New theory of periodical systems by finite interval inverse problem.

B. N. Zakhariev and V. M. Chabanov
Laboratory of theoretical physics, JINR,
Dubna, 141980, Russia; e-mail: zakharev@thsun1.jinr.ru

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1 Abstract

We show that the mechanism of gap formation has a resonance nature. The special real fundamental solutions were discovered which ‘paradoxically’ have knot distribution with a period coinciding with that of potential at all energies of the whole lacuna interval. In terms of these solutions resonance gap appearance gets the most direct explanation: ever repeating hits by the potential result in exponential increase (decrease) of the wave amplitudes in the forbidden zones. The analogous alternating hits from opposite sides are responsible for the wave beatings in allowed zones. The inversion technique gives rise to zone control algorithms – shifting chosen boundaries of spectral bands, changing degree of zone forbiddenness. All this cannot be achieved by the previous Bloch theory.

2 Introduction

It is well known that periodical potential perturbation splits the continuous spectrum creating bands of allowed zones separated by gaps of forbidden zones. The explanation of this statement by Bloch-Floquet formalism has seemed to be satisfactory since the appearance of this theory 70 years ago. However, the intrinsic mechanism of zone formation by a certain periodic
potential remained incompletely understandable: Bloch theory as a black box gives out only the spectral zones without qualitative explanations. Additional insight into the theory became possible due to inverse problem and SUSY QM formalisms that opened new horizons in quantum mechanics by their exactly solvable models, see our new book: "Submissive quantum mechanics" about the turnover from direct to inverse problem [1] (it can be found in internet http://thsun1.jinr.ru/~zakharev/).

We have found the following fact: there is some kind of deep-hidden 'resonance' which tears the spectrum. Namely, inside the gaps the period of the potential coincides with that of very special (we will call them 'smart', i.e. 'intellectual') solutions. Being periodically positioned, knots of these smart solutions are not the same, but interlaced with each other. Of these two linearly independent solutions, being a manifold of zero measure, the whole continuum of solutions with 'invisible resonance' can be constructed. They will have quite irregular disposition of knots at each energy value in the forbidden zone. Despite this 'irregularity camouflage' due to a resonant nature of constituents (coherent hits of perturbation in the successive periods), 'smart' solution oscillation amplitudes are forced to exponentially increase (or decrease) in opposite directions. This is characteristic to non-physical (forbidden) behaviour. Hence, arbitrary solutions tend asymptotically (as $x \to \pm \infty$) to pure smart solutions. On the one side, the discovered resonance mechanism seems to be very natural. On the other side, the property of smart solutions having the same period of knots (oscillations) on the finite energy interval contradicts the widely spread notion that the oscillation frequency increases with the energy, for instance, the initial free solution has a specified period at only one fixed energy point. In periodical potentials there are almost no periodical solutions except the zone boundaries. Bloch waves are products of functions with different periods. In forbidden zone nobody suspected of any periodicity. The unexpected periodical positioning of knots in rare smart solutions reveals almost evidently the resonance cause.

The above mentioned can be explained in the following way. Different solutions perceive the same potential as different effective potentials: more or less repulsive (attractive). It is due to different sensitivity of bumps and knots of (real) solution to the local values of the potential. So, for instance, if bumps of the smart solutions are at potential barrier positions there will prevail a repulsion, i.e., the effective kinetic energy will be weakened, which widens the distance between knots. This allows energy change complete com-
pensation needed to keep knot period constant all over the energy interval of the entire forbidden zone. So the inter-knot distance of smart solutions remains unchanged when shifting simultaneously the energy over the $E$-axis and the wave knot lattice over the $x$-axis.

It is worth to mention that the choice of purely real solutions was one of the key moments simplifying the investigations of this paper.

Splitting the unperturbed continuous spectrum into the band one by creating forbidden zones is essentially quantum effect. So we shall return later once more to clarify this basic features of wave behavior in periodical structures which is not at all 'non-physical' aspect of the theory. We shall also consider below somewhat less wonderful solutions in the allowed zones.

3 Inverse problem and SUSY QM spectral control

The complete sets of explicit inverse problem solutions on finite interval served us as a hint in constructing solutions to periodic potentials. Moreover, they give rise to a significantly broader class of exactly solvable models for periodic systems (infinite zone models).

