice with a *finite number of identical cells* N . The transition from free motion (outside the lattice) to the motion in the first cell of our chain and escape from the lattice to free motion can be described with the help of ‘boundary’ transfer matrices \hat{T}_\mp , similar to the matrices \hat{T} in (5), such that the full transfer matrix on the entire lattice of N cells becomes

$$\hat{T}_g^{\text{tot}} = \hat{T}_- \hat{T}^N \hat{T}_+. \quad (26)$$

⁶ In a simplified picture, $U = 0$ between the wells, and the basis wave functions outside the subcell take the form $\exp(\pm \kappa x)$, with $\kappa = (2m|E|/\hbar^2)^{1/2}$, whence the tunneling coefficient $D = \exp(-2\kappa a)$.

⁷ For example, for a lattice of δ -wells, an analysis of Eqn (44a) gives $C_\ell = 1/(2E_\ell)$; in the semiclassical case, $C_\ell \approx 4\pi/|E_\ell - E_{\ell+1}|$, where $E_{\ell+1}$ is the energy of the neighboring level in an individual cell.

Below, we discuss a lattice with free ends, $\hat{T}_\pm = 1$, in some detail. For other boundary conditions, $T_\pm \neq 1$, and the expressions for $T_{ij}^{\text{tot}}(E)$ become linear combinations of the four elements $T_{ij}^{\text{tot}}(E)$ given by (28). For $E < 0$, this leads to a shift in positions of levels within the allowed band found for the infinite lattice. This shift is quite noticeable if N is not large, but as N increases, the distances between the levels cease to depend on the boundary conditions. For $E > 0$, the positions of full transparency points (see below) and boundaries of opacity bands are displaced similarly.

4.1 Transfer matrix for a finite number of cells

Based on the transfer matrix \hat{T} in (5), we construct an auxiliary matrix $\hat{S}(z)$ using the equation with the initial condition $\hat{S}(0) = 1$,

$$\frac{d\hat{S}(z)}{dz} = \hat{T}\hat{S}(z), \quad \hat{S}(z) = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix},$$

or in components,

$$\frac{d}{dz} \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} = \begin{pmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{pmatrix} \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix}.$$

Taking definition (8) into account, we write the solution of this equation as

$$\begin{aligned} \hat{S}(z) = \exp(\hat{T}z) &\equiv R^{-1} \begin{pmatrix} \exp(\lambda_1 z) & 0 \\ 0 & \exp(\lambda_2 z) \end{pmatrix} \hat{R} \\ &\equiv \hat{F} \exp(\lambda_1 z) + \hat{G} \exp(\lambda_2 z), \end{aligned}$$

where we introduced matrices \hat{F} and \hat{G} with coefficients that are independent of z ; for example, $S_{12} = F_{12} \exp(\lambda_1 z) + G_{12} \exp(\lambda_2 z)$. A direct solution of equations for individual components decomposed with respect to the exponentials and initial conditions gives

$$\begin{aligned} S_{11} &= \frac{(\lambda_1 - T_{22}) \exp(\lambda_1 z) - (\lambda_2 - T_{22}) \exp(\lambda_2 z)}{\lambda_1 - \lambda_2}, \\ S_{21} &= T_{21} \frac{\exp(\lambda_1 z) - \exp(\lambda_2 z)}{\lambda_1 - \lambda_2}, \\ S_{12} &= T_{12} \frac{\exp(\lambda_1 z) - \exp(\lambda_2 z)}{\lambda_1 - \lambda_2}, \\ S_{22} &= \frac{(\lambda_1 - T_{11}) \exp(\lambda_1 z) - (\lambda_2 - T_{11}) \exp(\lambda_2 z)}{\lambda_1 - \lambda_2}. \end{aligned} \quad (27)$$

Hence, in particular, it follows that

$$\begin{aligned} (\hat{T}^N)_{11} &\equiv \left[\frac{d^N \hat{S}}{dz^N} \right]_{(z=0)} \Big|_{11} = \frac{(\lambda_1 - T_{22}) \lambda_1^N - (\lambda_2 - T_{22}) \lambda_2^N}{\lambda_1 - \lambda_2}, \\ (\hat{T}^N)_{12} &\equiv \left[\frac{d^N \hat{S}}{dz^N} \right]_{(z=0)} \Big|_{12} = T_{12} \frac{\lambda_1^N - \lambda_2^N}{\lambda_1 - \lambda_2}. \end{aligned} \quad (28)$$

4.2 The case $E < 0$

For $E < 0$, the problem lies in finding energies of stationary states. The condition for a level to exist for an energy E reduces to the requirement that the solution decaying on the right of the set of wells ($\exp(-\kappa x)$ for $x > Na$) not contain a contribution that grows without a bound on the left after passing through the entire chain (a function of the same form

$\exp(-\kappa x)$ for $x < 0$),

$$\hat{T}_{11}^{\text{tot}}(E) \equiv \left[\left(\hat{T}(E) \right)^N \right]_{11} = 0 \quad (\text{level for } E < 0). \quad (29)$$

This quantity was evaluated in (28). Inserting expressions $\lambda_i = \exp(\pm iqa)$ into (29) and using (7) and (10), we transform (29) to the form

$$(\hat{T}^N)_{11} = \frac{\sin[(N+1)qa] - T_{22} \sin(Nqa)}{\sin(qa)} = 0, \quad (30)$$

$$\text{where } 2 \cos(qa) = T_{11} + T_{22}.$$

This is an equation of degree N for $\cos(qa)$. Without a concrete form of entries in the transfer matrix, it only gives a solution of the problem in principle. Nevertheless, we can state that in each allowed band \mathcal{T}_p , Eqn (30) has, generally speaking, N solutions that correspond to the splitting of the original level of the individual well into ‘daughter’ levels of the set of wells. We arrive at an important conclusion: *the number of states in a band coincides with the number of periodicity elements N .*

If one of the boundaries of a band \mathcal{T}_p corresponds to a positive energy, the number of ‘daughter’ levels in the band with $E < 0$ can be smaller than N ; it can be said that some N ‘daughter’ levels are expelled into the region of positive energies.

