Formation of a quasistationary state by scattering of wave packets on a finite lattice

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The formation and further evolution of the quasistationary state that accompanies the scattering of wave packets in one-dimensional finite periodic structures are studied. The contributions in the spectral integral from the saddle point and simultaneously from the poles of the stationary scattering amplitudes are estimated analytically. They can have the additive character and give different peaks in the secondary packets formed by the nonstationary wave function evolution. The lifetime of the quasistationary state is long and increases significantly with the lattice length especially near the thresholds of transmission bands.

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I. INTRODUCTION

In the past decade the interest to the scattering of quantum wave packets by one-dimensional periodic structures of the finite length was aroused in connection with the intensive studies and practical applications of the nanocrystals, superlattices, and other multilayer systems.[1–11] Theoretical description of this phenomenon comes to the analysis of spectral integrals that characterize the structure of nonstationary wave function for different values of time and coordinate outside and inside of the lattice.

The process of the stationary wave scattering by one-dimensional finite periodic structures is well understood.[12–16] There are a few works where nonstationary scattering and tunneling propagation of wave packets in the one-dimensional finite periodic structures were discussed. The investigators took an interest in the reflected and transmitted packets delay time and in the propagating packets group velocity.[5–9] The peculiarities of these values are mainly determined by the vicinity of the stationary phase point in the under integral expression of the spectral integral.

In the present work, we show that the capture of particle in a long lived quasistationary state should take place near resonance of the transparency in the finite periodic structures in analogy with the electromagnetic or acoustic resonator excitation on the resonant frequency.

The concept of a quasistationary (metastable) state dates back to the famous G. Gamow's work about the alpha decay. In the framework of phenomenological theory the quasistationary state is approximately described by the particular solution of nonstationary Shrodinger equation satisfying to the boundary condition of existence of only outgoing wave on infinity. It permits to define the complex "self-energy" with the imaginary part that is inversely proportional to the lifetime of quasistationary state. Such an approach is available only in the limited region of coordinate and time because this solution cannot be normalized.[17,18] It is more constructive to describe a quasistationary state through the dynamics of the wave packet which is normalized superposition of the stationary scattering wave functions. The amplitudes of stationary scattering have poles in the complex energy plane. The real parts of these poles give the resonance energies and their imaginary parts determine the lifetimes of the quasistationary states.[18,19]

The quasistationary state is usually associated with the energy region close to a resonant level in continuous spectrum of the local potential well bounded by tunnel transparent barriers.[17–20] The length of the particle localization in this state is approximately equal to the width of well on the resonance level and the probability of localization decreases by the slow exponential law within sufficiently long time interval.

In this paper, we are mainly concerned with the peculiarities of forming and evolution of the original quasistationary state that accompanies the scattering of wave packet in the one-dimensional periodic lattice of finite length. It is not the state in a single well of a double barrier system but the state in a system composed of N identical wells and barriers. The length of this quasistationary wave function localization is approximately equal to the width of the lattice. The lifetime of this state increases significantly with the lattice length especially if the spectral function of the packet is narrow with its maximum lies closely to the lines of the total transparency near the thresholds of transmission bands. This effect resembles the effect of the slit diffraction intensification by the diffraction grating.

The energy of the packet spectral center can be both lower or higher the barriers height, i.e., the considered quasistationary states can be formed at the resonance energies not only by the tunneling under barriers, but also at scattering above the barriers. The shape of the potential in each elementary cell may be arbitrarily enough. The effect is most pronounced when the tight binding approximation is valid.

In the work in Ref. 10, the behavior of the poles of the stationary scattering amplitudes for the one-dimensional finite periodic structures has been discussed mainly for a high energy in the weak binding approximation, but the calculation of the wave packet evolution has not been performed. On the contrary, the authors of Ref. 9 performed some numerical and stationary phase approximation calculations for the wave packet evolution at scattering in the finite periodic structures. They explained the delay and trapping by the group velocity diminishing and by the tunneling time arising, but they did not consider the contributions of the poles of the stationary scattering amplitudes. Some numerical results are presented in Ref. 11 for the case of large energies without deep interpretation.

In contrast we show that the main peculiarities of forming and decaying of the quasistationary state at the scattering of the wave packet in the finite periodic lattice are determined by the competing of contributions in the spectral integral not

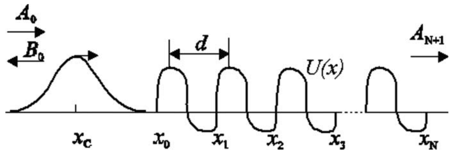

FIG. 1. Wave packet is falling on the one-dimensional periodic potential of the finite length.

only from the saddle point, but simultaneously from the poles of the stationary scattering amplitudes. These contributions can have the additive character and give different peaks of the secondary packets formed by the nonstationary wave function evolution which can be observable in real and numerical experiment. Our method of estimations of contributions in the spectral integral is analogical to Drukarev's method[19] that is described in the book.[18]

Also we derive the convenient form for the equations which determine positions of the reflection amplitude's zeroes and poles. We solve these equations in the tight binding approximation and find the positions of poles and therefore the lifetimes of quasistationary states in dependence of the lattice length and the intracell's potential parameters. The results very differ near thresholds and in the middle of transmission bands. In our discussion we operate in terms of the values that are directly measurable in the experiments by the scattering of wave packets in nanocrystals and superlattices: the probability of the particle finding in the lattice, the probability density, and the probability current. These values can demonstrate the interference peculiarities connected with the composition of the different resonance contributions type of ones discussed in the works,[20,21] but we emphasize here the most important role of the spectral function shape which extracts the contribution of one or a few resonances.

All represented analytical results were verified in our numerical experiment by the Gaussian wave packet scattering on the simplest finite periodic lattice composed of δ barriers. The results of these computations will be published in the following paper.[22]

II. SETTING OF A PROBLEM FOR A GENERAL MODEL

We consider the standard one-dimensional model situation of the quantum wave packet scattering. The packet is falling from the left on the periodic potential lattice of finite length composed by the sequence of N equal cells with the length d of elementary translation. The potential energy of the particle $U(x)$ in the area x from $x_0=0$ to $x_N=x_0+Nd$ is equal to the periodical function of the period d, and out of the lattice in regions $x\leq x_0$ and $x\geq x_N$ is equal to zero (Fig. 1).

The evolution of the wave packet is described by the time-dependent solution of nonstationary Schrodinger equation in the form of integral

$$\Psi(x,t) = \int c(E)\psi(E,x)\exp\left(-\frac{i}{\hbar}Et\right)dE, \tag{2.1}$$

where $\psi(E,x)$ are the solutions of stationary Schrödinger equation with the energy E forming the whole system, and the integral is taken over the whole spectrum of the scattering system. The wave function $\Psi(x,t)$ is normalized on the unit. The steady state wave functions of the continuous spectrum are normalized on the δ function of energy[17] and each wave function of the discrete spectrum is normalized on the unit and is orthogonal to other steady state wave functions. Due to the choice of the spectral function $c(E)$ the packet of any initial shape $\Psi(x,0)$ can be built of the steady state wave functions in the starting time $t=0$ and vice versa, defining of $\Psi(x,0)$ allows to find the spectral function

$$c(E) = \int_{-\infty}^{\infty} \psi^*(E,x)\Psi(x,0)dx. \tag{2.2}$$

Thus, for the determination of $c(E)$ and then $\Psi(x,t)$, we need full enough information about the structure of the steady state wave functions $\psi(E,x)$ in the lattice potential $U(x)$.

III. STATIONARY SCATTERING ON THE ONE-DIMENSIONAL LATTICE

A. Wave functions and scattering amplitudes

The lattice under our consideration is the one-dimensional diffraction grating. The stationary scattering in this system is well studied.[12–15] In course of description of the steady state wave functions in one-dimensional periodic lattices of finite length it is necessary to use the mathematical technique which generalizes the Bloch tools and describes the lattice coherent diffraction effects via the Chebyshev polynomials of the second kind presented as a trigonometric or hyperbolic functions of number of the cell.