The key point of the inverse problem is that spectral parameters (energy levels, normalizing constants, etc.) enter in the formalism as input data and corresponding exactly solvable models are generated by varying only a certain spectral parameter or a finite number of them (while living the others unaltered). Since spectral parameters form a complete set and completely determine properties of quantum systems, exact models corresponding to all possible variations of spectral parameters give rise embrace the whole manifold one- and multi-channel systems. Thus, there appears a possibility of changing at wish quantum objects by variation of these parameters (as if using control 'levers') and examine quantum systems in different thinkable situations. By the way, instead of about ten direct problem exactly solvable models which currently serve as a basis of the contemporary education one should also be guided by an infinite (!) number, even complete sets of such models from the inverse problem.

The laws of structure transformations and wave motions revealed by computer visualization of these models were reformulated into unexpectedly sim-
ple universal rules. The elementary "bricks and blocks" were discovered of which it is possible in principle to construct objects with any given properties [2].

Let us shortly formulate these rules [1, 4] because they will serve as suggesting considerations in constructing remarkable solutions with periodically spaced knots. Each real wave consists of bumps and knots. We now discuss two algorithms of transformation of one wave bump. They are easily demonstrated by the example of eigenvalue problem on a finite interval with zero boundary conditions (namely, for the ground state of the infinite rectangular well). First rule: To shift one energy level up (down) over the energy scale we must introduce a potential barrier (well) near the extremum of the bump where the wave is most sensitive to the potential ($V$), see Fig.1. Pay attention to the important immobility of the ground state knots that promoted us in revealing resonance ('smart') solutions. In addition, we need compensating wells (barriers) in the vicinity of knots if we want to keep all other energy levels at their previous places. So the different states see the same potential as different effective potentials. The second rule: for shifting the spatial localization of a wave bump over the finite interval to the right (left) we need potential perturbation as a barrier-well (well-barrier) block. These rules are applicable to wave bumps of each (bound or scattering) state and for any potential [4], see Fig.1, Fig.2.

As a result, we can transform any wave with arbitrary number of bumps. So we acquire the vision of the intrinsic logic of structure and behavior peculiarities of a great amount of thinkable systems, including real ones.

4 Waves in periodical potentials

Periodical perturbation 'stretches one spectral point' of initial free motion into continuous energy interval of forbidden zone with zero spectral density; in allowed zones the density is compressed [5].

Switching on the perturbation violates generally the periodicity (equidistance) of knots of the real solutions. There are continuum such solutions at any energy value and all solutions, unlike those for free motion, are quite different (they do not turn into one another by shifting $x$-variable).

Consider a free one-dimensional motion of waves over the $x$-axis. The Schrödinger equation has two linearly independent partial solutions. It suffice
to fix the position of any knot to determine the solution up to an inessential norming factor. For zero potential there is a continuous spectrum $E > 0$. A typical solution is $\sin(kx + \alpha)$ with the phase $\alpha$.

We shall choose, e.g., the periodic potential with the Kronig-Penney form, see Fig.3.

If the wave bumps (their extrema) are positioned above the middles of potential wells (see Fig.4C) and the knots inside the potential barriers, the wave 'must have' higher average kinetic energy and, hence, frequency of oscillations. Thus, we attained the same frequency as was in free motion but at a lower energy value $E_\prec$. This corresponds to pushing downward to the energy $E_\prec$ the ground state of the auxiliary problem of the infinite rectangular potential of width equal to the period (see Fig.1) with the potential wall positions coinciding with the knots. Remind that such a shift of levels is performed without moving the knots at the ends of the interval [2]. On the contrary, shifting the bump extrema of $\sin(kx + \alpha)$ to the middles of the barriers (see Fig.4A) would decrease in the average kinetic energy if we keep the energy $E = k^2$ unchanged. Consequently, one has to lift energy up to $E_\succ$ for the inter-knot distance to remain unaltered. The symmetry of potential between the knots according to the middle point between the knots in both the cases conserves the symmetry of the corresponding solutions on the periods. This allows their smooth periodic continuation. The solutions considered correspond to the upper and lower boundaries of the forbidden zone which is created by the potential perturbation.

