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Point interactions with bound states: A zero-thickness limit of a double-layer heterostructure

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A heterostructure composed of two parallel homogeneous layers is studied in the limit as their width and the distance between them shrinks to zero simultaneously. The problem is considered in one dimension and the squeezing potential in the Schrödinger equation is chosen in the form of a piecewise constant function. As a result, two families of point interactions with bound state energy are realized from this structure. The specific feature of these interactions is the resonant-tunneling transmission of electrons through one-point singular potentials under certain conditions described by transcendental equations. The solutions to these equations define so-called resonance sets of Lebesgue's measure zero. A particular example is the potential in the form of the derivative of Dirac's delta function. For a whole family of point interactions including this example, the existence of a bound state is proven, contrary to the widespread opinion on the non-existence of bound states in δ'-like systems.

Keywords: one-dimensional quantum systems, point interactions, resonant tunneling, bound states.

1. Introduction

The Schrödinger operators with singular zero-range potentials attract a considerable interest beginning from the pioneering work of Berezin and Faddeev [1]. These operators describe "contact" or "point" interactions which are widely used in various applications to quantum physics [2,3]. Intuitively, these interactions are understood as sharply localized potentials, exhibiting a number of interesting and intriguing features. The point interaction models are quite useful because they admit exact closed analytic solutions providing relatively simple situations, where an appropriate way of squeezing to zero can be chosen to be in relevance with a real structure. Applications of these models to condensed matter physics are of particular interest nowadays, mainly because of the rapid progress in fabricating nanoscale quantum devices. Particularly, the electron transmission through heterostructures composed of parallel planar layers (e.g., ultrathin layered sheets) can be investigated in the zero-thickness limit approximation when their width shrinks to zero [4,5]. These structures are not only important in various applications, but their study involves a great deal of basic physics. The electron motion in these systems is confined in the longitudinal direction (say, along x axis), which is perpendicular to the planes, and is free in transverse directions. The three-dimensional stationary Schrödinger equation of such structure can be separated into longitudinal and transverse parts, resulting in the reduced one-dimensional equation for bound states

$$-\psi''(x)+V(x)\psi(x)=E\psi(x),\ \ E=-\kappa^2 \tag{1}$$

with respect to the longitudinal component of the wave function $\psi(x)$ and the electron energy E. Here $V(x)$ is a real-valued function defined on the line $-\infty<x<\infty$. The dimensions are chosen through the relation $\hbar^2/2m^*=1$ with m^* being an effective electron mass.

2. Potential for a double-layer structure and its parametrization

In this article, we focus on the investigation of the existence of bound states in the planar heterostructure composed of extremely thin layers separated by small distances in the limit as both the layer thickness and the distance between the layers simultaneously tend to zero. Here, we restrict ourselves to the particular case of the structure consisting of two layers with widths l_1 and l_2 separated by distance r. Then the potential part in Eq. (1) can be written as

$$V(x)=\begin{cases} V_1 \ \text{ for } \ 0<x<l_1, \\ V_2 \ \text{ for } \ l_1+r<x<l_1+l_2+r, \\ 0 \ \text{ for } -\infty<x<0,\ l_1<x<l_1+r, \\ \qquad l_1+l_2+r<x<\infty, \end{cases} \tag{2}$$

where $V_j(x)$, $j = 1, 2$, are constants. In order to realize a zero-thickness limit, we introduce the parametrization of this potential via a dimensionless squeezing parameter $\varepsilon \to 0$ as

$$V_j = \varepsilon^{-\nu} a_j, \quad a_j \in \mathbb{R}, \quad l_j = \varepsilon d_j, \quad j = 1, 2, \quad r = \varepsilon^{\tau} c. \quad (3)$$

In the following we denote the parametrized form of potential (2) by $V_\varepsilon(x)$ regarding its $\varepsilon \to 0$ limit.

3. Existence set for a distributional δ'-potential

In general, the shrinking limit of potential (2) cannot be defined properly in terms of distributions, but this is not a necessary condition for realizing point interactions from Eq. (1) with parametrization (3) as $\varepsilon \to 0$. However, one particular case should be singled out regarding the convergence of the potential $V_\varepsilon(x)$ to the derivative of Dirac's delta function $\delta(x)$.

Let us determine the set on the $\{\nu, \tau\}$-plane (see Fig. 1), where the limit $V_\varepsilon(x) \to \gamma\delta'(x)$ is well-defined in the sense of distributions. Thus, using (2) and (3) as well as the fast variable $\xi = x/\varepsilon$, for any function $\varphi(x) \in C_0^\infty$, under the condition $a_1 d_1 + a_2 d_2 = 0$, we compute

$$\langle V_\varepsilon(x) \,|\, \varphi(x) \rangle = \int_0^{l_1 + l_2 + r} V_\varepsilon(x)\varphi(x)dx =$$

$$= -a_1 d_1 \left[\varepsilon^{2-\nu}(d_1 + d_2)/2 + \varepsilon^{1-\nu+\tau} c \right] \varphi'(0) +$$

$$+ O(\varepsilon^{3-\nu}) + O(\varepsilon^{2-\nu+\tau}) + O(\varepsilon^{1-\nu+2\tau}). \quad (4)$$

It follows from this asymptotic representation that the distributional $\varepsilon \to 0$ limit $V_\varepsilon(x) \to \gamma\delta'(x)$ takes place on the three-dimensional plane

$$\Sigma_0 := \{a_1, d_1, a_2, d_2 \,|\, a_1 d_1 + a_2 d_2 = 0\} \quad (5)$$

in the $\{a_1, d_1, a_2, d_2\}$-space.

