Theoretical Physics.
Quantum Mechanics

UDC 517.938 https://www.doi.org/10.33910/2687-153X-2022-3-1-37-42

Bound states for two delta potentials supported on parallel lines on the plane

A. S. Bagmutov[1], I. Y. Popov✉[1]

[1] ITMO University, 49 Kronverkskii Ave., Saint Petersburg 197101, Russia

Authors

Alexander S. Bagmutov, e-mail: Bagmutov94@mail.ru

Igor Y. Popov, ORCID: 0000-0002-5251-5327, e-mail: popov1955@gmail.com

For citation: Bagmutov, A. S., Popov, I. Y. (2022) Bound states for two delta potentials supported on parallel lines on the plane. *Physics of Complex Systems*, 3 (1), 37–42. https://www.doi.org/10.33910/2687-153X-2022-3-1-37-42

Received 21 November 2021; reviewed 10 January 2022; accepted 12 January 2022.

Funding: The research was supported by the Russian Foundation for Basic Research (Grant No. 20-31-90050).

Abstract. We consider a singular δ-potential supported on two parallel lines in R^2 as a model of two interacting macromolecules. The intensity of the potential is constant, but each line contains a finite segment with a variation. Using variational approach, we study continuous and discrete spectra and estimate the gap between the eigenvalue and the continuous spectrum as a function of shift between the line segments. The existence of bound states for the system is proven by test function with separated variables.

Keywords: spectrum, variational approach, potential supported on line.

Introduction

A great deal of recent research has focused on potentials supported on line in R^3 or R^2. Apart from the mathematical interest, the problem attracts researches due to its physical application as a potential can be considered a model of a long molecule. There is a series of works exploring the potentials supported on sets of zero measure (see, e. g.: Behrndt, Frank et al. 2017; Brasche, Teta 1992; Brasche et al. 1994; Exner, Ichinose 2001; Exner, Jex 2013; Exner, Kondej 2002; 2004; 2005; 2015; Exner, Pankrashkin 2014; Exner, Vugalter 2016; Exner, Yoshitomi 2002; Posilicano 2001; 2004). The background of the model is the theory of self-adjoint extensions of symmetric operators. An analogous model was also developed for narrow slits in the surfaces (Popov 1992a; 1993) and for potentials supported on hypersurfaces (Behrndt et al. 2016; 2017a; Exner et al. 2018). In the present paper we deal with 2D strip which boundaries are formed by potentials supported on lines. These potentials look like semitransparent boundaries (see, e. g., Bagmutov, Popov 2020; Popov 1992b; Vorobiev et al. 2020). The potentials are assumed to be negative (i. e., attractive, having a local perturbation and identical at each side of the strip but having some shift along the strip at one line in respect to the second line (Fig. 1). We prove the existence of eigenvalue caused by the local perturbation of the potentials and look after its behaviour if the shift of the perturbation changes.

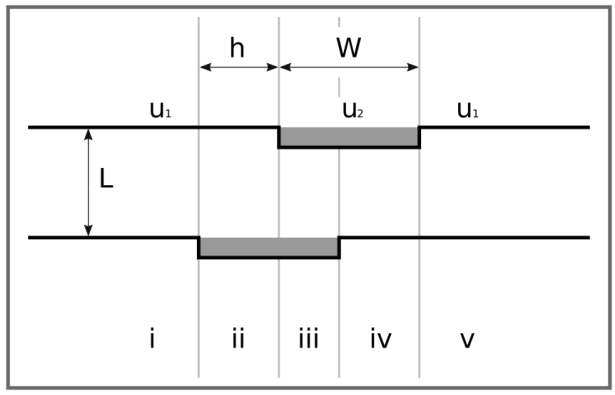

Fig. 1. System of two parallel lines with delta-potentials of varying intensity on them

The result has a biophysical character. It is related to molecule coupling, e. g., viruses coupling with cells or coupling of two DNA chains. Roughly speaking, the process looks as follows. One molecule recognises some label at the second molecule, keeps close to this position and forms a bond. In our simple model, molecules are represented by lines with potentials, a "label" is a perturbation of the potentials. A reasonable question begs itself: which factors can assist molecules to keep a small distance in proper position? If one considers electron in this system of two attractive potentials, there is a bound state due to its local perturbations. This state assists to keep molecules close. In real system this state can be destroyed by external perturbations (e. g., thermal vibration). The state is more stable if there is sufficient gap between the eigenvalue and the lower bound of the continuous spectrum. In our model, we show that an increase in the shift leads to a decrease in the gap, i. e., the most stable position is in the case of the shift absence. It means that the electron bound state is a factor assisting molecules to be in proper position.