In particular, in the case of tight binding, T_{22} is negligibly small, $T \equiv \theta\sqrt{D}$, and equation for energy levels (30) is simplified, taking the form $\sin[(N+1)qa]/\sin(qa) = 0$. The respective values of quasimomentum form the discrete set

$$qa = \frac{m\pi}{N+1}, \quad |m| \leq \frac{N}{2}. \quad (31)$$

Level energies can be expressed through the band width $2\Delta\varepsilon$ by directly inserting the found values of qa into the dispersion law,

$$E_{mk} = E_k + \Delta\varepsilon_k \cos\left(\frac{m\pi}{N+1}\right). \quad (32)$$

For $N = 2$ and 3 , these values match those that can be obtained in standard exercises of seeking states for two or three δ -wells or for a symmetric double well in the semiclassical approximation.

When N is odd, Eqn (32) with $d = (N+1)/2$ gives $E_d = E_k$. Accounting for the omitted term $T_{22} \equiv \theta\sqrt{D}$ gives the deviation $E_d - E_k \propto D$ (of the next order of smallness). For three δ -wells, this conclusion results from simple calculations.

4.3 The case $E > 0$

For $E > 0$, we are dealing with a scattering problem. In this case, it is convenient to assume that each cell begins from at least a vanishingly small region of free motion with $U = 0$, and we can therefore formally select solutions starting with $0 < x < \varepsilon$ in the form $\phi_{1,2} = \exp(\pm ikx)$ (the limit $\varepsilon \rightarrow 0$ is implied).

The aim is to understand the main features of the dependence of the transmission (and reflection) coefficient on energy. As is customary, for $x > Na$, we consider a wave incident from left to right (ϕ_1) and a reflected wave (ϕ_2), and for $x < 0$, a transmitted wave ϕ_1 ; for the scattering problem, relation (9) thus takes the form (the respective indices ℓ and r

label the states for $x < 0$ and $x > Na$)

$$\hat{T}^{\text{tot}} \begin{pmatrix} c_{1\ell} \\ 0 \end{pmatrix} = \begin{pmatrix} c_{1r} \\ c_{2r} \end{pmatrix}.$$

Normalizing the flux to the wave ϕ_1 on the right, we find that $1/T_{11}^{\text{tot}}(E)$ has the meaning of the transmission coefficient for the chain for a given energy E , and $T_{12}^{\text{tot}}(E)/T_{11}^{\text{tot}}(E)$ has the meaning of the reflection coefficient. Thus, different physical situations are realized for some $E > 0$:

$T_{12}^{\text{tot}}(E) = 0$: full lattice transparency, the band \mathcal{T}_p ,

$|T_{11}^{\text{tot}}(E)| \gg 1$: nearly complete opaqueness, the band \mathcal{S}_p .

According to (28),

$$(\hat{T}^N)_{12} = T_{12} \frac{\lambda_1^N - \lambda_2^N}{\lambda_1 - \lambda_2}. \quad (34)$$

Thus, full transparency is achieved for $\lambda_2^N = \lambda_1^N$, i.e., for $|A(E)| \leq 1$, in the allowed band \mathcal{T}_p . Because $\lambda_1\lambda_2 = 1$, this implies that $\lambda_2^N = \lambda_1^N = \pm 1$, i.e., full transparency is achieved for the quasimomentum $q = \pi r/N$, which corresponds to an integer number of half-waves within the entire chain. In other words, in each band \mathcal{T}_p , N full-transparency points appear, the transmission coefficient is close to 1 between them, and these points coalesce as $N \rightarrow \infty$ into a *band of full transparency* within the band \mathcal{T}_p .

In the same manner, in agreement with (28), the transmission coefficient $1/|T_{11}^{\text{tot}}(E)|$ for $|A(E)| > 1$, i.e., in the band \mathcal{S}_p , decreases with an increase in N as $\exp(-\beta aN)$, prohibiting electron transmission for sufficiently large N (a forbidden band). We note, however, that for large energies, β differs from 0 only slightly, Eqn (21), and the transmission is suppressed substantially only for a very large number of exactly identical cells $N > 1/\beta$.

A numerical example. In a model with a cell given by rectangular well (45) with the distance to the next cell $a - b = b$ and with the depth $V = 1$ eV, for $E = 10$ eV and $ka \approx 10\pi$, we obtain $\mu \approx 0.02$, and therefore a two-fold transparency suppression at the center of the forbidden band requires not less than $N = 50$ well-cells; in the middle between the center and the boundary of the band, the same suppression requires more than $N = 70$ identical well-cells.

In teaching, it would be helpful to illustrate these conclusions with simple computations and demonstrations. An analysis of scattering for a rectangular well, accessible in class, shows that the transmission coefficient increases with energy, reaching unity for some value of E , and then decays (usually not very strongly), reaches unity once again for another value of E , and further oscillates with ever smaller amplitude, regularly passing through unity. For scattering on $N = 2-15$ cells, the behavior can be more conveniently simulated with the help of the QUANTX software package [10]. It can be found that each initial maximum gives rise to a set of N close energies of full transparency (the transmission coefficient 1), alternating with bands of progressively decreasing transparency, acquiring, as N is increased, a form progressively closer to a rectangular one, with the bottom close to zero. The energy width of bands with low transparency decreases as E increases. For high energies, the transmission coefficient is indistinguishable from 1 for all E except for narrow forbidden bands.

