

BOUND STATES INDUCED BY INTERACTION POTENTIAL DEFORMATION

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Abstract. A simplified two-dimensional model of a quantum particle which interacts with another one through a one-dimensional Morse potential is studied. It is examined to what degree a small deformation of this one-dimensional interaction channel influences the ground state energy. The problem is important for the discussion on the deformation of various kinds of nanosurfaces such as carbon nanotubes. A deformation passing from the straight line geometry to ring geometry is considered. An upper bound for the number of oscillatory states is estimated and it is related to the deformation.

1. INTRODUCTION

The paper belongs to the line of research often called *singular perturbations* [1-3] used to study the low-dimensional quantum confinement effects. The corresponding quantum models are usually motivated by various kinds of nanostructured systems, like carbon nanotubes which exemplify 1D systems, quantum wires or 2D crystals. The electronic properties of such systems strongly depend on their geometric structure. In particular, the carbon nanotubes, depending on the diameter and helicity (described by (n,m) indices) of the tubes can be either metallic or semiconductor with energy gaps of different sizes [4]. For example, the (n,m) carbon nanotubes where $n - m = 3j$ and j is a non-zero integer would represent metals but due to the nanotube curvature, a small band gap appears and they become semiconductors [4]. If the tube radius R increases, then this gap decreases as $1/R^2$. An example of geometric confinement in other quantum systems can be the ground state properties of a toroidally trapped Bose-Einstein condensate where the curvature lowers the ground state energy [6] or the curvature-dependent conductance resonance in quantum cavities [6].

Let us suppose that we have a quantum particle confined in a narrow tube formed by some semiconductor material. Since the tube is very thin we can model it by a line Γ in \mathbb{R}^n where $n = 2, 3$. Some additional properties of Γ will be specified in further discussion. Furthermore, let us assume that the particle living in such a tube is interacting with another particle through the Morse-like potential

$$U(s) := \gamma(1 - e^{-a|s|})^2 - \alpha, \quad (1.1)$$

where γ, α and a are positive constants and argument $s \in \mathbb{R}$ determines the localization on Γ or, other words, it parameterizes Γ . The formula in Eq. (1.1) is a slight modification of the typical one-dimensional Morse potential which reads as $U(s) = \gamma(1 - e^{-as})^2$. On the other hand, the function (1.1) qualitatively corresponds to the three dimensional potential $V(r) = \gamma(1 - e^{-ar})^2$ considered by Morse in 1929 [7]. Another reason for such a modification is the fact that in this paper we are interested mainly in the bound states which are induced by the negative component of the interaction potential. Therefore, we believe that the results derived here do not change too much for the potential in Eq. (1.1), but

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the mathematical analysis is more involved. The interaction potential in Eq. (1.1) describes a situation when the reference system origin is associated with another particle such that a kind of a diatomic molecule is formed if the bound states exist. However, due to the possibility of *tunneling*, the whole space \mathbb{R}^n is admissible for the quantum particle; consequently the Hamiltonian of such a system can be symbolically written as:

$$-\Delta^{(n)} + U\delta(x - \Gamma), \quad (1.2)$$

where Γ , as before, describes the nanotube geometry, $\delta(\bullet)$ denotes the Dirac function and $-\Delta^{(n)}$ stands for the n -dimensional Laplacian; in the following we restrict ourselves to $n = 2$ and $\gamma = \alpha$. The kind of potentials which are localized on lower dimensional manifolds are often called *singular*. The main point of this paper is to show *how the geometry of the nanotube relates to the spectrum of the system*. The corresponding problem was already studied by P. Exner and others, (see [1,8,9] and references therein), however, in the models which have been considered so far the corresponding singular potentials are defined by coupling constants only; the interaction we consider here varies on Γ . On the other hand, the spectral analysis derived in [2] is given for a much more general case than singular perturbation given by a coupling constant (it is the so called *by dynamics* perturbation), however, the perturbation support is determined by a piece of a straight line and does not admit any deformation. Let us also mention that there are extensive literature sources where nanostructures are mathematically "realized" by graphs, cf. [10-12]. However these kinds of models, in contrast to our approach, do not take into account the possibility of tunnelling. The main result of this paper can be summarized as follows:

- The deformation of a nanotube described by Γ 'pushes down' the ground state energy. To be precise, if Γ is not related to a straight line (but asymptotically straight), then *the ground state energy is lower than in the case of a straight line*, see Theorem 2.3.
- We show how *an upper bound for the number of bound states relates to the nanotube deformation*, Theorem 2.3.