Let us consider a system shown in Fig. 1. It consists of two infinitely-stretching parallel lines at a distance L, on a 2D plane. Attractive delta-potential of a constant intensity $-u_1 < 0$ is located along the lines, except for a region of finite width W on each line, where intensity changes to $-u_2$, such as $-u_2 < -u_1$. Let us denote by $h < W$ a distance to which a region W on one line is shifted relative to the second line. We use the atomic system of units in which one has $m = 0.5$, $\hbar = 1$. Correspondingly, the Hamiltonian of the system is the Laplacian $H\hat{\psi} = -\Delta\psi$, with the domain consisting of continuous functions $\psi \in L^2(R)$ that satisfy the following conditions on the lines:

$$\frac{\partial\psi}{\partial y}\left(x, y_l + 0\right) - \frac{\partial\psi}{\partial y}\left(x, y_l - 0\right) = -\alpha_x \psi\left(x, y_l\right) \tag{1}$$

where $y_l = 0$ or L, and $\alpha_x = u_2$ is inside the perturbed region of the line W and $\alpha_x = u_1$, outside.

Continuous spectrum

Let us consider the continuous spectrum of the operator. As the system is a local perturbation of the corresponding one with two constant potentials $-\alpha = -u_1$ supported on two parallel lines, the continuous spectrum is the same as without this perturbation. In case of two parallel lines ($y = 0$, $y = L$) with constant potentials, separation of variables can be made, i. e, one can consider the wave function in the form $\psi(x,y) = \chi(x)\,\zeta(y)$. Correspondingly, the lower bound of the continuous spectrum for the Laplacian $\hat{H}$ with conditions (1) on the lines is given by the lowest eigenvalue for the transversal problem (for function $\zeta(y)$). To find it, we consider the operator $-\frac{d^2}{dy^2}$ on R with the following conditions at two points:

 https://www.doi.org/10.33910/2687-153X-2022-3-1-37-42

$$\begin{aligned}
\zeta(+0) &= \zeta(-0), \\
\zeta(L+0) &= \zeta(L-0), \\
\frac{d\zeta}{dy}(+0) - \frac{d\zeta}{dy}(-0) &= -\alpha\zeta(-0), \\
\frac{d\zeta}{dy}(L+0) - \frac{d\zeta}{dy}(L-0) &= -\alpha\zeta(L-0),
\end{aligned} \tag{2}$$

Theorem 1. *The lower bound of the continuous spectrum of the operator $\hat{H}$ is $-max_j\ \kappa_j^2$, where κ_j are real roots of the spectral equation:*

$$\frac{4}{\alpha^2}\kappa(\kappa + L) = e^{2\kappa L} - 1 \tag{3}$$

Proof. Differential equation for transversal eigenfunction $\zeta(y)$ of $-\frac{d^2}{dy^2}$ corresponding to eigenvalue k^2 at each part of is as follows: $-\frac{d^2\zeta}{dy^2} = k^2\zeta$. Taking its solutions $e^{\pm iky}$ and satisfying conditions (2), one obtains (3), where $\kappa = ik \in R_-$.

To have an eigenvalue, one needs a decay at infinity, i. e., $\kappa < 0$. Keeping in mind that the function in the left-hand side of (3) takes minimal value -1 at $\kappa = -\frac{\alpha}{2}$, one concludes that there is a root κ_1 of (3), $-\alpha < \kappa_1 < -\frac{\alpha}{2}$.