5. Some consequences of periodicity violation

Small chaotic violations. For $E < 0$, bands are formed through collectivization of states of the set of identical wells constituting the lattice, as discussed in Section 3.5.

We first consider an isolated well of arbitrary shape that corresponds to a single cell of the lattice. Let the well contain energy levels (from top down) $-E_1, -E_2, \dots, -E_k$ (in real crystals, these are electron energy levels in ions; in a typical case, the energy E_1 is about 1 eV, while the energies E_2, E_3 , and the following ones can be several dozen or hundred electron-volts). Each of these levels gives rise to an allowed energy band. The states in each of these bands are not localized in the vicinity of one of the wells, but are distributed among all wells.

For the top band with $E < 0$, the ‘parent’ states of individual electrons correspond to the largest value of the quantum number n , while the field of the nucleus is screened by other electrons, such that the effective nucleus charge is $Z = 1$. The size of the localization domain of a single ‘parent’ ion is comparable to the distance to the ‘neighbors’. The tunneling coefficient is therefore not very small and the top allowed bands for $E < 0$ are relatively wide.

For deeper bands, the ‘parent’ states of individual electrons correspond to smaller values of n than for the top level, and the effective nucleus charge is greater than 1 (fewer electrons participate in screening). Effective ion sizes are therefore smaller and the tunneling distance approaches the maximally possible value, the distance between ions (lattice constant) a . For these levels, the second factor in the integrand of the expression for the tunneling coefficient also increases in magnitude. For a major part of the classically forbidden domain governing the tunneling coefficient, $|E_k| \gg |V|$, therefore, (48) gives $D_k \approx \exp(-a\sqrt{2m|E_k|}/\hbar)$. This implies that the tunneling coefficient for the k th band D_k is very small, such that the set of allowed energies of deeply located bands is practically indistinguishable from the N -times-copied set of energies of an isolated ion.

A numerical example. For Al and Cu, the volume of one gram-atom is $\sim 10 \text{ cm}^3$. The mean interatomic distance in such a crystal is therefore $2.5 \times 10^{-8} \text{ cm}$. For the energy $E_k \approx -10 \text{ eV}$, $\hbar/\sqrt{2m|E|} \approx 0.6 \times 10^{-8} \text{ cm}$. For this level energy, $D_k \approx e^{-8} \approx 0.0003$, which gives a very small band width, $\Delta E_k \approx 0.003 \text{ eV}$. If we take a deeper level with the energy -100 eV , the band width is negligibly small: $\Delta E_k \sim 10^{-9} \text{ eV}$.

In a real crystal, the lattice periodicity is slightly perturbed by thermal oscillations (dislocations and impurities can also play a significant role). For this reason, the energies of electrons in neighboring quasi-isolated ions are slightly different. In agreement with the discussion in Appendix A for a pair of wells, insofar as such a difference δE_i^0 is small, the transformation of levels into a band only slightly differs from what happens in an ideal lattice. When the expected band width (25) becomes smaller than δE_i^0 , levels are not grouped, and electrons at deep levels stay localized around their ions.

Thus, in a crystal, states lying deep are localized close to ‘their’ ions, whereas the upper states are grouped into energy bands with the electrons freely propagating over the lattice.

For $E > 0$, we are dealing with resonances in a periodic structure (in the same way as in diffraction on a grating or in a Fabry–Pérot interferometer). As we have seen, in an ideal crystal, for some frequencies, destructive interference accompanying multiple reflections and refraction makes such a

resonator nontransparent. As a result, narrow forbidden bands also occur for large positive energies. At first glance, this violates the correspondence principle: *for large energies, the behavior should coincide with the classical one, and roughness of the potential should not be visible*. Here, again, deviations from periodicity save the situation. As we mentioned in Section 4.2, a substantial suppression of transparency can only happen for a large number of cells if the quasi-resonance conditions are satisfied, $k = \pi r/a$.

Small chaotic deviations from periodicity due to thermal motion, dislocations (even in neighboring linear chains), and (or) inaccuracy in crystal fabrication ‘smooth out’ destructive interference, and significant accumulation of nontransparency does not happen.

For large values of E in real substances, periodicity can be violated via one more mechanism. The approximation of fixed cell potential (1) becomes inapplicable for high-energy electrons. Interaction between an electron and a lattice ion can excite or even destroy the ion. For moderate energies, this is a low-probability process; however, its role increases as the energy increases.

6. Conclusions. Possible applications

From a unified standpoint, we studied the structure of levels (allowed and forbidden energy bands) and bands of transparency and opaqueness in one-dimensional repeating structures (cells), with transition from a finite cell set to an infinite one, to a periodic structure like a one-dimensional crystal. The appearance of a band structure is a general feature of such systems for cell potentials of an arbitrary shape. In a chain with a finite number of cells, the levels lie inside the bands found for the infinite crystal.

Two phenomena take place in solutions obtained for ideal lattices:

- (1) forbidden bands (bands of opaqueness) do not disappear even if the electron energy is arbitrarily large;
- (2) electrons on inner levels of an ion in a crystal must belong to energy bands, i.e., be delocalized, instead of being localized close to ions, as happens in reality.

These phenomena are not observed in nature. This implies that in order to describe the real world, the model of an ideal periodic lattice should be extended. Such an extension can account for small random deviations from periodicity (thermal motion, dislocations, impurities, excitation of lattice ions; see Section 5).

In addition to general results, the formulas given in Sections 2 and 4 offer a possibility of carrying out studies that are not done commonly.

- When the cell potential is known, the Schrödinger equation can be solved in a cell numerically. Based on these solutions, the dispersion law and positions of levels can be computed for finite lattices. Comparison with observational results would then allow estimating the quality of the available cell potential description.