Convention of the paper. The paper is mainly addressed to the physicists who are interested in nanostructure problems and, in our opinion, the results we obtain are important for nanostructure device engineering. However, these results are also strict from the mathematical point of view. To make

the reading easier, the involved technical details which require advanced mathematical tools are omitted or moved to the appendix. For readers who are interested in rigorous mathematical proofs we recommend [3,8,9].

2. HAMILTONIAN WITH SINGULAR PERTURBATION DEFINED BY THE MORSE POTENTIAL

We are interested in Hamiltonians with the interaction potential localized on a manifold of the lower dimension and described by the Morse-like function, see Eq. (1.1). We start with the simplest manifold, namely, let us consider the straight line in \mathbb{R}^2 being a graph of the function $s \rightarrow \Sigma(s) := (s, 0) \in \mathbb{R}^2$, $s \in \mathbb{R}$. We denote the line by Σ as well without any danger of confusion. The Hamiltonian we are going to discuss can be formally written as the following symbol:

$$H_{\gamma,a} = -\Delta^{(2)} + \left(\gamma(1 - e^{-a|s|})^2 - \alpha \right) \times \delta(x - \Sigma), \quad \alpha > 0, \quad (2.3)$$

where γ, a are positive constants and $\Delta^{(2)}$ stands for the two dimensional Laplace operator; finally $\delta(\cdot - \Sigma)$ denotes the Dirac function which is, in fact, a singular measure with support on Σ , i.e. $f(\Sigma(s)) = \int_{\mathbb{R}^2} \delta(x - \Sigma(s)) f(x) dx$. Once $H_{\gamma,a}$ is only a symbol, our first aim is to find a well defined self-adjoint operator in the Hilbert space $L^2 := L^2(\mathbb{R}^2)$ which we will later denote by H_V , and which preserves the intuitive properties of the above expression. In this paper we make use of a technical simplification putting $\alpha = \gamma$ and consequently denoting

$$V(s) \equiv V_{\gamma,a}(s) = \gamma(1 - e^{-a|s|})^2 - \gamma. \quad (2.4)$$

We postpone the discussion of the general case to a forthcoming paper. We will follow the notions $(\bullet, \bullet\bullet)$, $\|\bullet\|$ which denote the scalar product and the norm in L^2 . We employ the so called form sum method in order to give a physical sense to the symbol $H_{\gamma,a}$. Let us consider the energy quadratic form given by

$$\varepsilon_V(f, g) := \int_{\mathbb{R}^2} \nabla f \nabla \bar{g} dx + \int_{\mathbb{R}} V f|_{\Sigma} \bar{g}|_{\Sigma} ds, \quad (2.5)$$

where f, g are C^1 functions from L^2 with $\nabla f, \nabla g \in L^2$ and the symbol $f|_{\Sigma}$ stands for the restriction of f to Σ , precisely $f|_{\Sigma}(s) \equiv f(\Sigma(s)) = \int_{\mathbb{R}^2} \delta(x - \Sigma(s)) \times f(x) dx$. Relying on the results of [3] the operator H_V is associated to ε_V , i.e. $H_V(f, g) = \varepsilon_V(f, g)$ is self-adjoint and can be understood as a mathematical