Let us denote the base solutions of the Schrödinger equation with the energy $E>0$ describing the stationary scattering of the monochromatic waves falling from the left as

$$\psi(E,x) = \begin{cases} A_0 \exp(ikx) + B_0 \exp(-ikx), & x<0, \\ \psi_{0N}(E,x), & 0<x<x_N, \\ A_{N+1} \exp[ik(x-x_N)], & x>x_N, \end{cases} \tag{3.1}$$

where $k=\hbar^{-1}\sqrt{2mE}$ and A_0, B_0, A_{N+1} and partial amplitudes of the falling, reflected, and transmitted flat waves. The $\psi_{0N}(E,x)$ dependence of x is determined by the shape $U(x)$ in the area $0\leq x\leq x_N$. The amplitude of the falling wave should be equal to $A_0=\hbar^{-1}\sqrt{m/2\pi k}$ for the normalizing of the wave functions of the continuous spectrum $\psi(E,x)$ on the δ function of energy as shown in Ref. 17.

It is advisable to find the steady-state wave functions $\psi(E,x)$ and especially their intralattice part $\psi_{0N}(E,x)$ and the amplitudes of reflection $r(E)=B_0/A_0$ and transmission $t(E)=A_{N+1}/A_0$ by means of a transfer-matrix method that provides the automatic matching of piecewise solutions on the boarders of any segments of the x axis.

The simplest and the most natural definition of the transfer matrix $M(x,a)$ is provided by the relation

$$\begin{pmatrix} \psi(E,x) \\ \psi'(E,x) \end{pmatrix} = M(x,a)\begin{pmatrix} \psi(E,a) \\ \psi'(E,a) \end{pmatrix}.$$

It connects the column vectors composed of ψ and $\psi' = d\psi/dx$ in two points a and x by the linear transformation. Defined in such a representation the transfer matrix is real (as a consequence of the time reversibility), is unimodular ($\det M=1$), and is expressed in terms of the Wronski matrices of the stationary Schrödinger equation, taken in a and x points.[16]

If the matrix of the transfer across one cell of the periodic structure is M, then the matrix of the transfer across the n of sequential cells in the positive direction of the x axes is equal to M^n, and in the negative direction it is equal to $M^{-n} \equiv (M^{-1})^n$. The integer power of the two-dimensional unimodular matrix M^n is expressed through the matrix M and unite matrix I by means of Abeles formula (that is the form of Silvester's interpolation polynomial)[16,23,24]

$$M^n = U_{n-1}(y)M - U_{n-2}(y)I, \tag{3.2}$$

in which the exponent n can be negative and the coefficients are equal to the Chebyshev polynomials of the second kind $U_n(y)$ of the argument

$$y = \frac{1}{2}\mathrm{Sp}M, \quad \mathrm{Sp}M = M_{11} + M_{22}. \tag{3.3}$$

The matrix elements will be numerated by two subscripts as usual. The Chebyshev polynomials of the second kind for $n \geq 0$ in dependence of the value $|y|$ are described by the formulas:

$$\text{(a)}\ U_{n-1}(y) = \frac{\sin Knd}{\sin Kd}, \quad Kd = \arccos y, \quad |y| \leq 1, \tag{3.4}$$

i.e., they oscillate sinusoidally as the functions of the argument n or

$$\text{(b)}\ U_{n-1}(y) = (\mathrm{sgn}\, y)^{n-1}\frac{\mathrm{sh}\tilde{K}nd}{\mathrm{sh}\tilde{K}d},$$

$$\tilde{K}d = \mathrm{arch}|y| \equiv \ln(|y| + \sqrt{|y|^2 - 1}), \quad |y| \geq 1, \tag{3.5}$$

where the $\mathrm{sgn}\, y = \begin{cases} 1, & y > 0 \\ -1, & y < 0 \end{cases}$, i.e., they increase exponentially with n rising. Zeros of Chebyshev polynomials of the second kind, i.e., the roots of the equation $U_n(y)=0$ are real, simple, and contained in interval $(-1, 1)$ and equal to

$$y_m^{(n)} = \cos\frac{m}{n+1}\pi, \quad m = 1,2, \ldots ,n, \ n > 0. \tag{3.6}$$

The wave function $\psi = \psi_{0N}(E,x)$ and its derivation in the arbitrary point x inside the nth cell of the lattice $(n-1)d \leq x \leq nd$ can be expressed via their values on the left boundary of the lattice

$$\begin{pmatrix} \psi \\ \psi' \end{pmatrix}_x = M_x M^{n-1}\begin{pmatrix} \psi \\ \psi' \end{pmatrix}_{x_0},$$

$$\begin{pmatrix} \psi \\ \psi' \end{pmatrix}_{x_0} = L\begin{pmatrix} A_0 \\ B_0 \end{pmatrix}, \quad L = \begin{pmatrix} 1 & 1 \\ ik & -ik \end{pmatrix}, \tag{3.7}$$

where $M_x = M[x,(n-1)d]$. The oscillations with x of the elements of matrix M_x and of the functions $\psi(x)$ inside of each cell are defined by the number of the transmission band where the energy is lying, and the elements of matrix M^{n-1} provide the space modulation of these oscillations defining their amplitude envelopes and phases in cells as functions of the cell number n according to Eqs. (3.2)–(3.5).

For the infinite lattice in the both sides ($n \to \pm\infty$) the stability of solutions can be provided only in case (a) when $|y| \leq 1$ and $y = \cos Kd = 2^{-1}\mathrm{Sp}M$. From this, the Bloch theorem follows and all its sequences: Eigenvalues of the energy are grouped in the allowed zones and the envelopes of the wave functions oscillate in the space with the wave length $\lambda = 2\pi K^{-1}$, i.e., $\hbar K$ is the quasimomentum. However, in the finite lattice the eigenfunctions are defined by the case (b), i.e., $|y| = \mathrm{ch}\tilde{K}d = 2^{-1}|\mathrm{Sp}M| \geq 1$ appears along with the extended states ($|y| \leq 1$). The characteristic length of the exponential damping of such solutions near the lattice boundaries is $\delta x \sim \tilde{K}^{-1}$. This is the lattice analogue of the tunnel penetration under the reflecting barrier. In particular in points $x = x_0$ according to Eqs. (3.7) and (3.2) one may write

$$\begin{aligned} \psi_{0N}(E,x_0 + nd) &= (M^n)_{11}\psi(E,x_0) + (M^n)_{12}\psi'(E,x_0) \\ &= U_{n-1}(y)[M_{11}\psi(E,x_0) + M_{12}\psi'(E,x_0)] \\ &\quad - U_{n-2}(y)M_{11}\psi(E,x_0) \\ &= \begin{cases} \alpha_+ \exp(iKnd) + \alpha_-\exp(-iKnd), & |y| < 1 \\ \tilde{\alpha}_+ \exp(\tilde{K}nd) + \tilde{\alpha}_-\exp(-\tilde{K}nd), & |y| > 1, \end{cases} \end{aligned} \tag{3.8}$$

where the representations (3.4) and (3.5) of the Chebyshev polynomials were used in the last line. The factors $\alpha_+, \alpha_-, \tilde{\alpha}_+, \tilde{\alpha}_-$ can be named as effective partial amplitudes. They do not depend on the number n of cell and are expressible in terms of E, A_0, B_0, M_{11}, M_{12}.