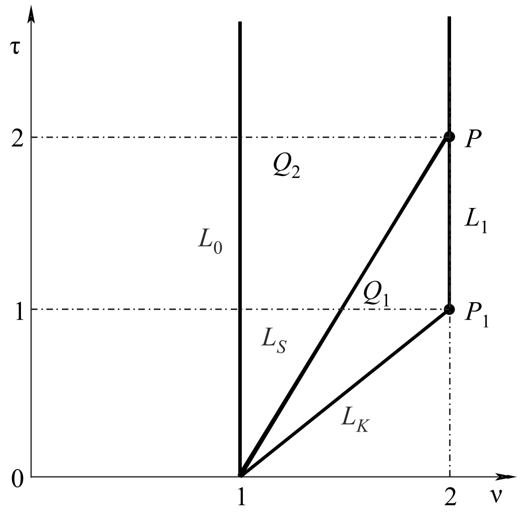

Fig. 1. Diagram of existence of distribution $\delta'(x)$ and point interactions with bound states. See text for details.

As illustrated by Fig. 1, on the $\{\nu, \tau\}$-plane, the support of the $\delta'(x)$ distribution is the line $L_{\delta'} := L_K \cup P_1 \cup L_1$ with $L_K := \{\nu, \tau \,|\, 1 < \nu < 2,\ \tau = \nu - 1\}$, $P_1 := \{\nu, \tau \,|\, \nu = 2,\ \tau = 1\}$ and $L_1 := \{\nu, \tau \,|\, \nu = 2,\ 1 < \tau < \infty\}$. The remainder of expansion (4) tends to zero as $\varepsilon \to 0$ because all the powers $3 - \nu$, $2 - \nu + \tau$ and $1 - \nu + 2\tau$ are positive on the $L_{\delta'}$-line. The strength (a dimensionless parameter) γ is the set function

$$\gamma = \frac{a_1 d_1}{2} \begin{cases} 2c & \text{on line } L_K, \\ 2c + d_1 + d_2 & \text{at point } P_1, \\ d_1 + d_2 & \text{on line } L_1. \end{cases} \quad (6)$$

4. Transmission matrix and its squeezed limit

The transmission matrix Λ of Eq. (1) for arbitrary regular potential $V(x)$ defined on the interval $x_1 < x < x_2$ connects the values of the wave function $\psi(x)$ and its derivative $\psi'(x)$ at the boundaries $x = x_1$ and $x = x_2$ through the matrix equation

$$\begin{pmatrix} \psi(x_2) \\ \psi'(x_2) \end{pmatrix} = \Lambda \begin{pmatrix} \psi(x_1) \\ \psi'(x_1) \end{pmatrix}, \quad \Lambda = \begin{pmatrix} \lambda_{11} & \lambda_{12} \\ \lambda_{21} & \lambda_{22} \end{pmatrix}. \quad (7)$$

The matrix elements λ_{ij} can be expressed in terms of the boundary values (given at x_1 and x_2) of linearly independent solutions to Eq. (1) [5]. Indeed, let $u(x)$ and $v(x)$ be linearly independent solutions of this equation. Then one can derive the following relations:

$$\lambda_{11} = W(x_1)^{-1}[u(x_2)v'(x_1) - u'(x_1)v(x_2)],$$

$$\lambda_{12} = W(x_1)^{-1}[u(x_1)v(x_2) - u(x_2)v(x_1)],$$

$$\lambda_{21} = W(x_1)^{-1}[u'(x_2)v'(x_1) - u'(x_1)v'(x_2)],$$

$$\lambda_{22} = W(x_1)^{-1}[u(x_1)v'(x_2) - u'(x_2)v(x_1)], \quad (8)$$

where $W(x)$ is the Wronskian:

$$W(x) = u(x)v'(x) - u'(x)v(x), \quad x_1 \le x \le x_2. \quad (9)$$

One can check from Eqs. (8) and (9) that the identity

$$\lambda_{11}\lambda_{22} - \lambda_{12}\lambda_{21} = 1 \quad (10)$$

holds true. There exists an infinite number of the linearly independent solutions $u(x)$ and $v(x)$. The representation of the Λ-matrix elements is essentially simplified if we choose these solutions obeying fixed initial conditions at $x = x_1$ or $x = x_2$. Thus, let the solutions $u(x)$ and $v(x)$ fulfill the initial conditions

$$u(x_1) = 1, \ u'(x_1) = 0, \ v(x_1) = 0, \ v'(x_1) = 1. \quad (11)$$

Inserting these values into Eqs. (8) and (9), one finds the following representation of the transmission matrix:

$$\Lambda = \begin{pmatrix} u(x_2) & v(x_2) \\ u'(x_2) & v'(x_2) \end{pmatrix}. \quad (12)$$