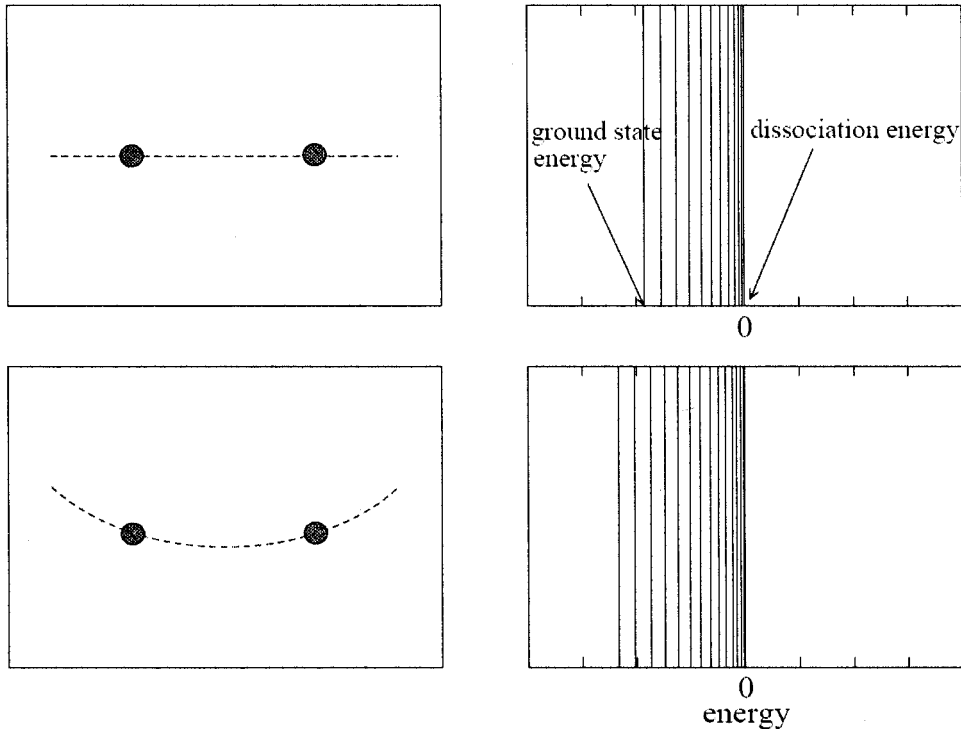


Fig. 1. Schematic draft of a diatomic molecule in the case of the straight line confinement for the constituent atoms and in the case of its deformation into a ring (left panels). A lowering of the ground state can be observed due to the curvature (right panels).

realization of (2.3). For more information about quadratic forms perturbed by singular measures we recommend [13]¹.

2.1. Spectrum of H_V

The aim of this section is to state some important facts about the spectrum of H_V . In particular, we will be interested in the discrete spectrum $\sigma_d(H_V)$ which determines the energies of the bound states of the quantum system governed by H_V . The completion $\sigma_{\text{ess}}(H_V) := \sigma(H_V) \setminus \sigma_d(H_V)$ is usually called in phenomenological literature a *continuous spectrum*, however keeping in mind the convention of the paper we introduce here the mathematical notion of the *essential spectrum* for $\sigma_{\text{ess}}(H_V)$.

Our first task is to recover the essential spectrum of H_V . It is well known that if the potential vanishes sufficiently fast at infinity, then it is not able to change the essential spectrum. In fact, this is our case; the Morse potential localized on Σ vanishes exponentially. *The stability of the essential spectrum of H_V with respect to Hamiltonian without interaction, i.e. $-\Delta^{(2)}$, is stated in the following lemma with the proof moved to Appendix.*

Lemma 2.1. *The essential spectrum of H_V is the same as $-\Delta^{(2)}$, i.e.*

$$\sigma_{\text{ess}}(H_V) = [0, \infty).$$

The stability of the essential spectrum is a natural consequence of the fact that the singular potential in our model vanishes at infinity. On the other hand, the potential in question is negative and it can induce some bound states with energies below 0. It is known that in a two-dimensional system a negative singular potential localized on compact line always has a discrete spectrum. In our problem we do not have a compact manifold. However, we can easily extend the mentioned result to our case since the potential V is negative and the essential spectrum threshold is 0. Therefore, we come to the following conclusion:

Lemma 2.2. *Hamiltonian H_V has at least one bound state with the corresponding energy below 0.*

Since the ground state energy of H_V will play an important role in the following discussion, it will be given symbol $\epsilon_{0,V}$; the ground state energy is nothing else but the infimum of the whole spectrum

$$\epsilon_{0,V} := \inf \sigma(H_V). \quad (2.6)$$

¹In fact, the operator associated to ϵ_V is called essentially self adjoint. This means that we need to take its closure to obtain self adjointness.

2.2. Deformation of Σ

Now, we turn to the main issue of this paper: *what happens* with the spectrum after a deformation of Σ or, physically speaking, whether a deformation of nanotubes changes the bound state energy spectrum of the quantum system. We define a deformed curve Γ in \mathbb{R}^2 , i.e. Γ does not coincide to Σ and assume that Γ is parameterised by the length of arc (the corresponding parameter will be denoted by s). To be precise, Γ is a graph of the C^2 function $\mathbb{R} \ni s \rightarrow \Sigma(s) \in \mathbb{R}^2$, and moreover it is assumed that Γ is asymptotically straight. This means that

(a1) there exists a compact set $M \in \mathbb{R}^2$ such that $\Gamma \setminus M \subset S$.

Consequently, the curvature $\kappa: s \rightarrow \kappa(s)$ of Γ is a function with compact support. The size of this support is denoted by D , i.e. D is the length of

$$\mathcal{D} := \text{supp } \kappa = \{s : \kappa(s) \neq 0\}^{\text{cl}}, \quad (2.7)$$

if \mathcal{D} consists of a finite number of disjoint connected sets, then D is a sum of lengths of the corresponding sets. Furthermore, we can measure the distance between two points living on Γ taking a usual Cartesian distance in \mathbb{R}^2 , i.e.

$$\rho(s, s') := |\Gamma(s) - \Gamma(s')| = \left(\sum_{i=1}^2 (\Gamma_i(s) - \Gamma_i(s'))^2 \right)^{1/2}, \quad s, s' \in \mathbb{R} \quad (2.8)$$

or moving along the curve

$$\sigma(s, s') := |s - s'|, \quad (2.9)$$

then $\sigma(s, s')$ states the Euclidean distance. Of course, due to the parameterization by the length of arc we have

$$\rho(s, s') \leq \sigma(s, s'). \quad (2.10)$$

To exclude self-intersections the second assumption is imposed which is a kind of an inverse inequality, namely

(a2) there exists a constant $C > 0$ such that $C\rho(s, s') \geq \sigma(s, s')$.

After these preliminaries we are ready to construct a Hamiltonian with a singular potential localized on Γ and determined by the Morse-like function.

Analogously as in (2.5) we consider:

$$\varepsilon_{v,\Gamma}(f, g) := \int_{\mathbb{R}^2} \nabla f \nabla \bar{g} \, dx + \int_{\mathbb{R}^2} V f|_{\Gamma} \bar{g}|_{\Gamma} \, ds, \quad (2.11)$$

and again we borrow the argument from [3] to conclude that the operator $H_{v,\Gamma}$ associated with $\varepsilon_{v,\Gamma}$ is self-adjoint. The Hamiltonian $H_{v,\Gamma}$ gives a mathematical meaning to the formal expression:

$$-\Delta^{(2)} + V\delta(x - \Gamma). \quad (2.12)$$

Repeating the argument from Lemma 2.1 we state the stability of the essential spectrum:

$$\sigma_{\text{ess}}(H_{v,\Gamma}) = [0, \infty). \quad (2.13)$$

Now the question is whether the deformation influences the bound state energies. A partial answer is contained in the following theorem:

Theorem 2.3. *Hamiltonian $H_{v,\Gamma}$ has at least one point of a discrete spectrum; moreover its ground state energy $\varepsilon_{0,v,\Gamma}$ satisfies*

$$\varepsilon_{0,v,\Gamma} < \varepsilon_{0,v}$$

Comment on proof. The idea of the proof is borrowed from [8] (see also [9]) and based on the so called Birman-Schwinger principle. In [8] an attractive singular potential localized on Γ and defined by a negative coupling constant has been considered. The Hamiltonian $H_{\alpha,\Gamma}$ of such a system can be formally written:

$$-\Delta^{(2)} - \alpha\delta(x - \Gamma), \quad \alpha > 0. \quad (2.14)$$

In particular, it has been shown in [8] that $\inf \sigma(H_{\alpha,\Gamma}) < \inf \sigma(H_{\alpha,\Sigma})$, i.e. the deformation pushes down the lowest energy². This model is slightly different from ours, however, the proofs of Lemmas 5.3, 5.4, 5.5 of [8] can be repeated with the obvious changes and adopted to our problem; we omit here the involved mathematical analysis and postpone it to a forthcoming paper. Theorem 2.3 shows that the deformation leads to pushing down the ground state energy of H_v .

3. UPPER BOUND FOR THE NUMBER OF BOUND STATES AS A FUNCTION OF CURVATURE

The aim of this section is to find an upper bound for the number of bound states of $H_{v,\Gamma}$; we use here the standard notation $\#_{\sigma_0}(H_{v,\Gamma})$ for the number of bound states (together with their multiplicity). We are especially interested in the question how the corresponding upper bound changes with the parameters corresponding to the deformation of Γ . Using the result of [14] we conclude that the following formulae:

²In fact, in [8] the authors have shown that the deformation induces bound states. In a system with a straight line interaction defined by a coupling constant there is only an essential spectrum, however, if we deform a Σ , then at least one point of the discrete spectrum appears below $\inf \sigma(H_{\alpha,\Sigma})$.

$$N_V := 1 + \int_{\mathbb{R}^2} |V_{\gamma,a}(s)| |V_{\gamma,a}(s')| \times \\ |C_1 \ln|s - s'| + C_2|^2 ds ds' \quad (3.15)$$

and

$$N_{V,\Gamma} := 1 + \int_{\mathbb{R}^2} |V_{\gamma,a}(s)| |V_{\gamma,a}(s')| \times \\ |C_1 \ln|\Gamma(s) - \Gamma(s')| + C_2|^2 ds ds' \quad (3.16)$$

state the upper bounds for the number of bound states of H_V and $H_{V,\Gamma}$ respectively. The constants C_1 and C_2 are given explicitly and they take the following form:

$$C_1 = -\frac{1}{2\pi}, \quad C_2 = \frac{1}{2\pi} \ln 2 - \gamma_E, \quad (3.17)$$

where γ_E is the Euler constant. Being consistent with the notation introduced in the previous discussion, we will use abbreviations $\sigma(s, s') = |s - s'|$ and $\rho(s, s') = |\Gamma(s) - \Gamma(s')|$.

Remark 3.1. Let us make some comments concerning the formulae (3.15) and (3.16). In fact, it has been shown in [14] that the number of bound states of Hamiltonian $-\Delta + W$ in L^2 satisfies:

$$\#\sigma_d(-\Delta + W) \leq 1 + \int_{\mathbb{R}^2 \times \mathbb{R}^2} |W(x)| |W(y)| \times \\ |C_1 \ln|x - y| + C_2|^2 dx dy \quad (3.18)$$

for all the $W(\bullet)$ potentials for which the above integral is finite. In this paper, we work with singular potentials which, of course, do not have this property. However, the result can be generalized for the singular potential case and (3.15) and (3.16) is obtained substituting the regular potential $W(\bullet)$ in (3.18) by a singular measure $V(\bullet)\delta(x - \Gamma(\bullet))$.

