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S.I.Serdyukova, B.N.Zakhariev

WHY THE QUANTUM LATTICE WAVE DOES NOT SLIDE DOWN THE POTENTIAL SLOPE

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Сердюкова С.И., Захарьев Б.Н. E4-91-237

Почему квантовая волна на решетке не спускается с потенциального склона?

В отличие от классической и квантовой частиц, скатывающихся с потенциального склона, квантовые волны на решетке запираются в связанных состояниях на потенциальном холме. Для линейных потенциалов спектр таких состояний эквидистантный. Хорошо известные функции Бесселя $J_\alpha(kr)$ с целым индексом α в качестве дискретной пространственной координаты (не r как обычно!) играют роль волновых функций связанных состояний — стоячих волн между потенциальным склоном и невидимой границей верхней запрещенной зоны. Эта точно решаемая модель проясняет некоторые специфические свойства более реалистических систем, например, межканального движения, где α означает дискретный номер канала.

Работа выполнена в Лаборатории теоретической физики и в Лаборатории вычислительной техники и автоматизации ОИЯИ.

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Serdyukova S.I., Zakhariev B.N. E4-91-237

Why the Quantum Lattice Wave Does not Slide Down the Potential Slope

Unlike the classical and quantum particles rolling down the potential slope the quantum waves on the lattice are confined in the bound states on the potential hill. For the linear potential there is an equidistant spectrum of these states. The well known Bessel functions $J_\alpha(kr)$ with the integer index α as a discrete spatial co-ordinate (not r as usual!) play the part of the bound state wave functions — standing waves between the potential hill and the invisible boundary of the upper forbidden zone. This exactly solvable model elucidates some peculiar features of more realistic systems, particularly, the interchannel wave motion where α means the discrete channel number.

The investigation has been performed at the Laboratory of Theoretical Physics and at the Laboratory of Computing Techniques and Automation, JINR.

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I. INTRODUCTION

Even Gell-Mann with his powerful quantum intuition considered quantum mechanics as the most unintuitive science. So there is a great need to make the behaviour of the nonrelativistic microworld more predictable. The new exactly solvable models may be extremely useful here. One such a simple model is suggested in this paper.

It is instructive to compare the peculiarities of the wave motion in the ordinary and in the discrete quantum mechanics [1]. In the last case we can use the finite-difference Schroedinger equation with the step $\Delta = x_{n+1} - x_n$ ($x_n = n\,\Delta$; $\Psi(x_n) \equiv \Psi(n)$; $h/2\pi = m = 1$):

$$- [\Psi(n + 1) - 2\Psi(n) + \Psi(n - 1)]/2\Delta^2 + V(n)\,\Psi(n) = E\,\Psi(n) \quad (1)$$

instead of the differential one

$$-\frac{1}{2}\,\Psi''(x) + V(x)\,\Psi(x) = E\,\Psi(x). \qquad (2)$$

It is important to mention that eq. (1) can be considered here not as a finite difference approximation to eq. (2) but as an example of equations for the description of the wave motion along the lattices. It is supposed that the discreteness of the variable corresponds here to the genuine nature of the described object.

The special feature of the "discrete Schroedinger equation" (1) is the finiteness of the width of the allowed energy zone. It is most clearly revealed in the case of free motion ($V \equiv 0$). Both equations (1) and (2) have the forbidden zone for the negative energy values. For $E < 0$ the equations (1) and (2) have the exponentially increasing or decreasing solutions : $\exp(\pm\varkappa x)$; $\exp(\pm\hat{\varkappa} n)$ with real $\varkappa = (-E)^{1/2}$, $\hat{\varkappa} = \mathrm{arch}(1-E\Delta^2)$. This can be verified by direct substitution. For $E > 0$ there is a continuous spectrum with oscillating solutions: linear combinations of $\exp(\pm ikx)$; with $k = (E)^{1/2}$ for eq. (2); and of $\exp(\pm i\hat{k}n)$ with $\hat{k} = \arccos(1-E\Delta^2)$ for eq. (1). But unlike eq. (2) the continuous spectrum of eq. (1) is bounded by the upper forbidden zone (see for example [1]): $E < 2/\Delta^2$, see Fig. 1. with a sandwich type structure of zones. Above this boundary the solutions of (1) are

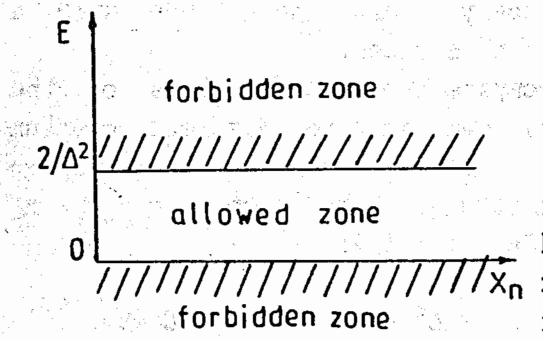


Fig. 1. The spectrum of the free motion over the lattice has the horizontal allowed zone between lower and upper forbidden zones.

combinations of $\exp(\pm i\pi n \pm\hat{\varkappa} n)$ with $\hat{\varkappa} = \mathrm{arcch}(E\Delta^2-1)$. That is they have exponentially increasing or decreasing oscillations above this boundary. For $V(n) = V_0 = \mathrm{const}$ the allowed zone is obviously shifted by V_0.