Remark. It is known that in the case of a single line, the lower bound of the continuous spectrum is $-\frac{\alpha^2}{4}$. In case of two lines with conditions (2), the limit of the threshold determined by (3) tends to $-\alpha_2$ when $L \to 0$. It corresponds to potential -2α at single line. Hence, for conditions (2), one has a summation of the two-line potentials.

Test functions

To find the discrete spectrum, we use a variational technique. We consider the ratio

$$E = \frac{(\hat{H}\psi, \psi)}{(\psi, \psi)}$$

which minimal value is the minimal eigenvalue of the operator $\hat{H}$. If a test function ψ is such that the value of the ratio is smaller than the lower bound of the continuous spectrum of $\hat{H}$, then there is an eigenvalue of $\hat{H}$ below the continuous spectrum and the value of the ratio gives one an upper estimation for this eigenvalue.

We will construct test functions which satisfy the condition (1) on the lines, but are not continuous along the X axis. However, it can be approximated with arbitrary accuracy by the functions from the operator domain. Specifically, we assume $\psi(x,y) = \chi(x)\zeta_x(y)$, where $\zeta_x(y)$ are five eigenfunctions of $-\frac{d^2}{dy^2}$, satisfying condition (2), one for each vertical strip with unique delta potentials on lines (denoted by Roman numerals in Fig. 1).

First, let us consider a transversal part $\zeta_x(y)$. There are 5 of them, with three unique sets of conditions (u_1,u_1), (u_1,u_2), (u_2,u_2). Let each of a_1 *and* a_2, $a_1 \le a_2$ take value of u_1 or u_2. The problem sometimes referred to as double delta-function potential in 1D. For the $L > L_0 = \frac{a_1 + a_2}{a_1 a_2}$, there are two solutions. When continually changing delta-function intensities to make them equal, one of them transforms into a symmetrical solution, and the other into an asymmetrical one. We will refer to them as solutions of symmetrical and asymmetrical types respectively. The restrictions on transversal energy levels $\tilde{E} = (0.5p)^2$ are as follows:

$$e^{-pL} = \frac{(p-a_1)(p-a_2)}{a_1 a_2}$$

Now, let us consider a longitudinal component $\chi(x)$ for the test function. The transversal variants create five regions with different energy $\tilde{E}_x$ each. These energies can be converted into a step-like potential for the longitudinal component constant in each region. We will consider two specific cases, corresponding to all transversal functions being either of symmetric or asymmetric types, which produces symmetric potentials with 3 different levels: a variation on square well potential, with additional step, hereafter referred to as step-well potential (see the example of potential, produced by symmetric type $\zeta_x(y)$, Fig. 2). Let V_1, V_2, V_3, denote constant levels of a potential, from the lowest to the highest. The solutions for $V_1 < E < V_2$ and $V_2 < E < V_3$, which we refer to as bottom and top ones respectively, satisfy different restrictions on energy levels. Let $k_1 = \sqrt{E - V_1}$, $k_2 = \sqrt{E - V_2}$, $k_3 = \sqrt{V_3 - E}$ and

$$T_r(E) = tan(k_1 r) \tag{4}$$

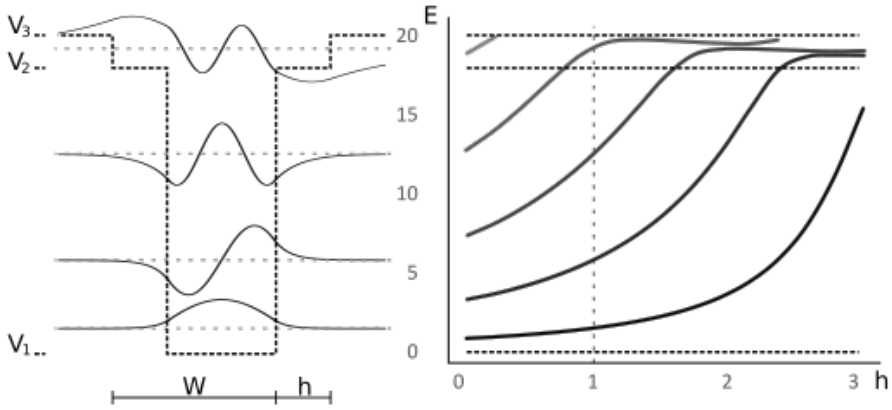

Fig. 2. Longitudinal component of the constructed function for the symmetric type $\zeta_x(y)$. Fixed values: $W = 3$, $V_1 = 0$, $V_2 = 18$, $V_3 = 20$. The plot shows dependence of energy levels on shift h. The left part shows a specific step-well potential, for $h = 1$, with energy levels and corresponding eigenfunctions.