In a squeezed limit one can set $x_1 \to -0$ and $x_2 \to +0$, so that *one-point* interaction (if realized) connects the two-sided boundary conditions at $x = \pm 0$ by the limit (called now connection) Λ-matrix. For instance, the point interaction realized from Eq. (1) with the potential $V(x) = \alpha\delta(x)$ is specified by the connection matrix

$$\Lambda = \begin{pmatrix} 1 & 0 \\ \alpha & 1 \end{pmatrix}, \quad \begin{pmatrix} \psi(+0) \\ \psi'(+0) \end{pmatrix} = \Lambda \begin{pmatrix} \psi(-0) \\ \psi'(-0) \end{pmatrix}. \tag{13}$$

We call this point interaction as *distributional* δ*-potential.*

The transmission matrix of the double-layer structure defined by potential (2) is the product $\Lambda = \Lambda_2\Lambda_0\Lambda_1$, where Λ_j is the transmission matrix of the *j*th layer ($x_1 = 0$ and $x_2 = l_j$, $j = 1, 2$) and Λ_0 describes the transmission across the free space distance with $x_1 = 0$ and $x_2 = r$. Let $u_j(\kappa_j, x)$ and $v_j(\kappa_j, x)$ be a pair of linearly independent solutions of Eqs. (1)–(3), each restricted to the *j*th layer. Then, using the initial conditions of type (11) for each subsystems (layers and distance) with parametrization (3), according general matrix representation (12), we get (adding the subscript ε)

$$\Lambda_{j,\varepsilon} = \begin{pmatrix} u_j(\kappa_j, \varepsilon d_j) & v_j(\kappa_j, \varepsilon d_j) \\ u'_j(\kappa_j, \varepsilon d_j) & v'_j(\kappa_j, \varepsilon d_j) \end{pmatrix}, \quad j = 1, 2, \tag{14}$$

where

$$u_j(\kappa_j, x) = \cosh(\kappa_j x), \quad v_j(\kappa_j, x) = \kappa_j^{-1}\sinh(\kappa_j x) \tag{15}$$

with

$$\kappa_j := \sqrt{\kappa^2 + V_j} = \sqrt{\kappa^2 + a_j\varepsilon^{-\nu}}, \tag{16}$$

and

$$\Lambda_{0,\varepsilon} = \begin{pmatrix} \cosh(\kappa r) & \kappa^{-1}\sinh(\kappa r) \\ \kappa\sinh(\kappa r) & \cosh(\kappa r) \end{pmatrix}. \tag{17}$$

In the following, for simplicity of notations, we introduce the abbreviations

$$\bar{\lambda}_{ij,\varepsilon} := \lambda_{ij} / \cosh(\kappa_1 l_1)\cosh(\kappa_2 l_2)\cosh(\kappa r),$$

$$t_j := \tanh(\kappa_j l_j), \; i, j = 1, 2, \; t_0 := \tanh(\kappa r). \tag{18}$$

Then, the explicit representation of the matrix elements of the product $\Lambda_\varepsilon = \Lambda_{2,\varepsilon}\Lambda_{0,\varepsilon}\Lambda_{1,\varepsilon}$ reads

$$\bar{\lambda}_{11,\varepsilon} = 1 + (\kappa_1/\kappa_2)t_1t_2 + [(\kappa_1/\kappa)t_1 + (\kappa/\kappa_2)t_2]t_0, \tag{19}$$

$$\bar{\lambda}_{12,\varepsilon} = (1/\kappa_1)t_1 + (1/\kappa_2)t_2 + [1/\kappa + (\kappa/\kappa_1\kappa_2)t_1t_2]t_0, \tag{20}$$

$$\bar{\lambda}_{21,\varepsilon} = \kappa_1 t_1 + \kappa_2 t_2 + [\kappa + (\kappa_1\kappa_2/\kappa)t_1t_2]t_0, \tag{21}$$

$$\bar{\lambda}_{22,\varepsilon} = 1 + (\kappa_2/\kappa_1)t_1t_2 + [(\kappa/\kappa_1)t_1 + (\kappa_2/\kappa)t_2]t_0. \tag{22}$$

In the squeezed limit (as $\varepsilon \to 0$), under parametrization (3), for the parameters in Eqs. (19)–(22) one can write the following asymptotic expressions [see notations (16) and (18)]:

$$\kappa_j \sim \varepsilon^{-\nu/2}\sqrt{a_j}, \quad t_j \sim \tanh\left(\varepsilon^{1-\nu/2}\sqrt{a_j}\, d_j\right) \tag{23}$$

and $t_0 \sim kr \to 0$. Therefore $|\kappa_j| \to \infty$ as $\varepsilon \to 0$, while the arguments of the tanh-function must be finite because a_j's may be negative ($a_j \in \mathbb{R}$). As follows from asymptotic representation (23) in the limit as $\varepsilon \to 0$, we have $\lambda_{12,\varepsilon} \to 0$ and the diagonal elements $\lambda_{11,\varepsilon}$ and $\lambda_{22,\varepsilon}$ have finite limits if the distance *r* tends sufficiently fast to zero.