The introduction of the linear potential $V(n) = n$ causes the inclination of the allowed zone (see Fig. 2.) so that for any fixed energy the waves are confined between the lower and the upper inclined boundaries. Indeed, the character of the solution (whether it corresponds to the allowed or to the forbidden zone) can be determined on the interval including three neighbouring points according to eq. (1) where the potential value is used at the middle point only. The width of the allowed zone depends on Δ and not on V. The variation of the potential $V(n)$ merely shifts the zone boundaries at different points n. For the linear potential the allowed zone has the corresponding linear boundaries.

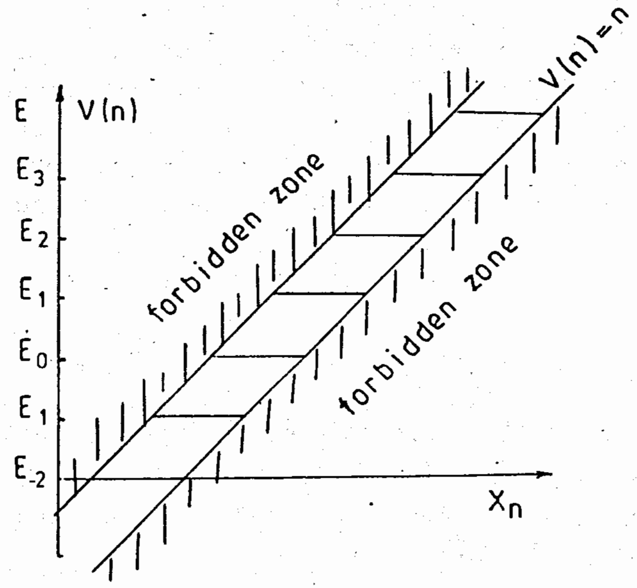


Fig. 2. The potential V linearly dependent on the spatial co-ordinate causes the inclination of the zones shown on Fig. 1. So for a fixed energy E waves have to oscillate between the two forbidden zones. There is an unbounded spectrum of equidistant levels $E_n = 1 \pm n/z$; $n = \ldots -1, 0, 1, \ldots$.

As it will be shown in sec. 2, the solutions of the corresponding Schroedinger equation are the Bessel functions $J_\alpha(z)$ with the discrete variable α playing the part of n in eq. (1). The Bessel functions with the integer α are the bound states (quadratically summable standing waves; see Fig. 4). Their spectrum is equidistant (as for the oscillator with the continuous co-ordinate) but unbounded: $E_m \longrightarrow \pm\infty$ as $m \longrightarrow \pm\infty$. The behaviour of this spectrum by the variation of the steepness of the potential slope of the suggested exactly solvable model allows one to understand the peculiarities of more general quantum systems. For example, the discrete oscillator well has the spectrum resembling one for the square well with the continuous co-ordinate. It becomes also clear what perturbations of the potential are required to change the spectrum in the desired way (new aspects of "spectral engineering" in addition to those considered in [1]). So we can produce a gap in the spectrum (Fig. 6) or to install an interval of dense levels in it (Fig. 7), To install bound states above the continuous spectrum (Fig. 9).

2. BESSEL FUNCTIONS

The first notion about the Bessel functions as the solutions of the finite-difference Schroedinger equation appeared in [2]. After that they were considered by [3] but only for infinite potential well. It appears that much more benefit can be achieved from exactly solvable models with the Bessel functions.

The well known recurrence equation for the Bessel functions

$$J_{\alpha+1}(z) + J_{\alpha-1}(z) = (2\alpha/z)\, J_\alpha(z) \quad , \qquad (3)$$

can be considered as the finite-difference equivalent (1) of the Schroedinger equation (2). Indeed, rewriting (3) in another form (by adding and subtracting $2J_\alpha$ and dividing both sides of the equation by $2\Delta^2 = 2$) we get

$$-\{J_{\alpha+1}(z) - 2J_\alpha(z) + J_{\alpha-1}(z)\}/2\Delta^2 - (\alpha/z)\, J_\alpha(z) = J_\alpha(z). \quad (3')$$

This is the finite-difference Schroedinger equation where the part of the discrete co-ordinate of the configurational space plays the index α as n in eq. (1) with the step $\Delta = 1$, fixed energy $E = 1$ and the potential $V(\alpha) = \alpha/z$ that is a linear function of α.