The restrictions for energies of symmetric and asymmetric solutions are as follows:

$$\begin{aligned} T_r(E) &= \frac{k_2}{k_1} tan\left(arctan\left(\frac{k_3}{k_2}\right) - k_2 h \right) \\ T_r(E) &= -\frac{k_2}{k_1} cot\left(arctan\left(\frac{k_3}{k_2}\right) - k_2 h \right) \end{aligned} \tag{5}$$

Let us denote the right-hand side of (5), as $K(E)$. These equations cover the case of $E < V_2$ with complex k_2. However, it might be convenient to use other expression for $K(E)$ with $\tilde{k}_2 = \sqrt{V_2 - E}$, which eliminates complex numbers:

$$K(E) = \frac{\tilde{k}_2}{k_1} tanh\left(arctanh\left(\frac{k_3}{\tilde{k}_2}\right) + \tilde{k}_2 h \right) =$$

$$= \frac{\tilde{k}_2}{k_1} coth\left(arccoth\left(\frac{k_3}{\tilde{k}_2}\right) + \tilde{k}_2 h \right)$$

 https://www.doi.org/10.33910/2687-153X-2022-3-1-37-42

Existence of bound states

The constructed functions can be used to create an upper bound on the discrete spectrum of $\hat{H}$.

Theorem 2. *The step-well potential (see Fig.2) always has at least one discrete eigenvalue below the essential spectrum* σ_{ess}.

Proof. We will prove that there is an interval where $T(E) - K(E)$ is continuous and takes values of different sign at the borders , where $T(E)$ (determined as (4)) and $K(E)$ are the left hand side and the right hand side of (5). Note, that for the edge cases $V_2 = V_1$, $V_2 = V_3$, $h = 0$ or $h = W$, the problem turns into a square well potential situation, for which the existence of an eigenvalue is proven.

First, let us note that $T(V_1) = 0$ and $K(+0) = +\infty$. The only discontinuities for the functions are the vertical asymptotes. Let us denote the smallest vertical asymptotes for T and K as A_T and A_K. Then $T(A_T - 0) = +\infty$, $K(A_K - 0) = -\infty$, and therefore, if $min\ (A_T, A_K) \le V_3$, then the interval $(0, min\ (A_T, A_K))$ is the required one.

Now, let us consider the case $min\ (A_T, A_K) \le V_3$. Fix some values of W and V_2. Here, $T(V_3) > 0$, let us prove that $K(V_3) \le 0$ for all relevant h. The equation for the asymptotes of $K(E)$ can be written as

$$cot\left(k_2 h\right) = -\frac{k_3}{k_2},$$

which shows that as h increases, A_K monotonically decreases, thus $K(E)$ continuous on (V_1, V_3), only for h from 0 to the point at which $A_K = V_3$. The function $K\left(V_3\right) = -\frac{k_2}{k_1} tan\left(k_2 h\right)$ is a monotonically decreasing function and when $h = 0$, one has $K(V_3) = 0$. That proves $K(V_3) \le 0$, when $A_K > V_3$, and, therefore, interval (V_1, V_3) is the necessary one.

Corollary 1. *The main operator* $\hat{H}$ *has at least one bound state.*

Proof. The essential spectrum of an operator is $\sigma_{ess}\left(\hat{H}\right) = \left(V_3, +\infty\right)$. The constructed function satisfies $\frac{\left(\hat{H}\psi, \psi\right)}{\left(\psi, \psi\right)} = E$, and can be approximated to an arbitrary degree by the functions from the operator domain. Therefore, the value E from Theorem 2 is the upper bound for the discrete spectrum of $\hat{H}$.