5. Resonance sets

The element $\lambda_{21,\varepsilon}$ as the most singular term in general diverges at $\varepsilon \to 0$. However, at certain values of the parameters a_1, d_1, a_2, d_2, a cancellation of divergences may occur resulting in finite limits $\lim_{\varepsilon\to 0}\lambda_{21,\varepsilon} =: \alpha \in \mathbb{R}$.

There are two ways of performing such a cancellation procedure [6]. One of the ways is to equate the total expression for $\lambda_{21,\varepsilon}$ in (21) to zero, resulting in the following constraints on the parameters a_1, d_1, a_2, d_2:

$$\frac{1}{a_1 d_1} + \frac{1}{a_2 d_2} + c = 0 \tag{24}$$

on the line L_K and

$$\frac{\coth(\sqrt{a_1}\, d_1)}{\sqrt{a_1}} + \frac{\coth(\sqrt{a_2}\, d_2)}{\sqrt{a_2}} + c = 0 \tag{25}$$

at the point P_1 (see Fig. 1). The solutions to both these equations form the so-called resonance sets in the $\{a_1, d_1, a_2, d_2\}$-space. Moving along the line L_K and approaching the point P_1 a splitting effect takes place describing the abrupt appearance of a countable set of hypersurfaces [6] which are solutions of transcendental equation (25). This family of point interactions is realized without bound states ($\alpha = 0$).

The point interactions with bound states (when $\alpha \neq 0$) can be realized if we equate to zero only the first two terms in expression (21) when it is possible that $\lim_{\varepsilon\to 0}\lambda_{21,\varepsilon} \neq 0$. In this case, we get the equations

$$a_1 d_1 + a_2 d_2 = 0 \tag{26}$$

on the line $L_S := \{\nu, \tau \mid 1 < \nu < 2, \; \tau = 2(\nu - 1)\}$ and

$$\sqrt{a_1}\tanh(\sqrt{a_1}\, d_1) + \sqrt{a_2}\tanh(\sqrt{a_2}\, d_2) = 0 \tag{27}$$

at the point $P_2 := \{\nu, \tau \mid \nu = \tau = 2\}$ (see Fig. 1), the solutions of which form the resonance sets Σ_0 and

$$\Sigma'_0 := \{a_1, d_1, a_2, d_2 \mid \sum_{j=1,2}\sqrt{a_j}\tanh(\sqrt{a_j}\, d_j) = 0\}. \tag{28}$$

In fact, Eqs. (26) and (27) coincide with Eqs. (24) and (25) where formally one can put $c = 0$ though indeed $c \neq 0$. Note that the set Σ_0 serves also as a condition for the exist-

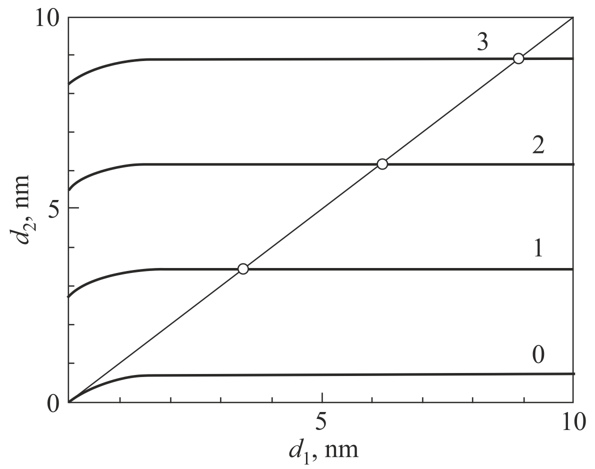

Fig. 2. The $\{d_1, d_2\}$-plane section of four (n = 0, 1, 2, 3) three-dimensional hypersurfaces being solutions to Eq. (28) with intensities $a_1 = -a_2 =: a = 0.5$ eV. The points of intersection of the bisector $d_1 = d_2$ with the curves $d_2 = d_2(d_1)$ correspond to the resonance set for the distributional δ'-potential. Here, $m^* = 0.1 m_e$ (m_e is an electron mass), so that 1 eV = 2.62464 nm^{-2}.

ence of the distribution $\delta'(x)$ [see Eq. (5)]. Similarly, moving along the L_S-line and approaching the P_2-point, we also encounter with splitting the set Σ_0 into the infinite series of hypersurfaces forming the resonance set Σ'_0. The first four curves numbered by n = 0, 1, 2, 3 are shown in Fig. 2 as a section in the $\{d_1, d_2\}$-plane, where the intensities $a_1 > 0$ (barrier) and $a_2 < 0$ (well) are fixed constant. As illustrated by this figure, there are periodic forbidden zones in the well depth d_2, while the barrier height is arbitrary.