As it follows from Eqs. (3.1) and (3.7) the partial amplitudes of plane waves solutions A_0, B_0 at $x < x_0$ and A_{N+1} at $x > x_N$ are connected by the relations

$$\begin{pmatrix} A_{N+1} \\ 0 \end{pmatrix} = M_{Nef}\begin{pmatrix} A_0 \\ B_0 \end{pmatrix}, \quad M_{Nef} \equiv L^{-1}M^N L, \tag{3.9}$$

and the reflection and transmission amplitudes

$$r(E) = -\frac{(M_{Nef})_{21}}{(M_{Nef})_{22}}, \quad t(E) = \frac{1}{(M_{Nef})_{22}} \tag{3.10}$$

depend on the energy E (or on the k parameter) via the elements of effective matrix M_{Nef}. It is easy to verify relations coming from the M_{Nef} definition and M reality

$$(M_{Nef})_{11} = (M_{Nef})^*_{22}, \quad (M_{Nef})_{12} = (M_{Nef})^*_{21}. \tag{3.11}$$

The reflection amplitude $r(E)$ and coefficient $R=|r(E)|^2$ are equal to zero at the full transparency energies when $(M_{Nef})_{21}=0$. The transmission coefficient $T=1-R=|t(E)|^2$ spectrum is composed of alternate transmission and attenuation bands[14–16] (Fig. 2 in the paper in Ref. 22). The almost full reflection in the attenuation bands $|y|>1$ takes place at $N\gg 1$ because $T\sim|(M_{ef})_{22}|^{-2}\sim|U_{N-1}(y)|^{-2}\sim\exp(-2\tilde{K}Nd)\to 0$ and $R\to 1$ at $N\to\infty$. In the transmission bands $|y|<1$ coefficients of transmission and reflection are modulated by Chebyshev polynomials of the second kind too. The oscillations of Chebyshev polynomial by $y=y(E)$ are defined by the sinus in the numerator of Eq. (3.4), and the envelope factor $1/\sqrt{1-y^2}$ plays the role of the amplitude function. At the increasing of N in each band $|y|<1$ the frequency of $U_{N-1}(y)$ oscillations is rising and the amplitude of the $|U_{N-1}(y)|\sim|(M_{ef})_{22}|\sim N$ is rising in the vicinity of $|y|\approx 1$. In each band $|y|<1$ the transmission coefficient T can have $N-1$ maximums about the unity situated at the full transparency energy near zeroes of $(M_{ef})_{21}$ (and R). Minimums where value T is defined by the envelope of Chebyshev polynomial $T\sim|U_{N-1}(y)|^{-2}\sim|1-y^2|$ lie between them. Thus at $N\gg 1$ the depth of modulation $T=T(E)$ significantly increases near the edges of transmission bands where there are narrow spectral lines of sufficiently strong nontransmission but during the moving away from points $|y|=1$ in the middle of transmission bands T is closer to unity. Narrow spectral maximums of $T(E)$ (the lines of transparency) correspond to energies at which $KNd/(2\pi)$ is natural, i.e., the natural number of half waves of envelope is kept within the length of lattice. The wave functions of stationary scattering with the energy in lines of transparency have the resonant character with their large amplitude inside the lattice (Fig. 3 in paper 22).

The amplitudes of reflection $r(E)$ and transmission $t(E)$ can also have the poles usually coinciding with the zeroes of matrix element $(M_{Nef})_{22}=0$ on the corresponding sheet of the Riemann surface of the complex variable E. We are first interested in those of them that describe the quasistationary states.

B. Equations for zeros and poles of the reflection amplitude

By the reason connected with the investigation of integrals convergence it will be more convenient to come from the variable E to the variable $k=\hbar^{-1}\sqrt{2mE}$. During the finding of zeros and poles of the reflection amplitude $r(k)$ of the finite lattice with arbitrary shape of potential inside the cell of periodicity it is also convenient to write the matrix elements included into Eq. (3.10) using the expressions (3.9) for M_{Nef} and (3.2) as

$$(M_{Nef})_{22}=(y+\bar{y})U_{N-1}(y)-U_{N-2}(y),$$

$$(M_{Nef})_{21}=\bar{\bar{y}}U_{N-1}(y), \tag{3.12}$$

where the values

$$y=\frac{1}{2}(M_{11}+M_{22}),\quad \bar{y}=\frac{i}{2}\left(\frac{1}{k}M_{21}-kM_{12}\right),$$

$$\bar{\bar{y}}=\frac{1}{2}\left[M_{11}-M_{22}+i\left(\frac{1}{k}M_{21}+kM_{12}\right)\right], \tag{3.13}$$

depend only on k and local parameters of the cell defining the form of elements of matrix M.

Inside the transmission bands $|y|<1$ the Chebyshev polynomials are proportional to the sinuses according to Eq. (3.4)

$$U_{N-1}(y)\sim\sin NKd\sim\exp(iNKd)-\exp(-iNKd), \tag{3.14}$$

where

$$Kd=\arccos y\equiv i\ln(y+\sqrt{y^2-1}).$$

Therefore, after the substitution (3.14) in (3.12), the extraction of the exponent $\exp(iNKd)$ and taking the logarithm it is easy to get the following forms both for the equation $(M_{Nef})_{21}\sim U_{N-1}(y)=0$ defining zeros of the reflection amplitude $r(k)$

$$\ln(y+\sqrt{y^2-1})=\frac{1}{2N}\,\mathrm{Ln}1, \tag{3.15}$$

and for the equation $(M_{Nef})_{22}=0$ defining its poles

$$\ln(y+\sqrt{y^2-1})=\frac{1}{2N}\,\mathrm{Ln}\left(1-\frac{2}{1+\dfrac{\bar{y}}{\sqrt{y^2-1}}}\right). \tag{3.16}$$

The dependence of the lattice length is taken into account by the factor $1/N$ in right sides.

Realizing the analytical continuation of the last expressions from the real axes into the complex plains of variables k or y it is necessary to take only the main branch of logarithm with $\ln 1=0$ in the left sides representing $Kd=\arccos y$. However the logarithms in the right sides arise from the $\sin NKd$ conversion and are the significantly manysheeted functions that have $\mathrm{Ln}\,1=i2\nu\pi$ where ν are integer numbers of the roots of equations. For the root function $\sqrt{y^2-1}$ it is also enough to take the main branch corresponding to $\sqrt{-1}=i$.

The roots of equations (3.15) of course coincide with the zeros of Chebyshev polynomials of the second kind (3.6), i.e., they give $Kd=\arccos y=\nu\pi/N$ that correspond to the real values of the energy E and wave number $k=k_R^0$ of the lines of full transparency distributed in the transmission bands as it described above.

The content of Eq. (3.16) is not so trivial. We divide it into the real and imaginary parts and get two equations defining the real $k_{R0}=\mathrm{Re}\,k_R$ and the imaginary $\Delta k_R=-\mathrm{Im}\,k_R$ parts of the poles $k_R=k_{R0}-i\Delta k_R$ of the reflection amplitude in dependence of the number N of the periodicity cells and their local parameters. It is evident that the equation slightly differs from Eq. (3.15) and poles of amplitudes $r(k)$ are situated closely to their zeros while the second term under the logarithm in the right side of Eq. (3.16) is small. In particular in case of the tight binding when $|\bar{y}|\gg 1$ the arguments of logarithm are close to unity by modulus both near the edges $|y|\approx 1$ and in the middle $|y|\ll 1$ of the transmission bands and we can restrict ourselves to the accounting of the lowest expansion terms. In this situation the dependencies of the poles positions (as well the lifetimes of quasistationary states τ_R) on N are given by some powers of N. The approximate solutions of Eqs.(3.15) and (3.16) for this case are given in Appendix A and the physical meaning of the results is discussed below in Sec. V.