This is confirmed by the consideration of other solutions with the energies between $E_\succ$, $E_\prec$. Take the solution with the knots at the boundaries of the potential wells and barriers (see Fig.4B,D). In this case, under each bump is the block ”well-barrier” or ”barrier-well” which slightly change the energy of the state which follows from the requirement of keeping inter-knot distance unaltered. Besides this there is strong violation of the symmetry of the bump, in particular, its derivatives at the knots (see discussion below). This leads to exponential growth of the solution oscillation amplitude as $x \to \pm \infty$. It follows from smooth connection of solutions on the neighbor periods. All other dispositions of the knots with respect to wells and barriers of the potential will lead to combinations of shifts over the energy scale and violations of symmetry of the initial bumps. So the whole spectral lacuna can be continuously filled by these solutions with gradual change in the 'degree of forbiddeness' of the zone from zero at one boundary to the maximum.
value somewhere near its middle and again to zero at the other boundary. This happens because of the increase-decrease of symmetry violation of the perturbing potential between the knots (pay special attention to the gradual shift of state over E and to the movement of bumps localization over x). Here the mathematically exact proof can be obtained without formulae (explanations ‘on fingers’ based, however, on the previous rules of quantum intuition). Arbitrary solution in forbidden zone has different asymptotically periodical displacement of knots because only increasing component of the corresponding linear combination of smart solutions survives at asymptotic distances (solution tends to one or another smart solution as \( x \to \pm \infty \)).

Above \( E > \) inside the allowed zone the frequency of knots begins to increase with \( E \) until the number of knots on one period increases by one. The solutions there have alternating increases and decreases of oscillation amplitudes. These beatings in allowed zones can be explained in the following way. There are no analogies of ‘smart’ solutions with equidistant knots except the zone boundaries where there is one periodic solution among the continuous set with disordered knots. With increase of energy the (average) density of ‘disordered’ knots also increases, as in free motion. There is difference in size of the potential period and the distances between solution knots. On the one side, it leads to oscillations of these knot positions with respect to potential periods along the \( x \) axis. On the other side, there is alternation of regimes of increase-decrease of oscillation amplitudes. The asymmetry of potential perturbations between the neighbor knots and inequality of solution derivatives there result in increasing and then decreasing (and so on) of swinging of the solutions, i.e., lead to beatings. In other words, at some moment, there may be more effective attraction, say, to the left and repulsion from the right between the knots of the solution. This will make the solution oscillation amplitude increase to the left. Later, due to shifting oscillations of the solution relative the potential periods, the situation changes to the opposite one: there will be excess of repulsion from the left and attraction from the right. The wave length of these modulated oscillations (beatings) will decrease from infinite value on the lower boundary of the allowed zone to a finite value of about the potential period size at the upper boundary.

At the energy zone boundaries, in addition to periodic solution, there is a solution linearly increasing in both directions. This reminds the situation with the solutions in vicinity of eigenstate with an energy \( E_\nu \) in a finite depth potential well. Above and below \( E_\nu \) there are two independent solutions
exponentially increasing (decreasing) to the right (left) sides and vice versa. Meanwhile at $E_\nu$ there are two solutions increasing and decreasing (bound state proper) in both directions.

Let us discuss once again the mechanism of zone formation by using somewhat different scheme. Let us at first consider an auxiliary problem of finding solutions and spectrum of the Hamiltonian with zero boundary conditions at the edges of the finite interval (period) $[\varepsilon, a+\varepsilon]$, for any $0 < \varepsilon < a$ and the potential $V^\varepsilon(x) = V_{\text{per}}(x)$, e.g., Kronig-Penney one, for $x$ belonging to this interval. The corresponding spectrum is discrete set $\{E_n^\varepsilon\}_{n=0}^\infty$. If we continue periodically (with the period $a$) this interval we will, of course, restore the periodical potential and, moreover, find particular solutions for $V_{\text{per}}(x)$ at the energies $E_n^\varepsilon$. In fact, the sought solutions may be obtained from the auxiliary problem eigenfunctions $\Psi_n^\varepsilon(x, E_n^\varepsilon)$. The wave continuity is guaranteed by vanishing of the eigenfunctions at the matching points $na + \varepsilon$ (points of contact of adjacent intervals). The smoothness of wave matching can be attained by multiplying neighbor eigenfunction by a factor being equal (modulo) to the ratio of the derivatives at the right and the left boundaries. If this factor is equal modulo to 1 the energy $E_n^\varepsilon$ will be at one of the zone boundaries. This case corresponds to such position of the interval $[\varepsilon, a+\varepsilon]$ that $V^\varepsilon(x)$ is a symmetric (with respect to the interval center) potential with a rectangular barrier (or well) in the middle, see Fig 4 A,C. When once the potential symmetry is violated (by altering $\varepsilon$), $\Psi_n^\varepsilon(x, E_n^\varepsilon)$ loses its previous symmetry, which results in either increasing or decreasing solution on the whole axis. Hence, the energy $E_n^\varepsilon$ turns out to be inside the forbidden zone. Simultaneously, the $E_n^\varepsilon$ is shifted downward (upward) since the potential $V^\varepsilon(x)$ becomes effectively less repulsive (attractive) as a result of shifting barrier (well) position on the interval. Thus, by varying the parameter $\varepsilon$ (as if scanning the potential by the interval $[\varepsilon, a+\varepsilon]$), the energy $E_n^\varepsilon$ runs the entire $n$th spectral gap.