6. Generalized δ- and δ'-potentials with bound states

All the point interactions realized in the limit as $\varepsilon \to 0$ on the $\{\nu, \tau\}$-plane (Fig. 1) have been listed in [6]. Within this family, the interactions with bound states can appear only on the resonance sets Σ_0 and Σ'_0 defined by the solutions of Eqs. (26) and (27). However, this happens if and only if the divergence of the product $\kappa_1\kappa_2$ in Eq. (21) is suppressed by an appropriate shrinking of the distance r, resulting in the appearance of a non-zero strength constant α. Therefore the separation of the layers by a non-zero distance r is the necessary condition for the existence of bound states. Under parametrization (3), a certain family of the interactions for which $\alpha \neq 0$ will be specified below for three cases: $\nu = 1$, $1 < \nu < 2$ and $\nu = 2$.

(i) $1 \le \nu < 2$: On this interval, in the limit as $\varepsilon \to 0$, using expressions (23) in Eqs. (19), (21) and (22), one finds the asymptotic representation of the Λ_ε-matrix elements as follows:

$$\lambda_{11,\varepsilon} \sim 1 + \varepsilon^{1-\nu+\tau} a_1 d_1 c, \quad \lambda_{22,\varepsilon} \sim 1 + \varepsilon^{1-\nu+\tau} a_2 d_2 c,$$

$$\lambda_{21,\varepsilon} \sim \varepsilon^{1-\nu}(a_1 d_1 + a_2 d_2) + \varepsilon^{2(1-\nu)+\tau} a_1 d_1 a_2 d_2 c. \quad (29)$$

It follows from these asymptotic expressions that in the limit as $\varepsilon \to 0$, the connection matrix $\Lambda = \lim_{\varepsilon\to 0} \Lambda_\varepsilon$ is of form (13) that corresponds to the δ-potential. Here, on the line $L_0 := \{\nu, \tau \,|\, \nu = 1,\ 0 < \tau < \infty\}$ (see Fig. 1), the total strength α is the algebraic sum of the layer strengths $\alpha_j := a_j d_j$, $j = 1, 2$, i.e., $\alpha = \alpha_1 + \alpha_2$ where a_1, d_1, a_2, d_2 are arbitrary parameters. Contrary, on the L_S-line, shown in Fig. 1, the total strength α is non-zero and finite only under the constraint $a_1 d_1 + a_2 d_2 = 0$, i.e., on set (5) which can be referred to as the resonance set for tunneling through the δ-potential. In particular, if $a_1 = -a_2$, this is a bisector shown in Fig. 2. Thus, on the resonance set Σ_0 being a plane in the $\{a_1, d_1, a_2, d_2\}$-space, we have

$$\lim_{\varepsilon\to 0} \lambda_{11,\varepsilon} = \lim_{\varepsilon\to 0} \lambda_{22,\varepsilon} = 1,$$

$$\lim_{\varepsilon\to 0} \lambda_{21,\varepsilon} =: \alpha = -(a_1 d_1)^2 c = -(a_2 d_2)^2 c. \quad (30)$$

In spite of the δ-like connection matrix (13), potential (2) with parametrization (3) does not converge at $\varepsilon \to 0$ to the distribution $\delta(x)$. Therefore the whole family of point interactions specified by the connection matrices of form (13) can be referred to as *generalized* δ*-potentials* which "cover" the subfamily of distributional δ-potentials. As illustrated by Fig. 1, the line L_S is a transient set that separates the interactions with full reflection (below line, region Q_1), except for the line L_K (where $\alpha = 0$), and fully transmitted interactions (above line, region Q_2) for which the Λ-matrix is the identity I. The similar definition of the δ-potential has been given by Šeba in [7], a point separating the half-axes with full reflection and perfect transmission was considered instead of the line L_S.