In case of weak binding the second term under logarithm in the right side of Eq. (3.16) can be not small even near the edges, then the dependence between N and the positions of poles becomes logarithmical.[10]

IV. NONSTATIONARY SCATTERING

A. Spectrum of scattering packet and the spectral integral

The spectral function of the scattering packet $c(E)$ in accordance with Eq. (2.2) is determined by the initial shape of the packet $\Psi(x,0)$ and by the structure of wave functions $\psi(E,x)$ of the stationary scattering. We consider some packet formed sufficiently far away on the left of the point $x=0$. It may be a packet of the type of Gaussian, Lorentz, and similar form with the initial width Δx and location of its maximum at $x=x_C<0$. We assume that spectral center is lying at energy $E_C=\hbar^2k_C^2/2m$ and spectral function coincides with the good accuracy with the spectral function of a free moving packet. The conditions of its usage are characterized by the chain of inequalities

$$k_C^{-1} \ll \Delta x \ll |x_C| \ll k_C(\Delta x)^2,$$

here the middle inequality $\Delta x \ll |x_C|$ allows us to change $\psi(E,x)$ in Eq. (2.2) by $A_0\exp(ikx)$ on the right of $x=0$. The right inequality $|x_C| \ll v_C t_C \approx k_C(\Delta x)^2$ guaranties that the packet cannot spread within the time of its falling on the lattice [where $v_C \approx \hbar k_C/m$ is the group velocity and $t_C \approx m(\Delta x)^2/\hbar$ is the time of spreading], the left inequality $k_C\Delta x \gg 1$ provides the coincidence of the two previous inequalities and allows to neglect the contribution into Eq. (2.2) of the reflected wave $B_0\exp(ikx)$ on the left of $x=0$. Besides for the initially narrow packets formed far away from the lattice we can neglect the contributions from the discrete spectrum of energies if the potential $U(x)$ has the potential wells with their bottoms below zero energy level. The length of lattice should be smaller than mean free path of the particles in the lattice because we neglect all dissipative processes.

Mathematical description of the wave function $\Psi(x,t)$ comes to the analytical or numerical integration (2.1) along the spectrum. The main difficulty is the existence of the quickly oscillating functions under the integral. It is more convenient to integrate by substituting of variable k

$$\Psi(x,t) = \frac{\hbar^2}{m}\int_0^\infty c[E(k)]\psi[E(k),x]\exp[-iE(k)t/\hbar]k\,dk, \tag{4.1}$$

where $E(k)=\hbar^2k^2/2m$. The wave packet can be formed near values of x and t for which the point of extremum phase of under integral expression is close to maximums of modules of the spectral function $c[E(k)]$ and of the amplitudes of the reflected $B_0(k)$ or transmitted $A_{N+1}(k)$ waves. The maximums are often defined by poles and other singular points of these functions in k value complex plain.

The numerical computation of the integral (4.1) is not a very complicated problem now. The results of such computation for the Gaussian wave packet scattering on the lattice formed by $N=50$ identical δ barriers are presented in our paper.[22]

The precise analytical integration is not possible. It can be made only approximately. Here we use the method of asymptotic evaluation of the main contributions in integral (4.1) that is analogical to Drukarev's[19] method and is described in the book by Baz, Zeldovich, and Perelomov.[18] This method combines the steepest descent (saddle point) and residue theory approaches. In Appendix B we explain the derivation of approximate formulas (B2) for nonresonant contribution $\Psi_S(x,t)$ from the saddle point and Eq. (B3) for resonant contributions $\Psi_{R\nu}(x,t)$ from the poles. We emphasize that the Eqs. (B2) and (B3) formulas characterize different contributions from different parts of the common integral contour. They are additive usually and describe the different secondary wave packet separated in space and time

$$\Psi(x,t) \approx \Psi_S(x,t) + \sum_\nu \Psi_{R\nu}(x,t). \tag{4.2}$$

The contribution from the pole $k_{R\nu}$ of number ν is proportional to the modulus of the spectral function in this pole vicinity $|c[E(k_{R\nu})]|$. As a result in such a way it is possible to describe the structure of the main peaks and edges in the form of the envelope function which are observed in real and numerical experiments. But in terms of quantity the position and the size of these structures are defined rather roughly.

In dependence on the form and spectral composition of the falling wave packet the lattice picks out the corresponding resonance components. All parts of the nonstationary wave function (falling, reflecting, and transmitting) are diffractively modulated outside and inside the lattice.

B. Region inside the lattice

In the region $x_0<x<x_N$ inside the lattice the envelope of the wave function is quite characterized by the value of this function on the nodes $x=x_0+nd$. The substitution of Eq. (3.8) in Eq. (2.1) allows us to write $\psi(x_0+nd,t)$ as

$$\Psi(x_0+nd,t) = \int_0^\infty \theta(1-|y|)|c(E)|(|\alpha_+|\exp i\Phi_+ + |\alpha_-|\exp i\Phi_-)dE + \int_0^\infty \theta(|y|-1)|c(E)| \times(|\tilde\alpha_+|\exp \tilde\Phi_+ + |\tilde\alpha_-|\exp \tilde\Phi_-)dE, \tag{4.3}$$

where the values

$$\Phi_+ = K(E)nd - \frac{Et}{\hbar} + \varphi_+(E), \quad \Phi_- = -K(E)nd - \frac{Et}{\hbar} + \varphi_-(E),$$

$$\tilde{\Phi}_+ = \tilde{K}(E)nd - i\left(\frac{Et}{\hbar} - \tilde{\varphi}_+(E)\right),$$

$$\tilde{\Phi}_+ = -K(E)nd - i\left(\frac{Et}{\hbar} - \tilde{\varphi}_-(E)\right),$$

are under exponents. The functions $\theta(x)=\begin{cases}1, x>0\\0, x<0\end{cases}$ provide the taking of the integral on the subregions of the energy admitted by inequalities $|y|<1$ or $|y|>1$, and $\varphi_\pm(E)$ and $\tilde{\varphi}_\pm(E)$ are the phases of the complex values $c(E)\alpha_\pm$ and $c(E)\tilde{\alpha}_\pm$.

The result of the integration strongly depends on the structure of the spectral function $c(E)$. If the modulus of the spectral function $|c(E)|$ has a sharp maximum located at $|y(E)|<1$ in some sth transmission band near the extreme phase point then the first integral in Eq. (4.3) becomes the main. In accordance with Eqs. (4.1) and (B2) it can describe the nonresonant wave packet with envelope function

$$\Psi_S(x_0 + nd,t) = \sqrt{\frac{-i2\pi\hbar^3}{mt}} k_S e^{-iE(k_S)t/\hbar} c[E(k_S)]\psi_{0N}[E(k_S),x_0 + nd]. \tag{4.4}$$

The saddle point coordinate k_S as function of nd and t we find from one of the equations $d\Phi_\pm/dk \sim d\Phi_\pm/dE=0$. These conditions of the extremality of the phases $\Phi_\pm=\Phi_\pm(E)$ can be written in the form

$$nd = \pm v_g(t - \Delta t_d), \tag{4.5}$$

where v_g is the group velocity in sth transmission band and Δt_d is the delay time that are defined as

$$v_g = \frac{1}{\hbar}\frac{\partial E_S(K)}{\partial K}, \quad \Delta t_d = \hbar \frac{\partial \varphi_\pm}{\partial E} \tag{4.6}$$

and $E_S(K)=E$ are the sth branch solutions of the equation $\cos Kd=y(E)$. In our case of the left falling packet the maximum of $|c(E(k))|$ is located at positive $k=k_C$, for the positive nd and t it corresponds to extremum of the phase Φ_+ and to the packet moving to the right side in the lattice.