- Construction of a lattice with a dispersion law desirable in some problem could be of interest; for example, a law such that the dependence $E(q)$ contains a point where $\partial E/\partial q = 0$ for $0 < q < \pi/a$ would lead to singularities in the distribution of the number of states over energies. In agreement with material in Section 2, it suffices to explore solutions of the Schrödinger equation in a single cell.

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7. Appendices

A. Slightly asymmetric double well

A basis for many physical discussions is provided by the case where the potential is given by a pair of wells separated by a region where $U_i = 0$. In the classical problem, the states of particles in each well are independent: they ‘do not know’ about each other. In the quantum case, ‘wings’ of wave functions of each of the wells reach the other well, and there is tunneling between the wells. Because wave functions decay rather rapidly outside the wells, tunneling is commonly a weak effect, modifying energy levels and wave functions only slightly. However, when the energies of levels in both isolated wells coincide, tunneling can lead to a ‘redistribution’ of states between the two wells, which is the reason why a band structure forms when the number of wells increases.

The main features of this problem can be conveniently studied with the example of a system with

$$U(x) = -G_1\delta(x+a) - G_2\delta(x-a). \quad (35)$$

We recall that for the potential $U(x) = -G\delta(x-b)$, the rules of matching for the wave function can be written as

$$\begin{aligned} \psi'(b+0) - \psi'(b-0) &= -2g_0\psi(b), \\ \psi(b+0) &= \psi(b-0), \quad g_0 = \frac{mG}{\hbar^2}. \end{aligned} \quad (36)$$

This system has one bound state with the energy and the wave function

$$E_0 = -\frac{\hbar^2 g_0^2}{2m}, \quad \psi_1(x) = \sqrt{g_0} \exp(-g_0|x|). \quad (37)$$

For a pair of wells and an arbitrary energy $E = -\hbar^2 \kappa^2 / (2m)$, subsequent application of matching rules at the points $x = \pm a$ gives an equation for the levels:

$$\begin{aligned} \kappa^2 - (g_{0,1} + g_{0,2})\kappa + g_{0,1}g_{0,2}(1 - D_a) &= 0 \\ \Rightarrow \kappa &= \frac{g_{0,1} + g_{0,2} \pm \sqrt{(g_{0,1} - g_{0,2})^2 + 4g_{0,1}g_{0,2}D_a}}{2}, \end{aligned} \quad (38)$$

where $g_{0,i} = mG_i/\hbar^2$, $D_a = \exp(-4\kappa a)$.

We consider the case $D_a \ll 1$.

- *A symmetric system, $G_1 = G_2 = G$.*

It follows from (38) that the initial level (37) is split into two levels with the energies

$$E_{\pm} = E_0 \pm \Delta_S, \quad \Delta_S = 2\sqrt{D_a} E_0 \ll E_0. \quad (39)$$

Inserting the solutions obtained in wave functions, we find that for the lower energy $E = E_0 - \Delta_S$, the wave function is symmetric, $\psi_{0r}(x) = \psi_{0l}(-x)$, whereas for the energy $E = E_0 + \Delta_S$, the wave function is antisymmetric, $\psi_{0r}(x) = -\psi_{0l}(-x)$. For small values of D , the wave functions of each of the well ‘halves’ differ only slightly from the wave function of an isolated well $\psi_0(x)$.

If a particle was initially located in the vicinity of the right well ($\psi(x, t=0) = \psi_{0r}(x)$), then, after the time $\pi\hbar/\Delta_S$, it occurs in the left well, i.e., the wave function oscillates,

$$\begin{aligned} \psi(x, t) &= \exp\left(-\frac{iE_0 t}{\hbar}\right) \left[\psi_0(x) \cos \frac{t}{\tau} + i\psi_0(-x) \sin \frac{t}{\tau} \right], \\ \tau &= \frac{\hbar}{\Delta_S}. \end{aligned}$$

- *Small deviations from symmetry, $|G_1 - G_2| \ll G_1$.*

It is convenient to introduce the notation

$$g_0 = \frac{g_{0,1} + g_{0,2}}{2} \Rightarrow E_0 = -\frac{\hbar^2 g_0^2}{2m}, \quad \delta g_0 = g_{0,1} - g_{0,2},$$

such that the energies of isolated wells are

$$E_{0l} = E_0 - \delta, \quad E_{0r} = E_0 + \delta, \quad \delta = \frac{\hbar^2 g_0 \delta g_0}{m} \ll E_0. \quad (40)$$

Direct substitution in solution (38) gives level energies in the form

$$E_{\pm} = E_0 + \Delta, \quad \Delta = \pm \sqrt{\delta^2 + \Delta_S^2}. \quad (41)$$

It then follows that for $\Delta_S < \delta$, tunneling leaves the levels almost intact. In contrast, for $\Delta_S > \delta$, the term splitting is close to that in the symmetric case (the system forgets about small asymmetry). Direct computation of the wave function in these limit cases shows the following.

- For $\Delta_S \gg \delta$, the splitting of initial terms δ is insignificant compared to the tunneling effect that mixes the states. For $\Delta < 0$, the wave function is symmetric (*the wave function of the ground state does not have zeros*), and for $\Delta > 0$, the wave function is antisymmetric, as in the case where the splitting of initial terms δ is absent. For stationary states, the probabilities of staying in the left and right wells are identical, just as for a symmetric well. If the initial state is confined near one of the wells, it passes to the other one with time, and beating with the frequency $\tau = 2\hbar/\Delta_S$ develops. It can be said that the system ‘hardly sees’ the initial level split.