Results

Now let us consider the constructed function energy levels as functions of h. As V_2 changes, note, that edge cases $V_2 = V_1$ and $V_2 = V_3$, produce square well potentials of widths $W + h$ and $W - h$, which, with an increase of h, get wider and narrower respectively. With V_2 fixed, an increase of h from 0 to W, transforms a narrow well (W, V_3), into a wide well $(2W, V_2)$, while continuously changing their energy levels.

As has been described above, the constructed functions, given large enough L, allow us to choose one of two transversal eigenvalues: $\tilde{E}_1 < a_1$ and $\tilde{E}_2 > a_2$ for each region, and while regions with $a_1 = a_2$ produce close values, regions with different intensities, which correspond to V_2, have a large gap between them. The choice between two values in each region corresponds to ψ of symmetric and asymmetric types. Using the results, we can conclude that their energy levels transform in different ways. Considering a symmetric type, we can see from Fig. 2 that the lowest eigenvalue is monotonically rising, until it escapes the strip below V_2 and reaches the lowest level of the wide square well $(2W, V_2)$. As for real systems, a larger gap between the eigenvalue and σ_{ess} ensures larger stability of the eigenstate in respect to perturbations. This means that the bound states with that behavior are more stable for small h.

As we mentioned in the Introduction, the considered system can be treated as a rough model for the description of some features of line molecules (e. g., DNA-like or protein-like) interactions. Particularly, it can be useful for understanding of the first stage of interaction between a virus and an organism molecule (recognition of a “label” and fixation near the molecule), see, e. g., (Li 2016; Shang et al. 2020).

Conflict of Interest

The authors declare that there is no conflict of interest, either existing or potential.

Authors contribution

The authors have made an equal contribution to the paper.

References

Bagmutov, A. S., Popov, I. Yu. (2020) Window-coupled nanolayers: Window shape influence on one-particle and two-particle eigenstates. *Nanosystems: Physics, Chemistry, Mathematics*, 11 (6), 636–641. https://doi.org/10.17586/2220-8054-2020-11-6-636-641 (In English)

Behrndt, J., Exner, P., Holzmann, M., Lotoreichik, V. (2017a) Approximation of Schroedinger operators with delta-interactions supported on hypersurfaces. *Mathematische Nachrichten*, 290 (8–9), 1215–1248. https://doi.org/10.1002/mana.201500498 (In English)

Behrndt, J., Frank, R. L., Kuhn, C. et al. (2017b) Spectral theory for schrodinger operators with δ-interactions supported on curves in R^3. *Annales Henri Poincare*, 18 (4), 1305–1347. https://doi.org/10.1007/s00023-016-0532-3 (In English)

Behrndt, J., Langer, M., Lotoreichik, V. (2016) Boundary triples for Schrodinger operators with singular interactions on hypersurfaces. *Nanosystems: Physics, Chemistry, Mathematics*, 7 (2), 290–302. https://doi.org/10.17586/2220-8054-2016-7-2-290-302 (In English)

Brasche, J., Exner, P., Kuperin, Yu. A., Seba, P. (1994) Schroedinger operator with singular interactions. *Journal of Mathematical Analysis and Applications*, 184 (1), 112–139. https://doi.org/10.1006/jmaa.1994.1188 (In English)

Brasche, J., Teta, A. (1992) Spectral analysis and scattering theory for Schrodinger operators with an interaction supported by a regular curve. In: *Ideas and Methods in Quantum and Statistical Physics*. Cambridge: Cambridge University Press, pp. 197–211. (In English)

Exner, P., Ichinose, T. (2001) Geometrically induced spectrum in curved leaky wires. *Journal of Physics A: Mathematical and General*, 34 (7), 1439–1450. https://doi.org/10.1088/0305-4470/34/7/315 (In English)

Exner, P., Jex, M. (2013) Spectral asymptotics of a strong δ' interaction on a planar loop. *Journal of Physics A: Mathematical and Theoretical*, 46 (34), article 345201. https://doi.org/10.1088/1751-8113/46/34/345201 (In English)