If the maximum of spectral function $|c(E(k))|$ lies near the poles of reflecting amplitude $r(k)$ then the relevant terms under the integral in Eq. (4.3) can describe the forming of the quasistationary state in the lattice when the transmitting and reflecting waves come in the mutual resonance forming damped standing waves in the lattice. In other words, the resonant contribution to the integral (4.1) from each of poles $k_R=k_{R0}-i\Delta k_R$ ($k_{R0}=\mathrm{Re}\, k_R, \Delta k_R=-\mathrm{Im}\, k_R>0$) of the reflecting amplitude $r(k)$ by Eq. (B3) has a form

$$\Psi_R(x_0 + nd,t) = -2\pi i \frac{\hbar^2 k_R}{m} e^{-iE(k_R)t/\hbar} \mathrm{Res}\{c[E(k_R)]\psi_{0N} \times [E(k_R),x_0 + nd]\}. \tag{4.7}$$

Here the time is counted off from some moment at the end of the transitional process of the initial propagation of transmitting and reflecting resonant waves through the lattice. It is approximately the moment when the line of the steepest descent cross the pole k_R in Fig. 3. The residue in Eq. (4.7) is usually proportional to $\mathrm{Res}\{r(k_R)\}$. The function $\psi_{0N}[E(k_R),x_0+nd]$ includes as factors the Chebyshev polynomials $U_n(y)\sim\sin(n+1)Kd$ which give to the space envelope $\Psi_R(x_0+nd,t)$ the character of resonance standing wave. The time behavior is described by the factor $\exp[-iE(k_R)t/\hbar]$ and it is a usual factor characterizing the evolution of the quasistationary state which has the energy $E_R=\mathrm{Re}\, E(k_R)$ and the lifetime $\tau_R=\hbar/\Gamma$, where $\Gamma=-\mathrm{Im}\, E(k_R)$, i.e.,

$$E(k_R) = E_R - i\Gamma,$$

$$E_R = \frac{\hbar^2}{2m}[k_{R0}^2 - (\Delta k_R)^2], \quad \tau_R = \frac{m}{2\hbar k_{R0}\Delta k_R}. \tag{4.8}$$

These slowly damping standing waves connected with different resonant poles $k_{R\nu}$ may be combined and exist after the wave packet (4.4) leaves the lattice. Their lifetimes $\tau_{R\nu}$ increase strongly with the increasing of the lattice length $L=Nd$.

If the spectral function $|c[E(k)]|$ has a maximum in the nontransmitting band $|y|>1$ then the main is the second integral in Eq. (4.3); it describes the damping of the wave packet in the lattice in analogy with the damping under the continuous potential barrier.

C. Region outside the lattice

On the left of the lattice at $x<x_0=0$ the term $A_0\exp(ikx)$ from Eq. (3.1) gives the main contribution to Eq. (4.1) for $t<-x_C/v_C$ and the saddle point $k_S=-m(x_C-x)/\hbar t$ determines the moving to the right and spreading of the packet falling on the lattice

$$\Psi_{Sf}(x,t) = \sqrt{\frac{-i2\pi\hbar^3}{mt}} k_S c[E(k_S)]A_0(k_S)e^{i[k_S x - E(k_S)t/\hbar]}.$$

Analogically, the term $B_0(k)\exp(-ikx)$ from Eq. (3.1) gives the noticeable contribution to Eq. (4.1) for $t>-x_C/v_C+\Delta t_r$ where Δt_r is the delay time of reflection, the saddle point $k_S\approx-m(x_C+x-v_C\Delta t_r)/\hbar t$ determines the moving to the left and spreading of the packet reflected by the lattice

$$\Psi_{Sr}(x,t) = \sqrt{\frac{-i2\pi\hbar^3}{mt}} k_S c[E(k_S)]r(k_S)A_0(k_S)e^{-i[k_S x + E(k_S)t/\hbar]}.$$

On the right of the lattice at $x>x_N$ the term $A_{N+1}(k)\exp[ik(x-x_N)]$ from Eq. (3.1) leads to the significant contribution to Eq. (4.1) in the same manner only for $t>-x_C/v_C+\Delta t_t$ where Δt_t is the transmission delay time; the saddle point $k_S\approx-m(x_C-x-v_C\Delta t_t)/\hbar t$ determines the moving to the right and spreading of the transmitted packet

$$\Psi_{St}(x,t) = \sqrt{\frac{-i2\pi\hbar^3}{mt}} k_S c[E(k_S)]t(k_S)A_0(k_S)e^{i[k_S(x-x_N) - E(k_S)t/\hbar]},$$

where $t(k_S)$ is the transmission amplitude but not a time.

The spectrally narrow initial packet especially on the edges of the transmission bands can form the quasistationary states determined by poles of the amplitudes $r(k)$ and $t(k)$. The decay of these states during the time τ_R is also accompanied by the resonance secondary packets coming out of the lattice to the left

$$\Psi_{Rr}(x,t) = -2\pi i \frac{\hbar^2 k_R}{m} \theta\left(\frac{\hbar k_{R0} t}{m} + x\right) c[E(k_R)] A_0(k_R) \times \text{Res}\{r(k_R)\} e^{-i[k_R x + E(k_R)t/\hbar]}, \tag{4.9}$$

following the reflected packet $\Psi_{Sr}(x,t)$ and to the right

$$\Psi_{Rt}(x,t) = -2\pi i \frac{\hbar^2 k_R}{m} \theta\left(\frac{\hbar k_{R0} t}{m} + x_N - x\right) c[E(k_R)] A_0(k_R) \times \text{Res}\{t(k_R)\} e^{i[k_R(x-x_N) - E(k_R)t/\hbar]} \tag{4.10}$$

following the transmitted packet $\Psi_{St}(x,t)$. Here as in Eq. (4.7) the time is counted off from some moment of quasistationary state formation and θ functions approximately describe the fronts of the secondary packets and provide the realization of the conditions of the achieving and capture of the pole by the steepest descent contour on Fig. 3. The contribution from the vicinity of the saddle point gives the smearing of the θ fronts in all rigorous integral (4.1).

V. MEASURABLE CHARACTERISTICS AND THE LIFETIME OF THE QUASISTATIONARY STATE

The quasistationary states arise in a solitary local potential well when surrounding barriers are weakly penetrated, therefore the corresponding resonant effects in the lattice display itself more brightly in case of a tight binding. We restrict ourselves to this case when the potential barriers in cells are weakly penetrated that provides the dependence of y from k and E is approximately linear inside the s is transmission band, then the energy of particle is connected with the quasimomentum K by the expression

$$E \approx E_S(k_0) + (-1)^S \Delta E_S \cos Kd. \tag{5.1}$$

where $E_S(k_0)$ is the electron energy at some threshold $k=k_0 \approx s\pi/d$ and ΔE_S are the bandwidth of sth transmission band.

The poles of $r(k)$ and $t(k)$ are disposed along the peculiar arc in the lower half plane,[10] and the extremes of them are located very closely to the real axes that results the long lifetime of the formed quasistationary states. The conditions of their formation are sufficient narrowness and the large value of the spectral function in the area of energy, corresponding to the real parts of the poles. These features of the system [peaks of the spectral function, zeros, and poles of the function $r(k)$] are fixed in the particular part of the k-plane. The saddle points corresponding to packets move with x and t, but the optimal for the resonance saddle points should be located in the same area. The spectral function is sufficiently narrow if the packet width Δx is larger or approximately equal to the length of the whole lattice $L \sim Nd \sim \pi/K(k_S)$.

The formation of described quasistationary state takes place in the lattice coincidentally with the transmitting of the non resonance main body of the wave packet. But when the lifetime is large enough $\tau_R > Nd/v_g$ the quasistationary state exists after the coming out the lattice of the reflected $\Psi_{Sr}(x,t)$ and transmitted $\Psi_{St}(x,t)$ packets. The probability of the particle detection inside the lattice is given by the integral

$$w_L = \int_0^L |\Psi(x,t)|^2 dx. \tag{5.2}$$

For the time when the superposition (4.2) is valid the contributions from different resonances in integral (5.2) are almost additive since the resonant wave functions are almost mutually orthogonal because of norming of the corresponding stationary wave functions on the δ function of energy. The oscillating interference terms in Eq. (5.2) are small and the next approximate equality is valid in the region of exponential decaying of the significant quasistationary states

$$w_L \approx \sum_\nu w_{0\nu} \exp\left(-\frac{t - t_{0\nu}}{\tau_{R\nu}}\right), \tag{5.3}$$

where $w_{0\nu}$ is the probability of νth quasistationary state forming at the moment $t_{0\nu}$.