Two linearly independent solutions $J_\alpha(z)$, $Y_\alpha(z)$ of eq. (3 or 3') are shown in Fig.3 (see [4], Fig.9.3). These Bessel

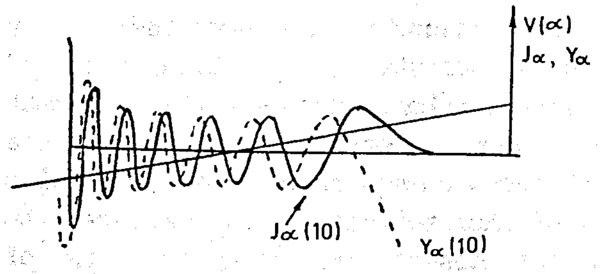


Fig.3 The dependence on index α of the Bessel functions of the first and second kind $J_\alpha(z)$, $Y_\alpha(z)$ (see [2] Fig.9.3).

functions of different kind with fixed z decrease and increase correspondingly as functions of index α inside the potential barrier $V(\alpha)$. Thus from a physical point of view Y_α are not appropriate. It may seem that J_α is also

physically unsuitable because the amplitude of oscillations of J_α is increased inside the upper forbidden zone (J_α is swinging more intensively with α moving to the left as we see in Fig. 3). Actually, there is a continuum of solutions represented by $J_\alpha(z)$, $Y_\alpha(z)$ in the Fig. 3. Choosing discrete values α with the step $\Delta = 1$, we get the α-lattice and relative discrete values of $J_\alpha(z)$, $Y_\alpha(z)$. Every shift of this lattice: $\alpha \longrightarrow \alpha' = \alpha + \varepsilon$; $\varepsilon < 1$ gives a new solution of eq. (4, 4'). For the integer α the functions J_α satisfy the condition ([4], eq.9.1.5):

$$J_{-\alpha}(z) = (-1)^\alpha\, J_\alpha(z) \qquad (4)$$

this provides the exponential decrease of J_α with integer α for $\alpha \longrightarrow -\infty$. So, among the continuum of different functions J_α there is a countable manifold of physically acceptable functions which are bound states confined between both forbidden zones (see Fig.4). These bound states form the equidistant spectrum because the energy shift $\delta E = 1/z$ is equivalent to the shift of the α-scale by $\delta\alpha = 1$ due to the linear dependence of the potential on α: $V(\alpha) = \alpha/z$.

It is convenient to number the bound states: $\Psi_0(\alpha) \equiv J_\alpha$; $\Psi_{\pm n}(\alpha) \equiv J_{\alpha\pm n}$. Those J_α which have fractional α represent the unphysical solutions for continuum of energy values between these levels $\Psi(E{=}\varepsilon{\pm}n/z;\ \alpha) = J_{\alpha+\varepsilon\pm n}$; $\varepsilon < 1$.

It is easy to predict, in accordance with Fig.4, that in the limit $z \longrightarrow \infty$ the discrete spectrum of eigenstates J_α becomes the continuum band as is required for the free motion along the lattice, and in the limit $z \longrightarrow 0$ there will be no levels (zero density of levels).

The model under consideration allows the variation of the value of the finite-difference step Δ. The change of Δ by factor s is equivalent to the change: $z \longrightarrow z/s^2$; $E \longrightarrow E/s^2$. So, the decreasing of Δ according to Fig.4 makes the spectrum more dence as the increasing of z.

If we changed the boundary conditions and install an infinite potential wall at $\alpha = 0$, the bound states would be