Exner, P., Kondej, S. (2002) Curvature-induced bound states for a δ interaction supported by a curve in R^3. *Annales Henri Poincaré*, 3 (5), 967–981. https://doi.org/10.1007/s00023-002-8644-3 (In English)

Exner, P., Kondej, S. (2004) Strong-coupling asymptotic expansion for Schroedinger operators with a singular interaction supported by a curve in R^3. *Reviews in Mathematical Physics*, 16 (5), 559–582. https://doi.org/10.1142/S0129055X04002084 (In English)

Exner, P., Kondej, S. (2005) Scattering by local deformations of a straight leaky wire. *Journal of Physics A: Mathematical and General*, 38 (22), 4865–4874. https://doi.org/10.1088/0305-4470/38/22/011 (In English)

Exner, P., Kondej, S. (2015) Gap asymptotics in a weakly bent leaky quantum wire. *Journal of Physics A: Mathematical and Theoretical*, 48 (49), article 495301. https://doi.org/10.1088/1751-8113/48/49/495301 (In English)

Exner, P., Kondej, S., Lotoreichik, V. (2018) Asymptotics of the bound state induced by δ-interaction supported on a weakly deformed plane. *Journal of Mathematical Physics*, 59 (1), article 013051. https://doi.org/10.1063/1.5019931 (In English)

Exner, P., Pankrashkin, K. (2014) Strong coupling asymptotics for a singular Schrodinger operator with an interaction supported by an open arc. *Communications in Partial Differential Equations*, 39 (2), 193–212. https://doi.org/10.1080/03605302.2013.851213 (In English)

Exner, P., Vugalter, S. (2016) On the existence of bound states in asymmetric leaky wires. *Journal of Mathematical Physics*, 57 (2), article 022104. https://doi.org/10.1063/1.4941139 (In English)

Exner, P., Yoshitomi, K. (2002) Asymptotics of eigenvalues of the Schroedinger operator with a strong delta-interaction on a loop. *Journal of Geometry and Physics*, 41 (4), 344–358. https://doi.org/10.1016/S0393-0440(01)00071-7 (In English)

Li, F. (2016) Structure, function, and evolution of coronavirus spike proteins. *Annual Review of Virology*, 3, 237–261. https://doi.org/10.1146/annurev-virology-110615-042301 (In English)

Popov, I. Yu. (1993) The helmholtz resonator and the theory of operator extensions in a space with indefinite metric. *Russian Academy of Sciences. Sbornik Mathematics*, 75 (2), article 285. https://doi.org/10.1070/SM1993v075n02ABEH003386 (In English)

Popov, I. Yu. (1992a) The extension theory and the opening in semitransparent surface. *Journal of Mathematical Physics*, 33 (5), 1685–1689. https://doi.org/10.1063/1.529697 (In English)

Popov, I. Yu. (1992b) The resonator with narrow slit and the model based on the operator extensions theory. *Journal of Mathematical Physics*, 33 (11), 3794–3801. https://doi.org/10.1063/1.529877 (In English)

Posilicano, A. (2001) A Krein-like formula for singular perturbations of self-adjoint operators and applications. *Journal of Functional Analysis*, 183 (1), 109–147. https://doi.org/10.1006/jfan.2000.3730 (In English)

Posilicano, A. (2004) Boundary triples and weyl functions for singular perturbations of self-adjoint operators. *Methods of Functional Analysis and Topology*, 10 (2), 57–63. (In English)

Shang, J., Wan, Y., Liu, C. et al. (2020) Structure of mouse coronavirus spike protein complexed with receptor reveals mechanism for viral entry. *PLOS Pathogens*, 16 (3), article e1008392. https://doi.org/10.1371/journal.ppat.1008392 (In English)

Vorobiev, A. M., Trifanova, E. S., Popov, I. Yu. (2020) Resonance asymptotics for a pair quantum waveguides with common semitransparent perforated wall. *Nanosystems: Physics, Chemistry, Mathematics*, 11 (6), 619–627. https://doi.org/10.17586/2220-8054-2020-11-6-619-627 (In English)