In the local quadratic by $\Psi(x,t)$ characteristics type of

$$|\Psi(x,t)|^2 \approx \left(\Psi_S(x,t) + \sum_\nu \Psi_{R\nu}(x,t)\right)^* \times \left(\Psi_S(x,t) + \sum_\nu \Psi_{R\nu}(x,t)\right), \tag{5.4}$$

the noticeable interference beats can become apparent on the difference frequencies $\Delta\omega_{\nu\mu} = (E_{R\nu} - E_{R\mu})/\hbar$ in time[21] and on the difference wave numbers $\Delta k_{\nu\mu} = k_{R0\nu} - k_{R0\mu}$ in coordinate if the corresponding resonance contributions in the superposition (4.2) are of the same order.

The exponential decay of the quasistationary states is accompanied by the comparatively weak impulses of the shape (4.9) and (4.10) coming out to the left and to the right from the lattice that follow the reflected and transmitted packets and generate corresponding pulses of current. The current of probability in some point is the most convenient value for observation of these interference effects

$$j_w = \frac{i\hbar}{2m}\left(\Psi(x,t)\frac{\partial \Psi^*(x,t)}{\partial x} - \Psi^*(x,t)\frac{\partial \Psi(x,t)}{\partial x}\right) \approx \frac{\hbar}{2m}\left[\left(\Psi_S(x,t) + \sum_\nu \Psi_{R\nu}(x,t)\right) \times \left(k_S \Psi_S(x,t) + \sum_\nu k_{R\nu}\Psi_{R\nu}(x,t)\right)^* + \text{c.c.}\right], \tag{5.5}$$

in points on the boundaries of the lattice for example. For a very lengthy packet at $\Delta x \gg Nd$ the spectral function is narrower than one line of resonant transparency and only one term is large in the previous sums so the beats are not observable.

In the tight binding approximation the analysis of Eqs. (3.15) and (3.16), the estimations of reflection amplitude zeros and poles, of the quasistationary states energies and lifetimes (4.8) are performed in Appendix A for the arbitrary cell potential. It is shown there that the resonance energies E_R are approximately given by the zone theory expression

(5.1) with $Kd=\nu\pi/N$. Near the top of the sth transmission band the estimated lifetime of a quasistationary state with number $\nu \ll N$ is as follows:

$$\tau_R = \frac{m}{2\hbar k_{R0}\Delta k_R} = \frac{mN}{2\hbar k_0}\left(\frac{N}{\nu\pi}\right)^2 \left| y'(k_0)\mathrm{Im}\,\frac{1}{\bar{y}(k_0)} \right|. \quad (5.6)$$

Near the bottom of the sth transmission band it is necessary to change $\nu \to \nu - N$. Thus the lifetimes of the near-threshold quasistationary states are very large proportionally to $(N/\nu)^2 \gg 1$ and increase according to the cube law $\sim (Nd)^3$ with the enlargement of the lattice.

In the middle of the sth transmission band we have

$$\tau_R = \frac{mN}{2\hbar k_0}\left| y'(k_0)\mathrm{Im}\,\frac{1}{\bar{y}(k_0)} \right|, \quad (5.7)$$

i.e., the lifetimes of the quasistationary states in the middles of the transmission bands are considerable in $2(N/\nu\pi)^2 \gg 1$ times smaller than the near-threshold ones and increase with the enlargement of the lattice according to the linear law $\sim Nd$.

The last estimations for τ_R are interesting to compare with the estimations for the time of transmission through the lattice $\Delta t = Nd/v_g$ of the nonresonance main wave packet (4.4) if its energy E_C of the spectral center is equal to the energy E_R of the quasistationary state. Using the relation $\cos Kd = y(E)$ we convert the first expression (4.6) for group velocity to the form

$$v_g = -\frac{d}{\hbar}\frac{\sqrt{1-y^2}}{(\partial y/\partial E)}, \quad (5.8)$$

from which it is seen that near the edges of zones the group velocity is diminishing and on edges $v_g=0$ because $|y|=1$ here. Differentiating y and $k=\hbar^{-1}\sqrt{2mE}\approx k_0 \approx s\pi/d$ we get $\partial y/\partial E = (\partial y/\partial k)(\partial k/\partial E) \approx (\partial y/\partial k)(m/\hbar^2 k)$. In the neighborhood of the νth resonant line near the top of the sth transmission band the approximate equalities $\sqrt{1-y^2}\approx\sqrt{2\Delta} \approx \pi\nu/N$ are valid in accordance with Eqs. (A4), (A3), and (A10). Thus we have the estimation

$$v_g \approx \frac{\hbar k}{m}\frac{d}{|y'(k_0)|}\frac{\nu\pi}{N} \approx v_{g0}\frac{d}{|y'(k_0)|}\frac{\nu\pi}{N} \ll v_{g0}. \quad (5.9)$$

where $v_{g0}=\hbar k/m \approx \hbar s\pi/md$ is a group velocity of the free moving packet, the last inequality is fulfilled at $\nu\pi d/[|y'(k_0)|N] \ll 1$, and

$$\Delta t \approx = \frac{m}{\hbar k}|y'(k_0)|\frac{N^2}{\nu\pi} \approx 2\frac{\nu\pi}{N}\tau_R \Bigg/ \left| \mathrm{Im}\,\frac{1}{\bar{y}(k_0)} \right| \ll \tau_R, \quad (5.10)$$

where inequality is fulfilled at $\nu\pi/[|\mathrm{Im}\,1/\bar{y}(k_0)|N] \ll 1$.

In the middle of sth transmission band $\sqrt{1-y^2}\approx 1$ and we have

$$v_g \approx \frac{\hbar k}{m}\frac{d}{|y'(k_0)|} \approx v_{g0}\frac{d}{|y'(k_0)|} \ll v_{g0}, \quad (5.11)$$

inequality is fulfilled at $d/|y'(k_0)| \ll 1$ and

$$\Delta t \approx = \frac{m}{\hbar k}|y'(k_0)|N \approx 2\tau_R \Bigg/ \left| \mathrm{Im}\,\frac{1}{\bar{y}(k_0)} \right| \ll \tau_R, \quad (5.12)$$

where inequality is fulfilled at $|\mathrm{Im}[1/\bar{y}(k_0)]| \ll 1$, i.e., v_g is larger and Δt is smaller than on the edges of transmission band in $N/\nu\pi$ times.

Thus the main result is that in the case of the tight binding approximation applicability and mentioned inequalities (see the model estimations and calculation in the paper in Ref. 22) in the whole transmission band $\Delta t \ll \tau_R$ and quasistationary state in lattice can exist long enough after the transmission and reflection of the nonresonant parts of the scattered wave packet.

VI. CONCLUSION

We showed that the quasistationary states inside the one-dimensional lattice of finite length can be formed by scattering of the wavepacket if the width of the packet is comparable or larger than the lattice length. The envelope of the quasistationary wave function inside the lattice is similar to the resonant stationary total transmission wave function envelope and its localization length is approximately equal to the length of the lattice. These states can exist after the coming away of the usual transmitted and reflected pulses. The lifetime of the quasistationary state increases with the lattice length more significantly for the resonance energy near the thresholds of transmission band than in the middle of the band. The interference effects can be significant at quasistationary state decaying.

The described regularities of formation and evolution of the quasistationary state in the lattice can become apparent in nanocrystals, superlattices, and multilayer systems of the finite length that is smaller than the quantum coherence length, i.e., the electron mean free pass in such systems. The received results and their consequences have the certain physical generality. It is possible to discover their analogs during the research of the electromagnetic or elastic wave packets scattering in the appropriate multilayer systems.