(ii) $\nu = 2$: This case corresponds to the point P_2 in Fig. 1 and the resonance set Σ'_0 defined by Eq. (28). This transcendental equation admits a countable number of solutions if at least one of the layer potentials has a well profile. There are no solutions if both the layers are barriers. The surface with $n = 0$ passes through the origin $a_1 = a_2 = d_1 = d_2 = 0$. The limit Λ-matrix elements defined on Σ'_0 are found from the asymptotic representation given by Eqs. (19) and (21)–(23). Setting $\lim_{\varepsilon\to 0} \lambda_{11,\varepsilon} =: \{\theta_n\}_{n=0}^{\infty}$ and $\lim_{\varepsilon\to 0} \lambda_{21,\varepsilon} =: \{\alpha_n\}_{n=0}^{\infty}$, at the point P_2, one finds

$$\theta_n = \frac{\cosh(\sqrt{a_1}\, d_1)}{\cosh(\sqrt{a_2}\, d_2)} = -\frac{\sqrt{a_1}\sinh(\sqrt{a_1}\, d_1)}{\sqrt{a_2}\sinh(\sqrt{a_2}\, d_2)}, \quad (31)$$

$$\alpha_n = c\sqrt{a_1}\sinh(\sqrt{a_1}\, d_1)\sqrt{a_2}\sinh(\sqrt{a_2}\, d_2). \quad (32)$$

Thus, the connection matrix defined on the resonance set Σ'_0 is the sequence of matrices, i.e.,

$$\Lambda = \{\Lambda_n\}_{n=0}^{\infty}, \quad \Lambda_n = \begin{pmatrix} \theta_n & 0 \\ \alpha_n & \theta_n^{-1} \end{pmatrix}. \quad (33)$$

The particular case of potential (2) with $r=0$ [8] has rigorously been treated by Golovaty with coworkers [9] for the whole family of regular functions $V_\varepsilon(x)$ that converge to $\delta'(x)$ in the sense of distributions as $\varepsilon\to 0$. For this family there are no bound states ($\lim_{\varepsilon\to 0}\lambda_{21}=0$) and the corresponding point interactions were suggested in [10] to be referred to as δ'-potentials. Here, we call all the point interactions which in general are realized with the connection matrix Λ of form (15), even if potential $V_\varepsilon(x)$ has no limit itself, generalized δ'-potentials. Then the point interactions realized from the potentials $V_\varepsilon(x)$ having the distribution $\delta'(x)$ in the limit as $\varepsilon\to 0$, appear to be a subfamily of generalized δ'-potentials.

The equation for the bound states with negative energy $E=-\kappa^2$ can be expressed via the elements of the transmission matrix for an arbitrary regular potential $V_\varepsilon(x)$ in Eq. (1) defined on a finite interval $x_1<x<x_2$ [11]. Indeed, the negative-energy solutions outside this interval are of the form

$$\psi(x)=\begin{cases} C_1 e^{\kappa x} & \text{for } -\infty<x<x_1,\\ C_2 e^{-\kappa x} & \text{for } \; x_2<x<\infty, \end{cases} \tag{34}$$

where C_1 and C_2 are arbitrary constants and $\kappa>0$. Inserting these expressions into matrix equation (7), we find the following compatibility equation:

$$\kappa\lambda_{12,\varepsilon}+\lambda_{11,\varepsilon}+\lambda_{22,\varepsilon}+\kappa^{-1}\lambda_{21,\varepsilon}=0,\quad \kappa>0, \tag{35}$$

where in general the Λ-matrix elements depend on κ [see Eqs. (19)–(23)]. However, in a squeezed limit, since $|V_j|\to\infty$, the κ-dependence in the elements of the Λ_ε-matrix vanishes because of asymptotic behavior (23) in the limit as $\varepsilon\to 0$. Consequently, using that $\lambda_{12,\varepsilon}\to 0$, the nontrivial bound state $\kappa>0$ becomes single-valued being defined only on one of the surfaces of the resonance set Σ'_0. In other words, on each nth surface of the Σ'_0-set defined by Eq. (28), the corresponding point interaction has only one bound state given by

$$\kappa_n=-\frac{\alpha_n}{\theta_n+\theta_n^{-1}},\quad n=0,1,\ldots, \tag{36}$$

with θ_n and α_n computed from Eqs. (31) and (32). Each κ_n is positive because $\alpha_n\theta_n<0$.

7. Persistence of a bound state

In general, for any potential (2) with finite fixed values V_1 and V_2, there exist several bound states if one of the wells is sufficiently deep. However, as derived above [see, e.g., Eq. (36)], in the squeezed limit only a single bound state is shown to exist. For instance, there is the conventional opinion that during shrinking a regular potential to the distribution $\delta'(x)$, all the bound states fall to $-\infty$, so that the δ'-potential has no bound state energies at all. However, this contradicts to the result given by Eq. (36) that indicates that one of these states survives under squeezing to one point. In order to resolve this puzzle, it is reasonable to control the behavior of bound states while shrinking potential (2) to a δ'-like profile. To this end, let us consider the function

$$\mathcal{F}_\varepsilon(\kappa):=\frac{\kappa\lambda_{12,\varepsilon}+\lambda_{11,\varepsilon}+\lambda_{22,\varepsilon}+\kappa^{-1}\lambda_{21,\varepsilon}}{\cosh(\kappa_1 l_1)\cosh(\kappa_2 l_2)\cosh(\kappa r)}, \tag{37}$$

so that the zeroes of this function correspond to the roots of Eq. (35). Explicitly, due to Eqs. (18)–(22), we have

$$\mathcal{F}_\varepsilon(\kappa)=\left[2+\left(\frac{\kappa}{\kappa_1}+\frac{\kappa_1}{\kappa}\right)t_1+\left(\frac{\kappa}{\kappa_2}+\frac{\kappa_2}{\kappa}\right)t_2\right](1+t_0)+ +\left[\frac{\kappa_1}{\kappa_2}+\frac{\kappa_2}{\kappa_1}+\left(\frac{\kappa^2}{\kappa_1\kappa_2}+\frac{\kappa_1\kappa_2}{\kappa^2}\right)t_0\right]t_1t_2. \tag{38}$$