We need the following lemma with a proof based on an elementary analysis to show how an upper bound for $\#\sigma_d(H_{V,\Gamma})$ depends on the curvature of Γ :

Lemma 3.2. *We have*

$$0 \leq \ln \sigma(s, s') - \ln \rho(s, s') \leq (\kappa_m D)^2 \quad (3.19)$$

for $s \neq s', s, s' \in \mathbb{R}$,

where $\kappa_m := \sup_{s \in D} \kappa(s)$ and D has been already defined as the size of support of the curvature function $s \rightarrow \kappa(s)$.

Proof. Using the analytical properties of the logarithmic function, in particular the fact that $-\ln x$ is convex and its derivative is given by $(\ln x)' = -1/x$, $x > 0$ and combining this with (2.10) we get:

$$0 < \ln \sigma - \ln \rho \leq (\sigma - \rho)/\rho,$$

where we abbreviate $\sigma = \sigma(s, s')$ and analogously for ρ . Furthermore, relying on the result of [8] we have:

$$\frac{\sigma(s, s') - \rho(s, s')}{\rho(s, s')} \leq \frac{1}{2\sigma(s, s')} \int_{s'}^{s_1} \left(\int_{s'}^{s_2} \kappa(s_2) ds_2 \right)^2 ds_1.$$

It is easy to see that the r.h.s. of the above expression can be bounded from above by $1/2 (\kappa_m D)^2$; this finally states the claim of lemma.

Using the above lemma we can show by a straightforward calculation the main theorem which shows how the upper bound for $\#\sigma_d(H_{V,\Gamma})$ changes with parameters associated with the curvature κ_m and D .

Theorem 3.3. *The following estimate:*

$$N_{V,\Gamma} \leq N_V + A(\kappa_m D)^2 + B(\kappa_m D)^4, \quad (3.20)$$

holds, for

$$A := \int_{\mathbb{R}^2} |V_{\gamma,a}(s)| |V_{\gamma,a}(s')| \times \\ |C_1 \ln|s - s'| + C_2|^2 ds ds' \quad (3.21)$$

and

$$B := \frac{1}{4} C_1^2 \left(\int_{\mathbb{R}^2} |V_{\gamma,a}(s)| ds \right)^2. \quad (3.22)$$

Proof. Using the explicit form for $N_{V,\Gamma}$ given by (3.15) together with the triangle inequality we estimate

$$N_{V,\Gamma} := N_V + 2|C_1| \int_{\mathbb{R}^2} |V_{\gamma,a}(s)| |V_{\gamma,a}(s')| \times \\ |C_1 \sigma(s, s') + C_2| \left| \ln \frac{\rho(s, s')}{\sigma(s, s')} \right| ds ds' + \\ C_1^2 \int_{\mathbb{R}^2} |V_{\gamma,a}(s)| |V_{\gamma,a}(s')| \left(\ln \frac{\rho(s, s')}{\sigma(s, s')} \right)^2 ds ds'.$$

Using the above inequality and the result of Lemma 3.2 we show by a straight-forward calculation that the expression

$$N_V + A(\kappa_m D)^2 + B(\kappa_m D)^4 \quad (3.23)$$

states an upper bound for $N_{V,\Gamma}$. This completes the proof.

To estimate the constants contributing to (3.20) we use the following upper bound

$$|\ln x| \leq \begin{cases} x^{-1/2} & \text{for } 0 < x < 1, \\ x + 1 & \text{for } x \geq 1. \end{cases}$$