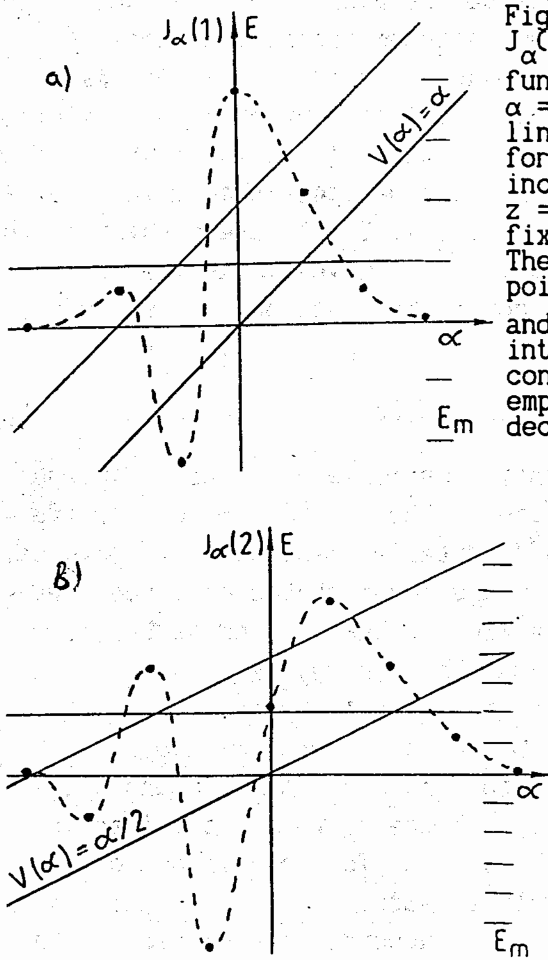
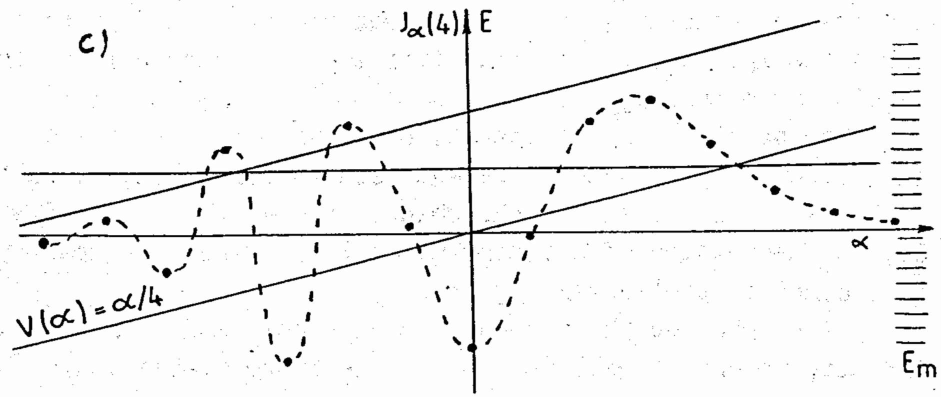


Fig. 4. Bessel functions $J_\alpha(z)$ as bound state wave functions on the lattice $\alpha = 0, \pm1, \pm2, \ldots$ with linear potential $V(\alpha) = \alpha/z$ for different values of inclination parameters z = 1 (a); 2 (b); 4(c) and fixed energy value E = 1. The exact sense have the point values of $J_\alpha(z)$ only and the dotted lines are introduced merely to connect these points. They emphasize the exponentially decreasing $J_\alpha(z)$ inside both the forbidden zones but with sighn oscillations in the upper one. For a less steep slope (b,c) the equidistant spectrum becomes more dense (see the ladders of the levels E_m in the right-hand side of Figs a,b,c). All bound state functions for the fixed potential are equivalent up to the shift of the co-ordinate α.



those J_α with the fractional α which are zero at $\alpha = 0$ (see [3]). But with increasing level number they become more and more close to our Bessel functions with iteger α.

All bound states J_α for fixed z are identical up to the α-shift (invariance for translations along the potential slope). Orthonormality condition and completeness relation coincide due to this fact (see Appendix):

$$\sum_{\alpha=-\infty}^{\alpha=+\infty} J_{\alpha+m}(z)\, J_\alpha(z) = \delta_{mo} \quad . \tag{5}$$

In the case of the continuous coordinate x the physically meaningful solutions of the Schroedinger equation are the Airy functions shown in Fig. 5.

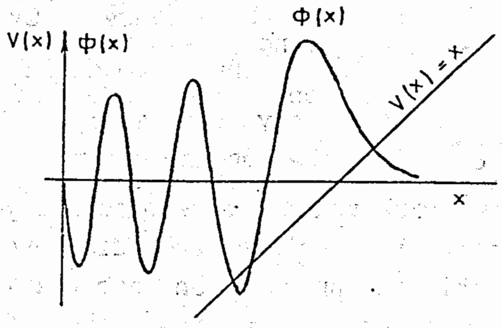


Fig. 5. Airy function - the solution of the Schroedinger equation (2) with the linear potential V(x) = x. Compare with its discrete analog J_α on Fig. 4 and Fig. 3. The Airy solution is not quadratically integrable and describes the wave which unlike J_α flies away down the potential hill.

The inverse problem approach [1] allows the transformation of spectra by shifting a finite number of levels and providing the corresponding perturbation $V(\alpha) \longrightarrow V(\alpha) + \Delta V(\alpha)$ of the potential and new eigenfunctions in the closed form (new exactly solvable models) expressed through $J_\alpha(z)$. In the case of the continuous coordinate x this was done by Calogero and Degasperis [5] and Grosse and Martin [6], see also [1].