Clearly, $\mathcal{F}_\varepsilon(\kappa)>0$ if both V_j's are positive and therefore no bound states exist. The same is true if one of V_j's or both ones are negative, but satisfy the inequalities $\kappa^2>|V_j|$, $j=1,2$. Without loss of generality, it is sufficient to analyze the case $V_2\le V_1$ ($V_2<0$). Then we have $t_2=i\tan(\sqrt{|V_2|-\kappa^2}\,l_2)$ and the presence of this factor in (38) leads to the existence of a finite number (say, p_0) of zeroes $\bar\kappa_{p,\varepsilon}$, $p=0,1,\ldots,p_0-1$ because the argument $\sqrt{|V_2|-\kappa^2}\,l_2$ as a function of ε is uniformly bounded from above. In the limit as $\varepsilon\to 0$, the escape of this finite number of zeroes to infinity follows from the inequalities

$$\frac{1}{\varepsilon}\sqrt{|a_2|-\left[\frac{(p+1)\pi}{d_2}\right]^2}<\bar\kappa_{p,\varepsilon}<\frac{1}{\varepsilon}\sqrt{|a_2|-\left(\frac{p\pi}{d_2}\right)^2} \tag{39}$$

valid for all $p=0,1,\ldots p_0$. On the other hand, since $|\kappa_j|\to\infty$ and $r\to 0$ as $\varepsilon\to 0$, the asymptotic representation of function (38) reduces to

$$\mathcal{F}_\varepsilon\sim 2+\frac{\kappa_1 t_1+\kappa_2 t_2}{\kappa}+\left(\frac{\kappa_1\kappa_2 r}{\kappa}+\frac{\kappa_1}{\kappa_2}+\frac{\kappa_2}{\kappa_1}\right)t_1t_2. \tag{40}$$

Here, the term $\kappa_1 t_1+\kappa_2 t_2$ in general diverges at $\varepsilon\to 0$ and in this case all the zeroes are moving to infinity. Equating this term to zero, one gets in the limit as $\varepsilon\to 0$ the resonance set Σ'_0 defined by Eq. (28). Next, because of (3), we have

$$\kappa_1 t_1\kappa_2 t_2 r\sim-\varepsilon^{\tau-\nu}a_1 c\tanh^2(\varepsilon^{1-\nu/2}\sqrt{a_1}\,d_1). \tag{41}$$

This term is finite on the set $L_S\cup P_2$ (see Fig. 1). According to Eqs. (30) and (35), on the line L_S, in the limit as $\varepsilon\to 0$ only one bound state level "survives", while the rest of levels tend to the accumulation point $\kappa=0$. Similarly to the conventional δ-potential, the bound energy level is

$$\kappa = \frac{1}{2}(a_1 d_1)^2 c = \frac{1}{2}(a_2 d_2)^2 c, \qquad (42)$$

valid only on plane (5). At the point P_2, we are dealing with the situation when all the zeroes of the function $\mathcal{F}_\varepsilon(\kappa)$ escape to $-\infty$ as $\varepsilon \to 0$, except for a one zero being located on one of the surfaces of the resonance set Σ_0'. Equating asymptotic expression (40) to zero and using (41) at the point P_2, we obtain the bound state value

$$\kappa_n = \frac{c a_1 a_2}{2 a_2 \coth^2(\sqrt{a_1}\, d_1) - a_1 - a_2}, \qquad (43)$$

valid on the nth surface of the resonance set Σ_0'. This expression coincides on Σ_0' with formula (36) where θ_n and α_n are given by Eqs. (31) and (32). Note that expression (43) does not depend on the parameter d_2, which was excluded because of the consideration on the set Σ_0'. On the other hand, on the set Σ_0', instead of formula (43), one can write a symmetric analogue

$$\kappa_n = \frac{c a_1 a_2}{2 a_1 \coth^2(\sqrt{a_2}\, d_2) - a_1 - a_2}, \qquad (44)$$

which now does not depend on the parameter d_1. Finally, one should emphasized that beyond the resonance sets Σ_0 and Σ_0', the point interactions with bound states do not exist at all. For these parameter values the system is opaque and the wave function satisfies at $x = \pm 0$ the boundary conditions of the Dirichlet type: $\psi(\pm 0) = 0$.