- For $\delta \gg \Delta_S$, the states stay localized on the right or on the left with high accuracy, tunneling barely changes the states, and beating does not occur. We can readily find that for $\Delta > 0$, the system is localized in the right well; the probability of finding it in the left well is very small. Similarly, for the state with $\Delta < 0$, it can be readily found that $w_r/w_l \approx (2\delta/\Delta_S)^2 \gg 1$, i.e., the system is localized in the right well, and the probability of finding it in the left well is very small. We can say that the system does not notice tunneling, and there are no delocalized states.

It is not difficult to draw similar conclusions also for a pair of smooth wells with the help of the semiclassical approximation (see, e.g., [4]).

B. Collection of exactly solvable models

B.1 A set of δ -wells (Dirac–Kronig–Penney model)

$$U(x) = -G \sum_{n=-\infty}^{\infty} \delta(x + na - \varepsilon), \quad k_0 = \frac{mG}{\hbar^2} > 0. \quad (42)$$

Here, ε is a small auxiliary quantity indicating that the boundary between the cells is located where the potential is smooth, and hence matching rules in form (4) can be used. We set ε to 0 in the end.

For $E < 0$, we select $\phi_1(x, E) = \exp(\kappa x)$ and $\phi_2(x, E) = \exp(-\kappa x)$. Simple application of matching conditions to a δ -well gives the coefficients $c_1^{(2)}$ and $c_2^{(2)}$ on the other side of the well, and toward the end of the cell, at the point $x = a - 0$, these coefficients acquire additional factors $\exp(\kappa a) = 1/\sqrt{D}$ in the left column and $\exp(-\kappa a) = \sqrt{D}$ in the right one. (The quantity $D = \exp(-2\kappa a)$ is the coefficient of tunneling between neighboring wells.) The resultant transfer matrix is

$$T = \begin{pmatrix} \left(1 - \frac{k_0}{\kappa}\right) \frac{1}{\sqrt{D}} & -\frac{k_0}{\kappa} \sqrt{D} \\ \frac{k_0}{\kappa \sqrt{D}} & \left(1 + \frac{k_0}{\kappa}\right) \sqrt{D} \end{pmatrix},$$

$$D = D_A \equiv \exp(-2\kappa a). \quad (43)$$

The case of positive energy, $E > 0$, follows by a simple replacement $\kappa \rightarrow ik \equiv i(2mE/\hbar^2)^{1/2}$ and $X = \kappa a \rightarrow Y = ka$.

The expression for the trace of the transfer matrix takes the form

$$A(E) = \begin{cases} \cosh(\kappa a) - \frac{k_0}{\kappa} \sinh(\kappa a), & E < 0, \\ \cos(ka) - \mu_A \sin(ka), \quad \mu_A = \frac{k_0}{k}, & E > 0. \end{cases} \quad (44a)$$

$$(44b)$$

For $|A(E)| \leq 1$, these relations turn into dispersion law (10), $\cos(qa) = A(E)$.

A detailed study of solutions of these equations is contained, for example, in [1–4]. We note that Eqn (44) has the same form as (20) (the difference lies in the definition of the parameter μ_A). For this reason, the results, at first glance, coincide with the respective results for the weak binding approximation. However, unlike the widths of forbidden bands in the general case considered in Section 3.4, which were decreasing for increasing E , the widths do not change as E increases in this model. It is an artifact of the model, rooted in the singularity of its cell potential.

B.2 Cell is a rectangular well with depth $-V$ and width b , the distance to the next well is $(a - b)$ (Kronig–Penney model)

$$U(x) = \begin{cases} -V, & na < x < na + b, \\ 0, & na + b < x < (n+1)a. \end{cases} \quad (45)$$

We set $k_0 = \sqrt{2mV/\hbar^2}$ and

$$k_1 = \sqrt{\frac{2m(E+V)}{\hbar^2}}, \quad z = k_1 b;$$

$$k = \sqrt{\frac{2mE}{\hbar^2}}, \quad Y = k(a-b) \text{ for } E > 0;$$

$$\kappa = \sqrt{\frac{2m|E|}{\hbar^2}}, \quad X = \kappa(a-b) \text{ for } E < 0.$$

Simple but cumbersome calculations show that for $E > 0$,

$$\hat{T} = \begin{pmatrix} \left(\cos z - i \frac{k^2 + k_1^2}{2kk_1} \sin z\right) \exp(-iY) & i \frac{k_0^2}{2kk_1} \sin z \exp(iY) \\ -i \frac{k_0^2}{2kk_1} \sin z \exp(-iY) & \left(\cos z + i \frac{k^2 + k_1^2}{2kk_1} \sin z\right) \exp(iY) \end{pmatrix}.$$

The case $E < 0$ is obtained by a natural change of variables.

The expression for the trace of the transfer matrix becomes

$$A(E) = \begin{cases} \cos z \cosh X - \frac{k^2 + k_1^2}{2kk_1} \sin z \sinh X, & E < 0, \\ \cos z \cos Y - \frac{k^2 + k_1^2}{2kk_1} \sin z \sin Y, & E > 0. \end{cases} \quad (46a)$$

$$(46b)$$

For $|A(E)| \leq 1$, these relations turn into dispersion law (10), $\cos(qa) = A(E)$.

An analysis of weak and tight binding approximations in this case presents a simple concretization of the results in Section 3.

B.3 Sinusoidal field

$$U(x) = 2V \cos \frac{2\pi x}{a}. \quad (47)$$

In this periodic field, the Schrödinger equation reduces to Mathieu's equation, solutions of which are considered, for example, in [11, 14] (and are studied in courses of mechanics in describing parametric resonance). In some discussions, the fact is used that in the momentum representation, the Schrödinger equation for this problem transforms into a difference equation [6].

The basic solutions ϕ_1 and ϕ_2 in a cell cannot be expressed through elementary functions in this case, and a tractable expression for the transfer matrix is unknown to the author.