The intuition which we get considering the exactly solved model of the Bessel eigenfunctions $J_\alpha(z)$ allows us to make qualitative predictions about the transformations of the linear potential required to change the initially equidistant spectrum. So, a gap in the sequence of levels can be produced by addition of a step potential

$$V(\alpha) = \begin{cases} 0 & \text{for } \alpha < 0 \\ V_0 & \text{for } \alpha \geq 0 \end{cases}$$

as is shown in Fig.6. To the vertical part of the potential

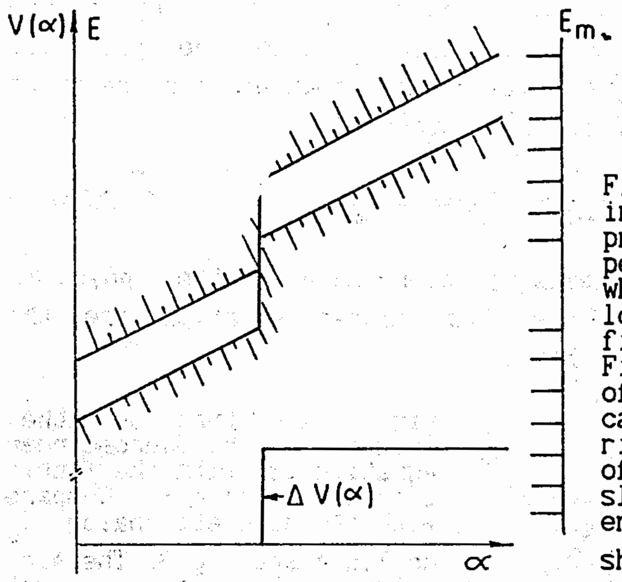


Fig.6. The energy gap in the level spectrum produced by the step perturbation $\Delta V(\alpha)$ which is shown in the lower part of the figure. According to Fig.4, the rarefying of the local spectrum can be caused by rising the steepness of the potential slope. The ladder of energy levels E_m is shown on the right.

shape (maximal steepness) there corresponds the zero density of levels. It is worth mentioning that unlike the discrete quantum mechanics it is impossible to produce an arbitrary gap in the spectrum by a local perturbation in the case of the ordinary Schroedinger equation with a continuous co-ordinate x.

The tightening of the levels in some region is caused by a beveled step potential

$$V(\alpha) = \begin{cases} 0 & \text{for } \alpha < 0 \\ \frac{\alpha}{Z} & \text{for } 0 \leq \alpha \leq N \\ -V_0 & \text{for } \alpha > N \end{cases}$$

as is shown in Fig.7.

So Figures 4,6 and 7 provide us with the intuition of spectrum structure for the arbitrary shape of the external field on the lattice. Numerical calculations confirm the predicted behaviour of the perturbed spectra as is

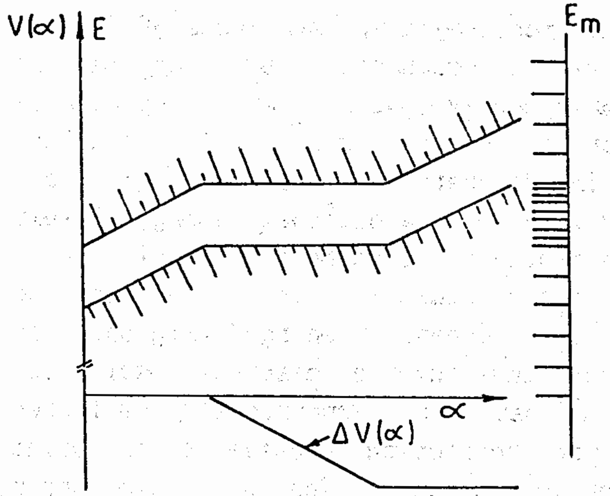


Fig.7. The local level condensation is caused by the perturbation $\Delta V(\alpha)$ producing the horizontal part of the allowed zone in accordance with Fig.4.

qualitatively shown in Figs 6 and 7. For example, it is evident that the spectrum of the discrete oscillator with the potential $V(n) = n^2$ on the half-axis ($n \geq 0$) is rarefied at