Combining the above estimate with the triangle inequality we get

$$\begin{aligned}
A &\leq |C_1| \int_{\mathbb{R}^2} V_{\gamma,a}(s) V_{\gamma,a}(s') |\ln|s - s'|| ds ds' + \\
|C_2| &\left(\int_{\mathbb{R}^2} V_{\gamma,a}(s) ds \right)^2 \leq 2|C_1| \int_{\mathbb{R}^2} \int_{s'}^{s'+1} V_{\gamma,a}(s) V_{\gamma,a}(s') \times \\
&(s - s')^{-1/2} ds ds' + 2|C_1| \int_{\mathbb{R}^2} \int_{s'+1}^{\infty} V_{\gamma,a}(s) V_{\gamma,a}(s') \times \\
&(s - s' + 1) ds ds' + |C_2| \left(\int_{\mathbb{R}^2} V_{\gamma,a}(s) ds \right)^2 \times \\
&\left(\int_{\mathbb{R}^2} V_{\gamma,a}(s') ds' \right)^2 \leq (3\gamma)^2 \left(|C_1| \left(2 + 2a^{-1} + (3a)^{-2} + 4a^{-3} \right) + |C_2| a^{-2} \right).
\end{aligned}$$

The last inequality has been obtained by integration by parts; we also take advantage of the fact that $V_{\gamma,a}(s) \leq 3\gamma e^{-a|s|}$. Furthermore, we have

$$B = \left(\frac{3\gamma C_1}{2a} \right)^2.$$

The above theorem gives the upper bound for the number of bound states of $H_{V,\Gamma}$ in the terms of parameter $\xi = \kappa_m D$ which characterizes the deviation of Γ from the straight line. The upper bound obtained is, in fact, a polynomial function of ξ . It is important to note from Eq. (3.20) that the difference of the corresponding upper bounds induced by the curvature $\Delta N_V = N_{V,\Gamma} - N_V$ generated by the dominating curvature κ_m in the region of a given size D can be qualitatively different for a small radius R of this curvature and a large one

$$\begin{aligned}
\Delta N_V &\leq \frac{BD^4}{R^4}; \text{ if } R \rightarrow 0, \\
\Delta N_V &\leq \frac{AD^2}{R^2}; \text{ if } R \rightarrow \infty,
\end{aligned} \tag{3.24}$$

It should be noted that the circle geometry case, when D is proportional to R , can be addressed to the geometric representation of the carbon nanotube as a model of a rolled up graphene sheet. It is not the case of ultra-small diameter carbon nanotubes ($R \sim 0.2$ nm) which can have the property of superconductivity [4]. In our opinion it would be very interesting to check whether an analogous polynomial behavior as in Eq. (3.24) is valid for the number of bound states, as well.

4. CONCLUSIONS

We have shown that it is possible to lower the ground state energy of a quantum particle by some defor-

mation of the "interaction channel" of the particle with other particles. The theoretical problem introduced in the above has a practical meaning for designing nanosurfaces of different shapes.

5. APPENDIX

Proof of Lemma 2.1. To present the claim we will use a standard method called Neumann bracketing, see [15]. Let B_R be an open ball in \mathbb{R}^2 and its boundary be denoted as ∂B_R . Let us consider the operator $H_V^{\text{int},R}$ in $L^2(B_R)$ with a singular potential on $\Sigma \cap B_R$ given by the Morse function and the Neumann boundary condition on ∂B_R . Analogously, we define $H_V^{\text{int},R}$ but in the space $L^2(\mathbb{R}^2 \setminus B_R)$. Then, using the results of [15] we have:

$$H_V^{\text{int},R} \oplus H_V^{\text{ext},R} \leq H_V,$$

for any $R > 0$. Since $H_V^{\text{int},R}$ is the Laplacian with the Neumann boundary conditions on ∂B_R it can produce a discrete spectrum only. Therefore, the H_V essential spectrum threshold is not less than the $H_V^{\text{ext},R}$ essential spectrum threshold. On the other hand, since the Morse potential vanishes exponentially at infinity, we can easily see that the whole $H_V^{\text{ext},R}$ spectrum threshold (i.e. the lowest energy) goes to 0 for $R \rightarrow 0$. This means that $\inf_{\sigma_{\text{ess}}}(H_V) \leq 0$. On the basis of the energy form (2.5) we can easily state that $\sigma_{\text{ess}}(H_V) \supseteq [0, \infty)$ and consequently this states the claim.

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