5 Shifts of zone boundaries

It appears that our ability to shift isolated bound state energy levels (over the $E$-scale) in the infinite potential well on a finite interval allows us to move some chosen upper (lower) boundaries of the spectral zones (bands) of periodic structures keeping infinite number of other upper (lower) boundaries
unperturbed.

For definiteness, we will consider shifting up and down the upper boundary of only the second allowed zone for the initial Dirac comb of periodic δ-barriers. For this purpose, we will use the SUSY QM formulas for only chosen energy level shift on the finite interval \([0, \pi]\) with potential \(V_0(x)\) [3]. Let \(\psi_0(x, E_n)\) be corresponding eigenfunction at the energy \(E_n\). We assume \(\tilde{\psi}_0(x, E_n + t)\) to be a non-physical auxiliary solution in the initial potential at shifted energy \(E_n + t\) with the symmetry being opposite to that of the \(\psi_0(x, E_n)\). With these solutions, we can construct the Wronskian

\[
\theta(x) = \psi'_0(x, E_n)\tilde{\psi}_0(x, E_n + t) - \psi_0(x, E_n)\tilde{\psi}'_0(x, E_n + t).
\]  

(1)

Shifting energy level \(E_n \rightarrow E_n + t\) is performed by special potential transformations. The corresponding final expressions for the transformed potential and solutions read

\[
V(x) = V_0(x) - 2t \frac{d}{dx}\left\{\psi_0(x, E_n)\tilde{\psi}_0(x, E_n + t)\theta(x)^{-1}\right\};  
\]  

(2)

\[
\psi(x, E) = \psi_0(x, E) - t\tilde{\psi}_0(x, E_n + t)\theta(x)^{-1}\int_0^x \psi_0(y, E_n)\psi_0(y, E)dy;
\]  

(3)

\[
\psi(x, E_n + t) = \psi_0(x, E_n)\theta(x)^{-1}.
\]  

(4)

The potential (2) can be periodically continued: \(V_{\text{per}}(x + l\pi) = V(x)\), \(l = 0; \pm 1; \pm 2; \ldots\) for \(x\) belonging to \([0, \pi]\). Such a scheme allows a spectral zone control. Let us consider this potential with an incorporated Dirac comb (equally spaced δ-potential barriers or wells \(\sum_{m=-\infty}^{\infty} v\delta(x - m\pi)\)), i.e., the following periodic potential: \(\sum_{m=-\infty}^{\infty} v\delta(x - m\pi) + V_{\text{per}}(x)\). The corresponding results are shown in Fig.5.

In the special case of *mergence of allowed zones* there is local compensation of attraction and repulsion, at the energy value \(E_m\) and \(\Delta E = 1\); as in the case of a free motion, any choice of boundary condition (position of some knot) gives solutions on periods with symmetric derivatives at the ends of the
interval (their invariance under arbitrary translations), which provides wave behavior without exponential growth. Any small change of energy leads to violation of this situation. A like mergence of the first and the second allowed zones see Fig.6. (something above $\Delta E = -2$ and below $\Delta E = 3$).