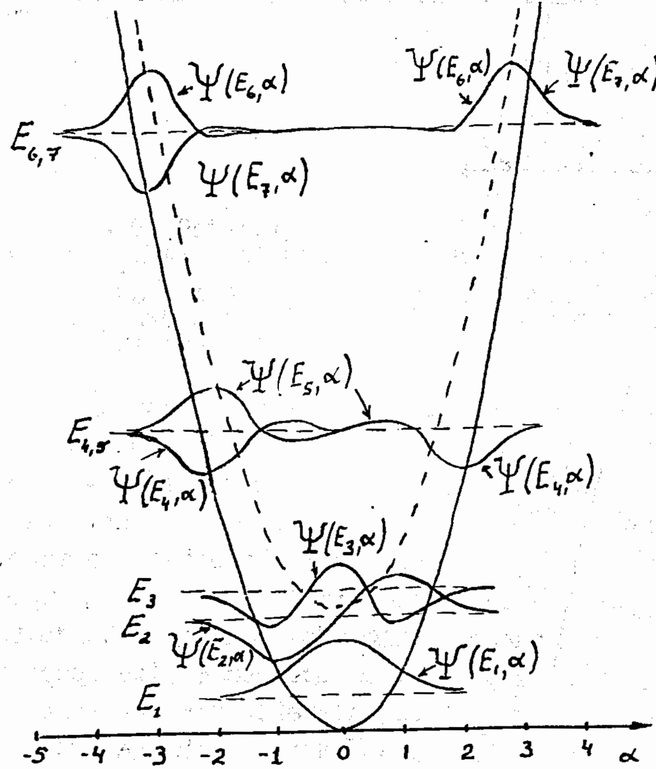


Fig.8a. The discrete oscillator has the upper forbidden zone inside the potential well (dashed line). The upper levels are almost degenerated.

high energies due to the increase in the steepness of V(n) at larger values of n unlike the equidistant spectrum in the continuous case. The upper energy levels E_m are proportional to $m^2 - 1$. This is almost as for the square well with the continuous co-ordinate. The discrete oscillator on the whole axis (n = 0, ± 1, ± 2,...) has additional energy levels corresponding to even eigenfunctions (symmetrical relative to the origin). These new levels become more and more near to ones of odd states with the increase in energy (Fig. 8a). It is also worth noting that the inverse discrete oscillator (Fig. 8b) with $V(n) = - n^2$ has the symmetrically reflected spectrum of the direct one (reflection relative to the point E = 1) unlike the continuous case. The unvisible upper boundary of the allowed zone is in this case outside the potential hill. The discrete oscillator spectrum is also changed if the middle point of the well is posed between the

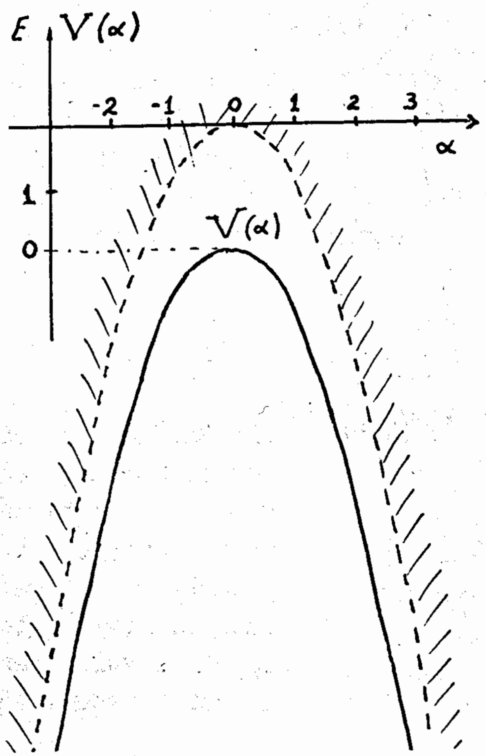


Fig. 8b. Inverted discrete oscillator. Its upper forbidden zone is outside the potential curve. Its spectrum is the reflection of one in the Fig. 8a with respect to the point E = 1.

discrete co-ordinate values. Another example of such a spectral symmetry is shown in Fig. 9 with discrete bound states above and under the continuous spectrum.