B.4 Lattice with a smoothly varying potential enabling a semiclassical description [7, problem 2-11]. For each given value of E , it is convenient to identify the left cell boundary with the left turning point; in this case, a_0 is the right turning point. (The shift of the origin does not cause serious complications if E is changed.)

The application of semiclassical matching rules in this case gives

$$T = \begin{pmatrix} \frac{2 \cos \sigma}{\sqrt{D}} & -\sqrt{D} \sin \sigma \\ \frac{\sin \sigma}{\sqrt{D}} & \sqrt{D} \cos \sigma \end{pmatrix}, \quad \sigma = \int_0^{a_0} \frac{p(x)}{\hbar} dx, \quad (48)$$

$$D \equiv D_D = \exp \left(-2 \int_{a_0}^a \frac{\sqrt{2m(U(x) - E)}}{\hbar} dx \right).$$

The expression for the trace of the transfer matrix takes the form

$$A(E) = \left(\frac{1}{\sqrt{D}} + \frac{\sqrt{D}}{4} \right) \cos \sigma. \quad (49)$$

For $|A(E)| \leq 1$, relation (49) turns into dispersion law (10), $\cos(qa) = A(E)$.

C. Light in a layered medium. Photonic crystals

We consider a structure consisting of N identical stacks of planar plates B placed one upon the other, using standard notation in the Gauss unit system with $\mu = 1 \Rightarrow n = \sqrt{\epsilon}$ [15].

C.1 General case. Matrix representation. Let a space be filled with layers $1, 2, \dots, N$ with dielectric permittivities $\epsilon_1, \epsilon_2, \dots, \epsilon_N$, such that the surfaces of all layers are perpendicular to the z axis, and layer thicknesses are d_2, d_3, \dots (layers 1 and N are semi-infinite). We assume for definiteness that ϵ_1 is a real value.

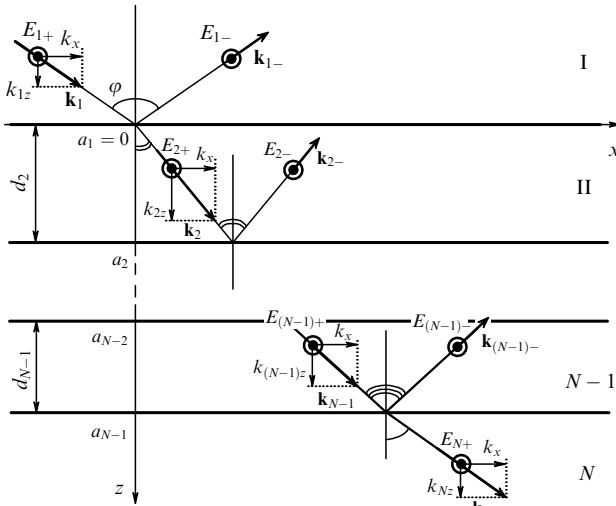


Figure. Fields in a layered medium (TE case).

We assume that light with a frequency ω is incident from medium 1 at an angle $\alpha = \varphi/2$ (see the figure) and its wave vector is located in the plane (x, z) . It is convenient to consider two possible light polarizations: when the electric field is perpendicular to the plane (x, z) , the TE polarization, and when the magnetic field is perpendicular to the plane (x, z) , the TM polarization. For definiteness, the figure shows the TE case.

In all layers, light has the same frequency and the same component of the wave vector parallel to the boundary, $k_x = (\omega/c)\sqrt{\varepsilon_1} \sin \alpha$. The components of wave vectors perpendicular to the boundaries in all layers are different,

$$k_{iz} = \sqrt{\left(\frac{\omega}{c}\right)^2 \varepsilon_i - k_x^2}. \quad (50)$$

They can be real (a transparent medium), imaginary (total internal reflection), or complex (a conducting medium).

The coordinates of layer boundaries are as follows: $z = a_1 = 0$ is the boundary between layers 1 and 2, $z = a_2 = d_2$ is the boundary between layers 2 and 3, $z = a_3 = d_2 + d_3$ is the boundary between layers 3 and 4, ..., $z = a_{N-1} = d_2 + d_3 + \dots + d_{N-1}$ is the boundary between layers $N-1$ and N . Furthermore, for example, the notation $z = a_2 - 0$ is used to denote a point in layer 2 'above' the boundary (2, 3), and $z = a_2 + 0$ for a point of layer 3 'under' this boundary.

The field in each layer is the sum of waves propagating 'down' (sign +) and 'up' (sign -),

$$\begin{aligned} \mathbf{E}_i &= \mathbf{E}_{i+}(a_m) \exp \{-i[\omega t - k_x x - k_{iz}(z - a_m)]\} \\ &+ \mathbf{E}_{i-}(a_m) \exp \{-i[\omega t - k_x x + k_{iz}(z - a_m)]\}, \\ \mathbf{H}_i &= \mathbf{H}_{i+}(a_m) \exp \{-i[\omega t - k_x x - k_{iz}(z - a_m)]\} \\ &+ \mathbf{H}_{i-}(a_m) \exp \{-i[\omega t - k_x x + k_{iz}(z - a_m)]\}. \end{aligned} \quad (51)$$

The idea of the problem solution is as follows. We assume that we know the field in medium I, i.e., down to the 'altitude' $a_1 - 0$. With the help of boundary conditions, the field in medium II at the 'altitude' $a_1 + 0$ can then be determined. Then the field in medium II at the 'altitude' $a_2 - 0$ is readily

computed. The same procedure is repeated for the transition into medium III, and we obtain the field at the 'altitude' $a_3 - 0$. Eventually, we arrive at the description of fields in medium N , at the 'altitude' $a_N + 0$, which we seek. Technically, the transformations from one layer to another outlined above can be conveniently expressed with the help of matrices as the transformation of the column

$$\begin{pmatrix} E_{1+}(a_1) \\ E_{1-}(a_1) \end{pmatrix} \rightarrow \begin{pmatrix} E_{1+}(a_N) \\ E_{1-}(a_N) \end{pmatrix}$$

and a similar column for the magnetic field.