Exactly solvable models allow one to demonstrate the control of ‘forbiddenness’ at any chosen energy point by changing the derivative of finite interval solution at the left boundary, the spectral weight vector $c$ [9, 11]. Below are given the formulas for the potential and wave functions transformations corresponding to variations of the spectral weight factor $c_n$ of a chosen bound state at the energy $E_n$. Let $\psi_n(x)$ be the eigenfunction of the initial Hamiltonian corresponding to $m$th energy eigenvalue, $\hat{c}_m$’s are the initial spectral weight factors. Then changing $\hat{c}_m \rightarrow c_m$ gives

$$\psi_n(x) = \psi_n(x) + \frac{(1 - \frac{c_m^2}{\hat{c}_m^2}) \psi_m(x)}{1 - (1 - \frac{c_m^2}{\hat{c}_m^2}) \int_0^x \psi_m^2(y) dy} \times \int_0^x \psi_m(y) \psi_n(y) dy,$$

(5)

$$V(x) = \hat{V}(x) + 2 \frac{d}{dx} \frac{(1 - \frac{c_m^2}{\hat{c}_m^2}) \psi_m^2(x)}{1 - (1 - \frac{c_m^2}{\hat{c}_m^2}) \int_0^x \psi_m^2(y) dy}.$$

(6)

Again, we periodically continue these results. Changing $c$ leads to previous symmetry violation for the initial wave function $\psi_n(x) = \sqrt{(2/\pi)} \sin(nx)$ (we put $\hat{V}(x) = 0$ and the interval to be $[0, \pi]$). As a result, the whole axis wave function, ‘sewed’ from $\psi_n(x)$, will asymptotically diverge. The factor $c$ just represents the index of divergence rate, ‘forbiddenness’. See results on the corresponding control in Fig.7, [1] (in particular, we can thus tear the continuous spectrum at energy point $E_n$).

Instructive are some simple examples of shifting only the upper or only lower boundaries of zones. They can be achieved by introducing $\delta$-peaks or $\delta$-wells at the middle of the periodical potential barriers or wells. Take
into account that the δ-potentials do not influence the solution if they are coincident with the knots, but push the energy of state maximally up or down, being disposed at the maximum modulo of the wave bumps.

Analogous reasoning is applicable to other forbidden zones. We only need to use the initial free sine-like solutions at higher energies corresponding to knot frequency twice (and more times) in comparison with the periodic oscillations of the potential.

We can generalize the theory for arbitrary periodic potential for which it is impossible to choose the period with symmetrical potential shape (with respect to the center of period). In spite of asymmetry in this case there are such positions of solution knots relative to potential at specific energies $E_\langle,\rangle$ that the derivatives at knots become equal modulo. So we get the boundaries of zones. See Fig.8. as an example potential with peak of barriers and bottoms of wells at the same points. In this case $\Psi; \Psi_1; \Psi_2; \Psi_3$ correspond to spatial shifts to the right, left and $E$-shifts up and down.

It is worth to mention the possibility to create localized bound states in periodic structures in analogy with transformation of free motion (soliton-like potentials which are transparent for Bloch waves [6, 7].

Everything we have learned about the periodic structures (smart solutions in forbidden zones, beatings in allowed zones) is applicable to the finite interval potentials created from truncated periodic potentials (i.e., becoming periodic when continuing over the entire $x$-axis), in particular, to resonance tunneling through finite number of periodic potential barriers where multiplets of resonances correspond to allowed zones and gaps between them to forbidden zones.

It is worth to mention that we have found examples for complex periodic potentials [8]) which do not create lacunas.

6 Some multichannel models.

We hope to generalize our theory to systems of coupled Shrödinger equations. As the first steps in this direction can be considered the following models illustrating some important features of complex systems.

1. Let $V_{11}(x) = V_{22}(x)$ (with equal periods) and the thresholds of both the channels are equal $\varepsilon_1 = \varepsilon_2 = 0$. For uncoupled (independent) channels the one-channel theory is obviously generalized. There are separate spectral
bands in both the channel spectral branches. Now let us switch on some interchannel coupling \( V_{12}(x) = V_{21}(x) \). So, the interaction matrix is symmetrical with respect to channels. If we choose boundary conditions for both the channels equal, the partial channel functions will be equal \( \Psi_1(x) = \Psi_2(x) \). This allows one to make the substitution \( V_{12}(x)\Psi_2(x) \rightarrow V_{12}(x)\Psi_1(x) \) in the equation for the first channel and analogous transformation in the second channel. This results in their effective separation (coupling disappearance: 'diagonalization' of the interaction matrix) with new effective interaction matrix elements

\[
V_{11}^{\text{eff}} = V_{11} - V_{12}c_2/c_1; \quad V_{22}^{\text{eff}} = V_{22} - V_{21}c_1/c_2.
\]

All this leads, e.g., to two branches of potential oscillations accompanied by natural effect for the band structure (widening or narrowing of forbidden zones).