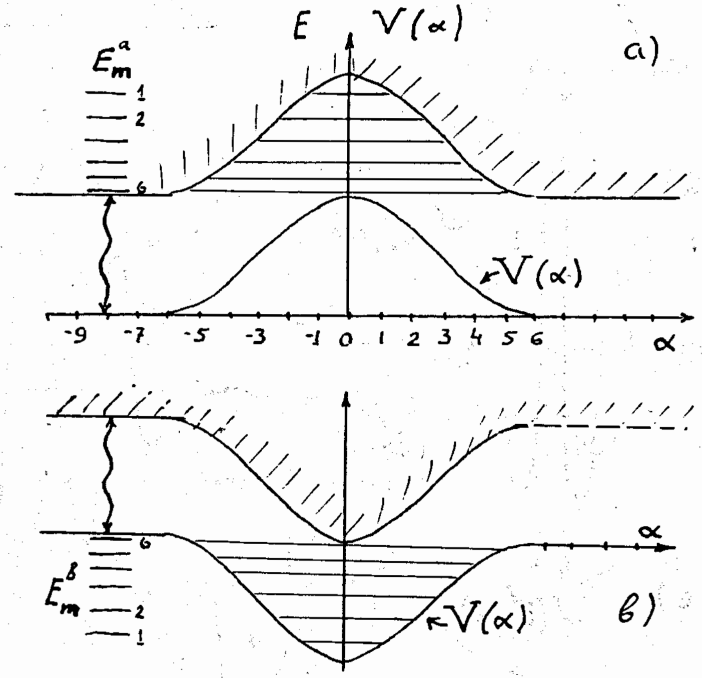


Fig. 9. Potential barrier (a) and well (b) with bound states E_m above (a) and under (b) the continuous spectrum. The upper boundaries of the allowed zones are shown with the dotted lines here. The wiggly lines denote the bands of the continuous spectra.

The wave functions corresponding to some bound states for potentials in Fig. 9 are shown in Fig. 10. Solid lines there are wave functions for E_1, E_2, E_6 (for bound states below the continuous spectra: a, b, c ; and for bound states above it: a', b', c').

The considered finite-difference model can also be the step to the better understanding of the corresponding multi-dimensional systems and the systems with the periodical plus additional potential (for exact solutions with the continuous variable for periodical plus linear potential see the paper [7]).