Transmission through the interface between two media.

• In a TE wave, the electric field is directed along the y axis, $\mathbf{E} = (0, E, 0)$. The continuity condition at the boundary of two layers, for example, the second and third ones, can be written as a condition for field amplitudes:

$$\begin{aligned} E_{2+}(a_2 - 0) + E_{2-}(a_2 - 0) &= E_{3+}(a_2 + 0) + E_{3-}(a_2 + 0), \\ k_{2z}(E_{2+}(a_2 - 0) - E_{2-}(a_2 - 0)) &= k_{3z}(E_{3+}(a_2 + 0) - E_{3-}(a_2 + 0)). \end{aligned}$$

This implies that the field amplitudes in the next layer are expressed in terms of the amplitudes in the current layer via relations conveniently written with the help of the transfer matrix⁸ (this is a matrix form of the known Fresnel formulas)

$$\begin{pmatrix} E_{3+}(a_2 + 0) \\ E_{3-}(a_2 + 0) \end{pmatrix} = \hat{T}_{32}^{\text{TE}} \begin{pmatrix} E_{2+}(a_2 - 0) \\ E_{2-}(a_2 - 0) \end{pmatrix}, \quad (52)$$

$$\hat{T}_{32}^{\text{TE}} = \frac{1}{2} \begin{pmatrix} 1 + r_{23}^E & 1 - r_{23}^E \\ 1 - r_{23}^E & 1 + r_{23}^E \end{pmatrix}, \quad r_{23}^E = \frac{k_{2z}}{k_{3z}}.$$

• In a TM wave, the magnetic field is directed along the y axis, $\mathbf{H} = (0, H, 0)$. The continuity condition at the boundary of the same second and third layers can be written as the condition for field amplitudes

$$\begin{aligned} H_{2+}(a_2 - 0) + H_{2-}(a_2 - 0) &= H_{3+}(a_2 + 0) + H_{3-}(a_2 + 0), \\ \varepsilon_3 k_{2z}(H_{2+}(a_2 - 0) - H_{2-}(a_2 - 0)) &= \varepsilon_2 k_{3z}(H_{3+}(a_2 + 0) - H_{3-}(a_2 + 0)). \end{aligned}$$

From this condition, the field amplitudes in the next layer are expressed in terms of amplitudes in the current layer with the help of relations conveniently written in matrix form as

$$\begin{pmatrix} H_{3+}(a_2 + 0) \\ H_{3-}(a_2 + 0) \end{pmatrix} = \hat{T}_{32}^{\text{TM}} \begin{pmatrix} H_{2+}(a_2 - 0) \\ H_{2-}(a_2 - 0) \end{pmatrix}, \quad (53)$$

$$\hat{T}_{32}^{\text{TM}} = \frac{1}{2} \begin{pmatrix} 1 + r_{23}^M & 1 - r_{23}^M \\ 1 - r_{23}^M & 1 + r_{23}^M \end{pmatrix}, \quad r_{23}^M = \frac{\varepsilon_3 k_{2z}}{\varepsilon_2 k_{3z}}.$$

Transmission through a layer. In passing through layer 3, waves change their complex amplitudes. In matrix form, this operation (transmission to the other layer boundary) for the

⁸ The sense of indices on the matrices: in (52), the superscript b means boundary transmission, TE labels the wave type; the subscript 32 labels transmission to medium 3 from medium 2; in (54), the superscript d implies translation over d and the subscript labels the layer.

TE wave is written as

$$\begin{pmatrix} E_{3+}(a_3 - 0) \\ E_{3-}(a_3 - 0) \end{pmatrix} = \hat{T}_{\{3\}}^d \begin{pmatrix} E_{3+}(a_2 + 0) \\ E_{3-}(a_2 + 0) \end{pmatrix}, \quad (54)$$

$$\hat{T}_{\{3\}}^d = \begin{pmatrix} \exp(ik_{3z}d_3) & 0 \\ 0 & \exp(-ik_{3z}d_3) \end{pmatrix}.$$

The expression for the TM wave is the same up to the replacement $E \rightarrow H$; the matrix $\hat{T}_{\{3\}}^d$ preserves its form.

Transmission through a stack of plates. It is now clear that for both polarizations we can write

$$\begin{pmatrix} E_{N+}(a_N + 0) \\ E_{N-}(a_N + 0) \end{pmatrix} = \hat{T}_{\text{TE}}^{\text{tot}} \begin{pmatrix} E_{1+}(a_1 - 0) \\ E_{1-}(a_1 - 0) \end{pmatrix},$$

$$\hat{T}_{\text{TE}}^{\text{tot}} = \hat{T}_{N,N-1}^{\text{bTE}} \hat{T}_{\{N-1\}}^d \cdots \hat{T}_{21}^{\text{bTE}};$$

$$\begin{pmatrix} H_{N+}(a_N + 0) \\ H_{N-}(a_N + 0) \end{pmatrix} = \hat{T}_{\text{TM}}^{\text{tot}} \begin{pmatrix} H_{1+}(a_1 - 0) \\ H_{1-}(a_1 - 0) \end{pmatrix}, \quad (55)$$

$$\hat{T}_{\text{TM}}^{\text{tot}} = \hat{T}_{N,N-1}^{\text{bTM}} \hat{T}_{\{N-1\}}^d \cdots \hat{T}_{21}^{\text{bTM}}.$$