2. Let the thresholds be unequal \( \varepsilon_1 < \varepsilon_2 \), \( V_{11}(x) = V_{22}(x) = 0 \) and the coupling of channels be some constant \( V_{12}(x) = V_{21}(x) = \text{const} \). Let us choose the boundary conditions as follows: \( \Psi_i(0) = \Psi_i(\pi) = 0; \ i = 1, 2 \). It means the requirement of equidistancy of knots in different channels with quite different partial channel energies \( E_i = E - \varepsilon_i \). This 'paradoxical' situation can exist despite the difference of the thresholds if the effective kinetic energies in both the channels, e.g., ground state are equal. This can be achieved by choosing different spectral weights of partial components which are proportional to one another: \( \Psi_1(x) = c_1/c_2\Psi_2(x) \). Really, the partial channel equations can be rewritten as uncoupled ones using the substitution \( \Psi_1(x) \) by \( c_1/c_2\Psi_2(x) \) and vice versa:

\[
-\Psi_1''(x) = (E - \varepsilon_1 - V_{12}c_2/c_1)\Psi_1 - \Psi_2''(x) = (E - \varepsilon_2 - V_{21}c_1/c_2)\Psi_2. \quad (7)
\]

The expressions in brackets in the right hand sides are effective kinetic energies and they become equal if

\[
c_2/c_1 = \Delta \varepsilon_{12}/2V_{12} \pm \sqrt{\Delta \varepsilon_{12}^2/(4V_{12}^2) + 1}.
\]

3. Again let \( \varepsilon_1 < \varepsilon_2 \), \( V_{11}(x) = V_{22}(x) = 0 \), but with the modified boundary conditions \( \Psi_i(\pi/i) = \Psi_i(\pi/i) = 0; \ i = 1, 2 \) and interchannel coupling
$V_{12}(x) = V_{12}\delta(x)$. In this model the effective kinetic energy in the second channel with smaller partial energy $E - \varepsilon_2$ must be even greater than in the first channel in order to provide the two times smaller distance between the knots ($\pi$ in comparison with $2\pi$ for the first channel).

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Figure captions

Fig 1. The potential perturbation of the bottom of the infinite rectangular well which results in lowering (shown by arrow $\Delta E_1$) only one level $\hat{E}_1 = 1 \rightarrow E_1 = -4$ of the ground state. The bold black arrow directed downward points to the well (dashed-dotted line $\Delta V(x)$) acting on the most sensitive, central, region of the wave function to shift the level downward. The same arrows directed upward near the walls of the initial well, where the function $\Psi_1$ has knots and where it is the least sensitive to potential changes, point to the barriers needed to keep all other energy levels $E_i \neq 1$ from shifting. The transformations of the wave functions $\Psi_{1,2} \rightarrow \Psi_{1,2}$ are shown by thin dashed lines. The instructive value of this picture consists in that it demonstrates qualitative features of universal, elementary transformation for a single bump of a wave function. It allows one to understand the rule of the wave transformations of arbitrary states with many bumps and in arbitrary potentials, see also other pictures. b) Evolution of the $\Psi_1$ when $\Delta E = -1, -3$. Note that the knots at the edges of the interval (equal to period, see text) do not move c) Evolution of the potential when $\Delta E = -1, -2, -3$. Do not confuse the cases b, c) with motions in the system: we mean changes of $\Psi_1, V$ under successive transitions from one system to another ("in the space of different models").