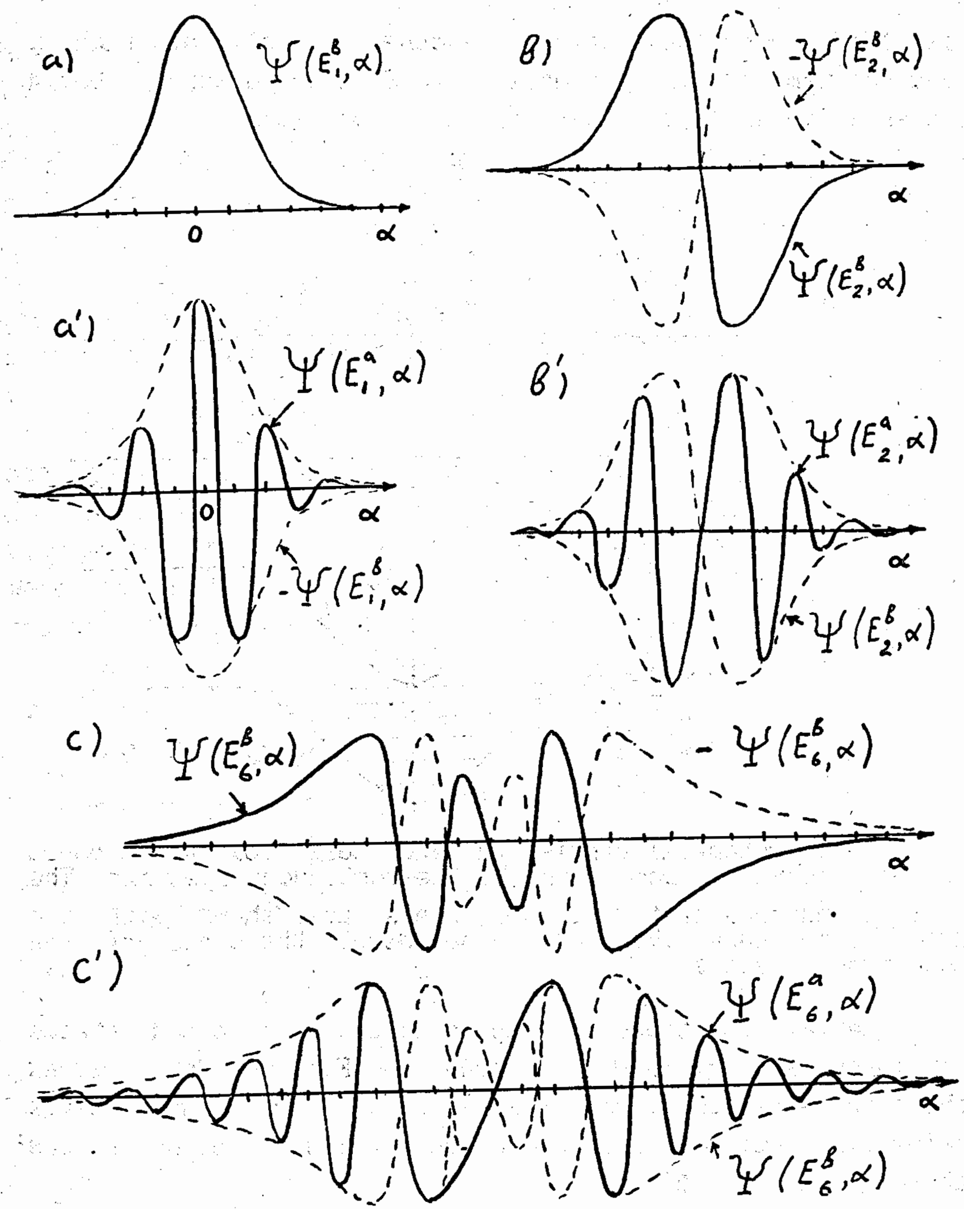


Fig. 10. Bound states under (a, b, c) and above (a′, b′, c′) the continuous spectrum for potentials shown in Figs. 9b, 9a, correspondingly. The symmetrical states (a and a′, b and b′, c and c′) are equal up to the sign. Dashed lines in b, c are $-\Psi$, and in a′, b′, c′ are $\pm\Psi$ from a, b, c. The lines are only connecting discrete values of $\Psi(E, \alpha)$.

CONCLUSION

The suggested model is a new one of the set of exactly solvable models [1] revealing the rules of spectral engineering: construction of quantum systems with the arbitrary allowed spectra.

The experience we get with the Bessel functions can be applied to the consideration of the interchannel motion [8]: motion over the discrete co-ordinate numbering of the coupled Schroedinger equations.

The authors are thankful to A.I.Shirokova for numerical calculations which allowed to make clear some significant details of the finite-difference solutions.

APPENDIX. COMPLETENESS AND ORTHONORMALITY OF $J_n(z)$.

At first, it is easy to check that both the orthogonality and completeness conditions

$$\sum_{\alpha=-\infty}^{\alpha=+\infty} \Psi_m(\alpha)\, \Psi_n(\alpha) = \delta_{nm} \; ; \quad \sum_{n=-\infty}^{n=+\infty} \Psi_n(\alpha)\, \Psi_n(\alpha') = \delta_{\alpha\alpha'} \qquad (6)$$

can be written in the same form (5):

$$\sum_{\alpha=-\infty}^{\alpha=+\infty} J_{\alpha+m}(z)\, J_\alpha(z) = \delta_{mo} \qquad (5)$$

Indeed changing $\Psi \longrightarrow J$ and the summation variables we get:

$$\sum_{\alpha=-\infty}^{\alpha=+\infty} J_{\alpha+m}\, J_{\alpha+n} = \delta_{nm} \longrightarrow \sum_{\alpha'=-\infty}^{\alpha'=+\infty} J_{\alpha'+m-n}\, J_{\alpha'} \longrightarrow \sum_{\alpha=-\infty}^{\alpha=+\infty} J_{\alpha'+p} J_{\alpha'} =$$

$= \delta_{po}$ which is the same as (5), and analogously

$$\sum_{n=-\infty}^{n=+\infty} J_{\alpha+n}\, J_{\alpha'+n} = \delta_{\alpha\alpha'} \longrightarrow \sum_{\beta=-\infty}^{\beta=+\infty} J_\beta\, J_{\beta+\alpha-\alpha'} \longrightarrow \sum_{\beta=-\infty}^{\beta=+\infty} J_\beta\, J_{\beta+p} = \delta_{po}.$$

Now let us derive the orthogonality condition. According to eq.(3) we have

$$J_{\alpha+m+1}(z) + J_{\alpha+m-1}(z) = \{2(\alpha + m)/z\}\, J_{\alpha+m}(z) \quad , \qquad (7)$$

$$J_{\alpha+n+1}(z) + J_{\alpha+n-1}(z) = \{2(\alpha + n)/z\} J_{\alpha+n}(z) \qquad (8)$$

Multiplying eq.(7) by $J_{\alpha+n}(z)$ and eq.(8) by $J_{\alpha+m}(z)$, and summing them over all α we get the same expressions in the rhs. Subtracting the resulting equations we get:

$$\{2(m - n)/z\} \sum_{\alpha=-\infty}^{\alpha=+\infty} J_{\alpha+n}(z)\, J_{\alpha+m}(z) = 0 \,. \qquad (9)$$

This implies for $m \neq n$ the orthogonality condition. From the well known integral representation

$$J_n(z) = \frac{1}{2\pi} \int_{-\pi}^{\pi} \exp(iz \sin\phi + in\phi)\, d\phi$$

we get the normalizing condition (using $\sum_n \exp(in\phi) = \delta(\phi)$):

$$\sum_{\alpha=-\infty}^{\alpha=+\infty} |J_n(z)|^2 = 1 \,.$$

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