APPENDIX A: REFLECTION AMPLITUDES ZEROS AND POLES. THE ENERGY AND LIFETIME OF THE QUASISTATIONARY STATE IN THE LATTICE OF THE FINITE LENGTH (TIGHT BINDING APPROXIMATION)

A. Premise expressions

As noted above, the resonant effects display themselves more brightly in case of a tight binding. We consider the case when the potential of each periodicity cell provides the linear dependence of y from k inside the transmission bands in the main approximation (Fig. 2).

We will reckon the energy (5.1) and the wave number from the top of sth transmission band $|y|<1$ that corresponds to some values $k=k_0$, $\bar{y}=\bar{y}(k_0)$, $\bar{\bar{y}}=\bar{\bar{y}}(k_0)$, and $y(k_0) = (-1)^S$. For the complex variable $k=k_1+ik_2$, where $k_1 = \mathrm{Re}\,k$, $k_2=\mathrm{Im}\,k$, in the region of sth transmission band

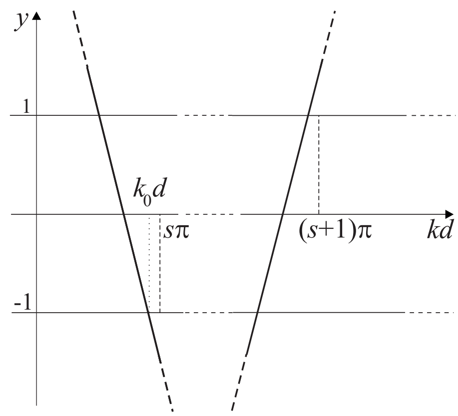

FIG. 2. Linear parts of the function $y(kd)$ in tight binding approximation near two regions of transmission.

$$k_1 = k_0 - \Delta k_1, \tag{A1}$$

at that Δk_1 as k_2 is the small value $|\Delta k_1|, |k_2| \ll 1/d < |k| \approx s\pi/d$. We will write the parameter y as

$$y = (-1)^S(1-\varepsilon), \tag{A2}$$

where in the main linear order

$$\varepsilon = (-1)^S y'(k_0)(\Delta k_1 - ik_2) \tag{A3}$$

and $y'(k_0)=dy(k_0)/dk$ is the derivation in the point k_0. It follows from the definitions (3.13) and the model estimations (see the paper in Ref. 22) that in the tight binding approximation $|y'(k_0)| \gg d$ and $|\bar{y}(k_0)| \gg 1$. In the region of transmission band $|y| < 1$ it should be $0 < \mathrm{Re}\,\varepsilon < 2$; the top of the band $\Delta k_1 = 0$ corresponds to $\mathrm{Re}\,\varepsilon = 0$ and the bottom of the band $\Delta k_1 = 2(-1)^S/y'(k_0) \ll 1/d$ corresponds to $\mathrm{Re}\,\varepsilon = 2$.

We get the approximate expressions for Δk_1 and k_2 near the thresholds and in the middle of the transmission band. First we consider the regions near the thresholds $|y| \approx 1$. The small deviations from them by variable y we will denote as Δ. Thus $y = 1-\Delta$ where $|\Delta| \ll 1$, we have at $\Delta = \varepsilon$ for the even s and at $\Delta = 2-\varepsilon$ for the odd s, and $y = -1+\Delta$ where $|\Delta| \ll 1$, we have at $\Delta = \varepsilon$ for the odd s and at $\Delta = 2-\varepsilon$ for the even s. In both cases

$$\sqrt{y^2-1} \approx \sqrt{-2\Delta}\left(1 - \frac{\Delta}{4}\right) \tag{A4}$$

with its own Δ, but

$$y + \sqrt{y^2-1} \approx \pm 1 + z,$$

$$z = \sqrt{-2\Delta} \pm \Delta - \frac{\Delta}{4}\sqrt{-2\Delta},$$

where the upper sign we take near the threshold $y=1$ and the lower sign near the threshold $y=-1$. Further we use a well-known expansion of logarithm[25]

$$\mathrm{Ln}(1+z) = i2\nu\pi + \ln(1+z), \tag{A5}$$

$$\ln(1+z) = z - \frac{z^2}{2} + \frac{z^3}{3} - \frac{z^4}{4} + \cdots, \tag{A6}$$

where ν is a whole number.

For the left parts of Eqs. (3.15) and (3.16), as mentioned above, we will use Eq. (A6), then near the threshold $y=1$ we have

$$\ln(y + \sqrt{y^2-1}) \approx i\sqrt{2\Delta}\left(1 + \frac{\Delta}{12}\right) \approx i\sqrt{2\Delta}, \tag{A7}$$

and near the threshold $y=-1$ using $\ln(-1+z) = \ln(-1) + \ln(1-z)$ and $\ln(-1) = i\pi$ we have

$$\ln(y + \sqrt{y^2-1}) \approx i\left[\pi - \sqrt{2\Delta}\left(1 + \frac{\Delta}{12}\right)\right] \approx i(\pi - \sqrt{2\Delta}). \tag{A8}$$

In the middle of the transmission band $|y| \ll 1$, so in the linear approximation $y + \sqrt{y^2-1} \approx i + y = i(1-iy)$ and

$$\ln(y + \sqrt{y^2-1}) \approx i\left(\frac{\pi}{2} - y\right), \tag{A9}$$

where the first term of the expansion (A6) and $\ln i = i\pi/2$ are used.

B. Estimate expressions

We will get the approximate expressions for Δk_1 and k_2 for the arbitrary cell potential providing the linear dependence (A2) and (A3).

Let us consider the regions near the thresholds. In Eq. (3.15) the right part is equal to $i\pi\nu/N$. Equating it successively to the expressions (A7) and (A8), solving the equations for Δ and using the noted connections $\Delta = \varepsilon$ or $\Delta = 2-\varepsilon$ with the help of Eq. (A3) we verify in considered order that zeros of $r(k)$ have imaginary parts that are equal to zero $k_2 = 0$ and the roots k_R^0 are given by the right part of Eq. (A1) and condense to the thresholds inside the band of transparency according to the quadratic law because near the top

$$\Delta k_1 = \frac{(-1)^S}{2y'(k_0)}\left(\frac{\nu\pi}{N}\right)^2 \tag{A10}$$

and near the bottom

$$\Delta k_1 = \frac{(-1)^S}{2y'(k_0)}\left[4 - \pi^2\frac{(\nu-N)^2}{N^2}\right], \tag{A11}$$

where the roots are reckoned from the top of transmission band.

Considering Eq. (3.16) we can substitute the parameter $\bar{y}$ and $\sqrt{y^2-1}$ as Eq. (A4) into the right part of it; then we can expand the logarithm by Eqs. (A5) and (A6). As a result the right part (3.16) in the main order by Δ is equal to

$$i\frac{\nu\pi}{N} - \frac{i}{N}\frac{\sqrt{2\Delta}}{\bar{y}(k_0)}.$$

We equate it successively to the right parts of Eqs. (A7) and (A8) and express Δ connected with ε as above. After the separation of the real and imaginary parts of the equations we can verify that in the main order under consideration the real parts $k_{R0}=\mathrm{Re}\,k_R$ of the reflection amplitude poles $k_R=k_{R0}-i\Delta k_R$ identical to the roots k_1 are equal to

$$k_{R0}=k_0-\Delta k_{R1}, \quad (A12)$$

where Δk_{R1} are given by the expressions

$$\Delta k_1=\frac{(-1)^S}{2y'(k_0)}\left(1-\frac{2}{N}\,\mathrm{Re}\,\frac{1}{\bar{y}(k_0)}\right)\left(\frac{\nu\pi}{N}\right)^2, \quad \nu\ll N$$

near the top and

$$\Delta k_1=\frac{(-1)^S}{2y'(k_0)}\left[4-\left(1-\frac{2}{N}\,\mathrm{Re}\,\frac{1}{\bar{y}(k_0)}\right)\pi^2\frac{(\nu-N)^2}{N^2}\right], \quad N-\nu\ll N$$

near the bottom of the transmission band. In particular, if $|\mathrm{Re}[1/\bar{y}(k_0)]|\ll N$, they are equal to the right parts of Eqs. (A10) and (A11).