Fig 2. The (a,b) transformation of the infinite rectangular potential well $\hat{V} \rightarrow V$ and eigenfunctions $\hat{\Psi}_1 (x)$ (a,d), $\hat{\Psi}_2 (x)$ (a,c) by increasing spectral weight factor (SWF) $c_1 \rightarrow c_1$, the derivative $\Psi'_1(x = 0)$ at the left wall. The scales of the functions $\Psi_1, \Psi_2$ (a) are shifted up to the corresponding energy levels $E_1, E_2$. In (b,c,d) the evolution of the potential and functions with increasing $c_1 2, 5, 10, 20$ times is demonstrated. Meanwhile all ! energy levels $E_n$ and all SWF, except one $c_n \neq 1$, remain unchanged, as is seen for $\Psi_2$ (a,c). The parameter SWF $c_1$ controls the localization of the wave function $\Psi_1(x)$ (a,d,e) in space: by increasing $c_1$ the ground state is pressed to the left potential wall, as is shown by arrows in (a,d). This is performed by the potential barrier in (a,b) on the right which shifts the function $\Psi_1(x)$ to the left, and the potential well on the left which simultaneously compensates the influence of the barrier on the energy levels and keeps them all at the same places. All wave functions, except the ground state, undergo some recoil in the opposite direction which is demonstrated by $\Psi_2(x)$ (a,c). So there is separation of the bound state from others.
Fig. 3. The wave functions of a free motion \( \sin(kx + \alpha) \) at energy \( E = k^2 \) corresponding to frequency of periodic potential \( V(x) \) oscillations. These solutions of the Shrödinger equation are chosen with different values \( \alpha \) so that the knots coincide with: the middle of the potential barriers, or wells, or left sides of the barriers (wells). All free waves have the equidistant distribution of knots, and switching on the perturbing periodic potential must violate this. However, we can find such values of \( E_> ; E_<; \) etc. (shifted from \( E_1 \), see vertical arrows) at which we can choose perturbed solutions with the same equidistant distributions of knots. Horizontal arrows correspond to the shifts of space localization of the wave bumps (see Fig. 4.C, D) without shifting the knots.

Fig. 4. The same as in Fig. 3, but the cases with a different shift of knots are considered separately: A,B) the perturbed solution is shifted up without violation of the distance between knots; B) shift to the right (mainly) of localization of any wave bump; C) shifting down the solution with keeping equidistant distribution of its knots. D) shift to the left. Transformations of wave bumps are shown separately at the left sides of the figures (see also Fig. 5).

Fig. 5. Perturbations of the initial free wave functions with the different x-shifts (\( \alpha \)) by the periodic potential with the period equal to the distance between the wave knots. The perturbed solutions are considered at energy values (A: \( E_> \); B: \( E_< \), etc.) where their knots do not change their positions. C) Exponential increase of swinging amplitude of solutions in forbidden zone is demonstrated by introducing big negative factors \( f, f^2, f^3 \ldots \) which provide the smooth junction of solutions on neighbor periods (the corresponding potential perturbation is shown in Fig. 5.D.).

Fig. 6. Shifting the upper boundary of the second allowed spectral zone (shown with arrows). Pay attention to the merging of this zone with the upper one at \( \Delta E = 1 \). Find two another examples of merging of first and second zones.

Fig. 7. (Upper part) Changes in zone structure corresponding to relative variations of a derivative at one end of a period (spectral weight factor) \( c/\hat{c} \) at energy point \( E = 2 \). The initial periodic potential \( \hat{V} \delta(x - n\pi) \) has Dirac comb peaks with the strength \( \hat{V} = 4 \) and period \( \pi \). The wave function at \( E = 2 \) is on each period an eigenfunction of the eigenvalue problem with the boundary conditions on the edges of a period specified so that the auxiliary
discrete energy level just coincides with the chosen point $E = 2$. (Lower part) Changes of the imaginary part of quasi-momentum $ImK(E)$ which characterize the degree of forbiddenness, the index of exponential swinging of solutions.

Fig.9. Schematic illustration of the set of ‘smart’ solutions with periodic knots (curved line) which are a zero measure manifold among all other solutions in the chosen forbidden zone (rectangular shadowed area corresponding to $\pm \Delta x$ on the finite interval having a length of the period).

The continuum of free periodic solutions of the type shown in Fig.3 at ‘resonance’ energy $E_r$ (shown here as a line with points) are transformed by periodic perturbation $V$ into exponentially increasing (decreasing) solutions of a forbidden zone which splits the initial continuous spectrum.
Fig. 1
Fig. 2
Fig. 3
Fig. 4
Fig. 5
Fig. 6
Fig. 7
continuum of free solutions $\hat{\Psi}(x)$ at $E_r$

'resonance' energy $E_r$

zero measure sets of smart solutions among all others in forbidden zone

relative shift of $\Psi(x)$ vs. $V(x)$

two smart solutions at fixed $E$

Fig. 9