The scenario of escaping the bound energy levels to infinity (except for one level) is illustrated in Fig. 3 for a distributional δ'-potential. This point interaction is realized

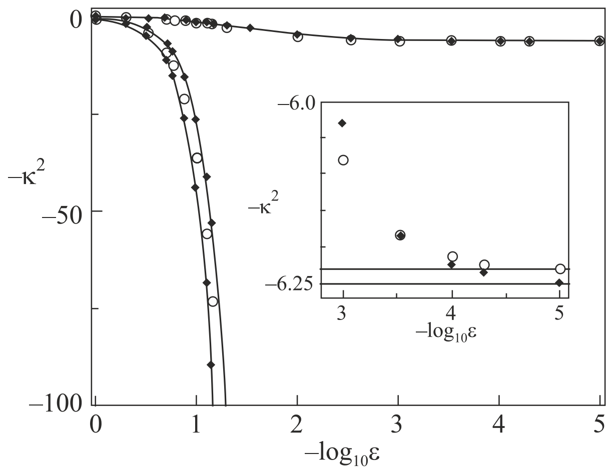

Fig. 3. Dependence of the bound state energy $E = -\kappa^2$ on the squeezing parameter ε for $\nu = \tau = 2$, $a_1 = -a_2 = 0.5$ eV and $c = 10$ nm. The ○ (◆) markers correspond to the first (second) subset of resonance set Σ_0' [see Eq. (28)] with $d_1 = d_2 =$ 5.6 (10) nm. The inset shows the asymptotic behavior of energy E as $\varepsilon \to 0$. Solid straight lines correspond to the exact values of E according to Eq. (36).

at the point P_2 lying on the line $L_{\delta'}$. The data with $a_1 = -a_2$ and $d_1 = d_2 =: d$ immediately provide its location on the $L_{\delta'}$-line. Next, for the existence of a bound energy level as $\varepsilon \to 0$, these data must satisfy Eq. (28). Therefore the resonance set for the distributional δ'-potential is $\Sigma_0' \cap \Sigma_0$.

Then, for this potential $\kappa_0 = 0$ and for the numerical calculations presented in Fig. 3, we use the first two nontrivial values of d ($d = 5.6, 10$ nm) that correspond to the subsets of Σ_0' with $n = 1$ and $n = 2$. As shown in Fig. 3, for the data with $n = 1$, there are two zeroes of $\mathcal{F}_\varepsilon(\kappa)$, where $\bar{\kappa}_{1,\varepsilon} \to \kappa_1$ and $\bar{\kappa}_{2,\varepsilon}$ diverges at $\varepsilon \to 0$. For the data with $n = 2$, there are three zeroes, where $\bar{\kappa}_{1,\varepsilon} \to \kappa_2$, while $\bar{\kappa}_{2,\varepsilon}$ and $\bar{\kappa}_{3,\varepsilon}$ diverge.

8. Concluding remarks

There exists an ubiquitous opinion that the bound state energy levels for Schrödinger equation (1) with a regularized potential $V_\varepsilon(x)$ escape to $-\infty$ as $V_\varepsilon(x) \to \gamma\delta'(x)$ in the sense of distributions (γ is a strength constant). However, in general this is not true, except for the point interactions with an additional δ-like potential [12], when $V(x) = \alpha\delta(x) + \gamma\delta'(x)$. On the basis of both the analytic arguments and the numerical computations, we prove that for the family of δ'-regularized potentials, a single bound energy level converges to a finite value, whereas the rest of energy levels escapes to $-\infty$. This is also true for the two families of point interactions, called in this article generalized δ- and δ'-potentials, that cover their distributional analogues. These interactions are realized asymptotically as a one-point approximation of double-layer heterostructures, when the thickness of layers and the distance between them squeeze simultaneously to one point. The separated distance between the layers plays a crucial role in the existence of bound states for the families of generalized δ- and δ'-potentials as defined in the present paper.

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Точкові взаємодії зі зв'язаними станами: наближення нульової товщини для двошарової гетероструктури

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Гетероструктура, що складається з двох паралельних шарів, досліджується в наближенні, коли товщина шарів та відстань між ними зменшуються до нуля. Проблема вивчається в одновимірному випадку, потенціал у рівнянні Шредінґера обрано у вигляді кусково-сталої функції. Для такої структури отримано два сімейства точкових взаємодій зі зв'язаними станами. Специфічною характерною рисою цих взаємодій є резонансно-тунельне проходження електронів через точковий сингулярний потенціал за певних умов, що задаються трансцендентними рівняннями. Рішення цих рівнянь визначають так звані резонансні множини нульової міри Лебега. Конкретним прикладом є потенціал у вигляді похідної від дельта-функції Дірака. Для всього сімейства точкових взаємодій, включаючи і цей приклад, доведено існування зв'язаних станів всупереч поширеній думці про неіснування зв'язаних станів у δ'-подібних системах.

Ключові слова: одновимірні квантові системи, точкові взаємодії, резонансне тунелювання, зв'язані стани.