The imaginary parts of the reflection amplitude poles k_R are given by the roots k_2 that are equal near the top of the transmission band to

$$\mathrm{Im}\,k_R=-\Delta k_R=-\frac{1}{|y'(k_0)|}\left|\mathrm{Im}\,\frac{1}{\bar{y}(k_0)}\right|\frac{1}{N}\left(\frac{\nu\pi}{N}\right)^2, \quad (A13)$$

and differ by the changing to $\nu\rightarrow\nu-N$ near the bottom. They are condensed to the thresholds according to quadratic law. Thus, in the main order by the small parameters of tight binding approximation, the reflection amplitude poles lie under its zeros. Eliminating ν from Eqs. (A12) and (A13) we get the angle coefficient γ (near the top edge $\Delta k_R=\gamma\Delta k_{R1}$, for example) which characterizes the coming of the arc of localization to the real axes

$$\gamma\approx\frac{2}{N}\left|\mathrm{Im}\,\frac{1}{\bar{y}(k_0)}\right|, \quad (A14)$$

if $|\mathrm{Re}(1/\bar{y}(k_0))|\ll N$.

Now we consider the region in the middle of the transmission band where $|y|\ll 1$, so we use the linear approximation (A9). Equation (3.15) with the right part $i\pi\nu/N$ gives $k_2=0$ of course and the roots Δk_1 defining by Eq. (A1), the zeros of $r(k)$ distributed in the middle of the band almost according to the linear law

$$\Delta k_1=\frac{(-1)^S}{y'(k_0)}\left(1+(-1)^S\frac{\pi\nu_1}{N}\right), \quad (A15)$$

where $\nu_1=\nu-N/2$ enumerates these roots from the middle of the transmission band.

In the right part of Eq. (3.16) we substitute $\sqrt{y^2-1}\approx i$ and expanding the logarithm we get that this right part in the middle of the transmission band in the main order is equal to

$$i\frac{\nu\pi}{N}-\frac{i}{N}\frac{1}{\bar{y}(k_0)}.$$

We compare the real and imaginary parts of the last expression with analogical parts of the formula (A9) where y is given by Eqs. (A2) and (A3). It is evident that the real parts of the reflection amplitude poles are defined by the roots k_1 and are given by the expression (A15) in which Δk_{R1} is equal to

$$\Delta k_1=\frac{(-1)^S}{y'(k_0)}\left[1+(-1)^S\frac{\pi}{N}\left(\nu_1-\frac{1}{\pi}\,\mathrm{Re}\,\frac{1}{\bar{y}(k_0)}\right)\right], \quad \nu_1\ll N$$

and if $|\mathrm{Re}(1/\bar{y}(k_0))|\ll\nu_1$ they are equal to the right part of Eq. (A15) now, i.e., k_{R0} almost coincides with the values of zeros of $r(k)$. The imaginary parts of the reflection amplitude poles k_R are given by k_2; in the middle of the transmission band they are approximately equal to

$$\mathrm{Im}\,k_R=-\Delta k_R=-\left(\frac{1}{y'(k_0)}\,\mathrm{Im}\,\frac{1}{\bar{y}(k_0)}\right)\frac{1}{N}. \quad (A16)$$

This value characterizes the maximum deviation of arc of the poles localization from the real axes. It is seen that it is inversely proportional to length Nd of the lattice.

In order to receive the approximate expressions for the energy E_R and the lifetime τ_R of the quasistationary state it is necessary to substitute k_{R0} and Δk_R into the formulas (4.8). Since the tight binding approximation is $\Delta k_R\ll\Delta k_{R1}\approx\Delta k_1\ll k_{R0}\approx k_R^0\sim s\pi/d$ (see the model estimations in 22) then for the energy E_R with good accuracy we may use the solution of Eq. (3.15), i.e., the usual expression of the zone theory (5.1) with $Kd=\nu\pi/N$. In order to estimate the lifetime τ_R it is enough to substitute $k_{R0}\approx k_0$ into the second of the formulas (4.8) in accordance with Eq. (A12) and Δk_R from Eq. (A13) or Eq. (A16). We get the law (5.6) near the thresholds and the law (5.7) near the middle of the transmission band.

APPENDIX B

After the substitution $\psi[E(k),x]$ from Eq. (3.1) and $c[E(k)]$ to Eq. (4.1) the integrals appear

$$I=\int_0^\infty F(k)\exp[-i\beta_t(k-k_S)^2]dk, \quad (B1)$$

where $\beta_t=\hbar t/2m$, k_S, and $F(k)$ depend on x, t, and parameters of the problem. The function $F(k)$ can have the poles k_R or other singularities in value k complex plain defined by the singularities of $c[E(k)]$ and of amplitudes of reflecting and transmitting waves. The integral (B1) is usually evaluated by the method of steepest descent (of saddle point).[26] If the value β_t is very large the main contribution in it is connected with the so-called stationary point k_S on the real axes that is the saddle point for the function $\mathrm{Re}[-i\beta_t(k-k_S)^2]$ relative to $\mathrm{Re}\,k$ and $\mathrm{Im}\,k$ variables and the line of the steepest descent of this function is the straight line I transmitting the complex plain of the value k via k_S under the angle $-\pi/4$ to the real axes (Fig. 3).

In accordance with the general rule, the contribution from the vicinity k_S is found by displacement of the integration contour in the analyticity domain from the real axis to the line I of the steepest descent crossing the saddle point. The contribution of the saddle point is usually evaluated by the

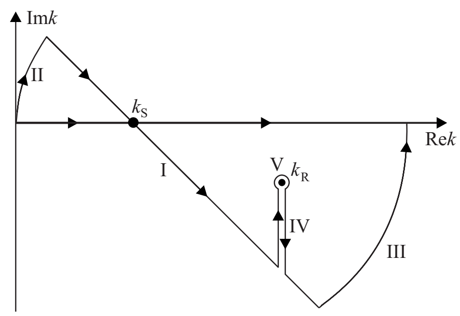

FIG. 3. Displacement of the integration contour in the analyticity domain from the real axis to the line I of the steepest descent crossing the saddle point k_S; the pole k_R is going around by a small circle V.

Poisson integral along the line I; it is equal to

$$I_S = F(k_S)\sqrt{\frac{-i\pi}{\beta_t}}. \tag{B2}$$

In comparison with it the contributions of other parts of deformed contour (lines II and III in picture Fig. 3) are usually small. If the pole k_R or the branch point of $F(k)$ is met during the shift of the contour near the saddle point then they should be walked around by the way of IV and V types as shown in the picture.

In case of poles the contributions of the IV parts are mutually cancelling and the contribution of the small circle V around the pole k_R is equal to the residue in this pole and can be not small in comparison with contribution I_S of the saddle point

$$I_R = \pm 2\pi i \mathrm{Res}\{F(k_R)\}\exp[-i\beta_t(k_R - k_S)^2]. \tag{B3}$$

The plus sign is taken if the pole is localized in the II sector of the upper half-plain, and the minus in the III sector of the lower half-plain as it is shown in Fig. 3.

The result of the usage of the saddle point method strongly depends on the width and position of the saddle in the complex plain, its remoteness from the original, and on the form of the spectral function of the packet, scattering amplitudes, and on the position and types of their singularities. The positions of the scattering amplitudes poles on the complex k plain, and of spectral function $c[E(k)]$ do not depend on time. However, the saddle point and the line of I type at fixed x move along with the t to the origin usually according to the rule $k_S \sim 1/t$ absorbing the singularities of the stationary scattering in the II and III sectors. This defines the appearance of the x and t edge conditions that provides a special pattern of different maximums and fronts in the form of the envelope of the wave function $\Psi(x,t)$.

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