We recall that the determinant of a matrix product is the product of determinants. We can readily find that

$$\det \hat{T}_{\{k\}}^d = 1, \quad \det \hat{T}_{k+1,k}^{\text{bTE}} = r_{k+1,k}^{\text{E}}, \quad \det \hat{T}_{k+1,k}^{\text{bTM}} = r_{k+1,k}^{\text{M}}. \quad (56a)$$

Accordingly, the determinant of the full transfer matrix takes the simple form

$$\det \hat{T}_{\text{TE}}^{\text{tot}} = r_{21}^{\text{E}} r_{32}^{\text{E}} \cdots r_{N,N-1}^{\text{E}} = \frac{k_{zN}}{k_{z1}},$$

$$\det \hat{T}_{\text{TM}}^{\text{tot}} = r_{21}^{\text{M}} r_{32}^{\text{M}} \cdots r_{N,N-1}^{\text{M}} = \frac{\varepsilon_1 k_{zN}}{\varepsilon_N k_{z1}}. \quad (56b)$$

Notably, if the stack of plates B begins and ends in the same medium, then $\det \hat{T}_{\text{B}} = 1$.

The simplest stack B consists of a pair of plates: one with a width d_2 and dielectric permittivity ε_2 and the other with a width d_1 and dielectric permittivity ε_1 . For this stack, the transfer matrix is $\hat{T}_{\text{B}} = \hat{T}_{21}^{\text{b}} \hat{T}_{\{2\}}^d \hat{T}_{12}^{\text{b}} \hat{T}_{(1)}^d$. Inserting expressions (52)–(54) and performing simple manipulations, we find the determinant and trace of the transfer matrix in the form⁹

$$\det \hat{T}_{\text{B}} = 1,$$

$$2A \equiv \text{Tr}(\hat{T}_{\text{B}}) = 2 \cos \alpha_1 \cos \alpha_2 - \left(r + \frac{1}{r}\right) \sin \alpha_1 \sin \alpha_2,$$

$$k_{zj} d_j = \alpha_j, \quad r_{\text{TE}} = \frac{k_{2z}}{k_{1z}}, \quad r_{\text{TM}} = \frac{\varepsilon_1 k_{2z}}{\varepsilon_2 k_{1z}}. \quad (57)$$

For transparent media, the quantity A is real. To see this, we recall that when the angle of incidence does not exceed the angle of total internal reflection for the transition from medium I to medium II, all quantities entering (57) are real. If the incidence angle exceeds the angle of total internal reflection for the transition from medium I to medium II,

k_{2z} becomes imaginary, $k_{2z} = i\kappa$. As a consequence, r is also imaginary. In the same way, the phase $\alpha_2 = i\kappa d_2 \equiv i\gamma$ becomes imaginary. This implies an obvious change $\cos \alpha_2 \rightarrow \cosh \gamma$, $\sin \alpha_2 \rightarrow i \sinh \gamma$. Under this change, the realness of A is preserved.¹⁰

Thus, stack B is an analog of the crystal lattice cell studied in previous sections, and the transfer matrix \hat{T}_{B} has the same properties as the total transfer matrix for linear quantum chain (5) with the same equation for the eigenvalues.

C.2 Large stacks of identical plates. We now consider a structure composed of N identical plate stacks B placed one upon another. The results that follow for this structure are in many aspects similar to those discussed in Section 4; an essential difference is related to the difference in the number of periodicity elements: it is $N = 10^4 - 10^8$ for a crystal, whereas one can hardly have $N \gtrsim 10^2$ for the optical structure being considered.

We demonstrate with several examples that for different parameters of our stacks, incidence angles, and light frequency, both possibilities $|A| > 1$ and $|A| < 1$ can be realized.

First, if the plates are sufficiently thin, i.e., $\alpha_1 \ll 1$ and $\alpha_2 \ll 1$, then the first term in expression (57) is slightly smaller than 2, and the second is also not large, whence $1 > |A| > 0$, our structure is transparent, and the condition for an allowed band to exist is satisfied: a stack of a large number of such plates can be perfectly transparent.

More interesting are cases where plates are not very thin. We here discuss only the case of real k_{iz} (and hence real r).

If an integer number of half-waves fits one of the plates, i.e., $\alpha_1 = m\pi$ or $\alpha_2 = m\pi$, then $|A| \leq 1$, and the existence condition for an allowed band is satisfied: a stack of a large number of such plates can be perfectly transparent.

If, in contrast, an odd number of quarter-waves fits the width of one of the plates, e.g., $\alpha_1 = (m + 1/2)\pi$, then, because $(r + 1/r) > 2$, for a wide range of values of α_2 it turns out that $|A| \geq 2$, i.e., the condition for the existence of a forbidden band is realized: a stack of a large number of such plates is opaque.

The function A is a smooth function of its arguments. For this reason, conditions for the existence of allowed and forbidden bands are realized in some reasonably wide domain of frequencies and (or) incidence angles. We stress that the allowed and forbidden bands differ for TE and TM waves.

Thus, in the system considered, the sets of allowed and forbidden bands form in the same way as for the electron in a crystal. Such an object is interpreted as a photonic crystal (see, e.g., [9]). A convenient advantage of a photonic crystal over a semiconducting crystal is that in the optical case, by various means one can control, in addition to elements of periodicity (the material and plate thickness), not one parameter but two: the frequency and the incidence angle.

Exotic possibilities occur when

- (a) one of the layers in stack B is a thin metal plate;
- (b) total internal reflection takes place at the interface of two media, e.g., k_{2z} is a purely imaginary quantity.

⁹ We draw attention to the similarity to the transfer matrix for model B.2, Eqn (46).

¹⁰ The formulas above offer an opportunity to consider a set of traditional optical problems for a planar plate from a single standpoint: a single plate, including the case where an integer number of half waves fits its width (*blue optics*), the case of a dielectric mirror, a plate in the case of total internal reflection, and a thin metal plate [15].

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