GEOMETRICALLY INDUCED TWO-PARTICLE BINDING IN A WAVE GUIDE

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Abstract. For mathematical models of quantum wave guides we show that in some situations two interacting particles can be trapped more easily than a single particle. In particular, we give an example of a wave guide that can not bind a single particle, but does have a geometrically induced bound state for two particles that attract each other. We also show that Neumann boundary conditions are 'stickier' for two interacting particles than for a single one.

1. Introduction

Over the last two decades a considerable amount of research has been done on mathematical models for quantum wave guides (see e.g. [1, 2, 3, 4, 5, 6] and references therein). Typically a particle in such a structure is modelled by a Schrödinger operator on some tube-like domain in two or three dimensions. The main object of interest is the spectrum of these operators, and especially their low-lying eigenvalues which indicate the presence of bound states for the particle. Such trapped modes have been proven to exist, e.g., for tubes with local deformations, bends, or mixed boundary conditions. Much less is known though about the binding of several interacting particles in such settings [7, 8, 10]. In the present article we will show that under certain conditions a system of two interacting particles can be bound more easily than one particle alone.

Our work is inspired by the analogous effect for Schrödinger operators in free space: Consider for a particle of mass m the operator

$$H = -\frac{1}{2m}\Delta + V(x)$$

in $L^2(\mathbb{R}^n)$ with a non-trivial, compactly supported and bounded potential $V \leq 0$. It is well known that for $n > 2$ the attractive potential V may be too weak to have bound states, i.e., H may not have negative eigenvalues. If this is the case, the same potential may still give rise to bound states of a system of two particles that attract each other. This can be understood by physical intuition if one assumes that the two particles act in some sense like one particle of the double mass. After all, as far as the existence of eigenvalues is concerned, doubling

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the mass has the same effect as doubling the strength of the potential. In the present article we discuss whether an analogous effect can occur for purely geometrically induced bound states in wave guides.

More precisely, we describe a quantum mechanical particle in a wave guide by the Dirichlet Laplacian $-\Delta$ in $L^2(\Omega)$, where Ω is a straight strip or tube. The spectrum of this operator is purely continuous and contains every real number above some threshold, which is the lowest eigenvalue of the Laplace operator on the cross section of Ω. It is known that geometrical perturbations like bending the tube or local deformations of the boundary can give rise to eigenvalues of $-\Delta$ below this threshold. In analogy to the case of the Schrödinger operator with a weak attractive potential, we ask the following question: Does a wave guide exist that doesn't have a bound state for one particle, but that does have a bound state for a system of two interacting particles?

This question is not so easy to answer by physical intuition, because the existence or non-existence of geometrically bound states for one particle doesn't depend on the mass of the particle in question. This means that the intuitive 'double mass argument' for two particles in an attractive potential doesn't apply to this situation. Despite that, we will show in the following two sections that the answer to the question above is 'yes'.

2. Two-particle bound states in deformed wave guides

We assume our wave guide to be the domain $\Omega \subset \mathbb{R}^2$ given by

$$\Omega = \{(x, y) : |y| < f(x)\}$$

where

$$f(x) = \begin{cases} \frac{1}{2} & \text{for } |x| > L/2, \\ \epsilon/2 & \text{for } x = \pm L/2, \\ h/2 & \text{for } |x| < L/2 \end{cases}$$

with $L > 0, h > 1$ and $0 < \epsilon < 1$. We impose Dirichlet conditions on $\partial\Omega$, which includes the 'barriers' at $x = \pm L/2$. Our geometry can be interpreted as a cavity of length L and width h coupled weakly (if ϵ is small) to two semi-infinite straight wave guides. We choose to set $m = \frac{1}{2}$, such that the one-particle Hamiltonian is simply $H_1 = -\Delta$. Then standard arguments imply that

$$\sigma_{\text{ess}}(H_1) = [\pi^2, \infty).$$

Eigenvalues may occur depending on the choice of the parameters L, h and ϵ, but we will show:

Lemma 2.1. *If $L^{-2} + h^{-2} > 1$ then for small enough ϵ there are no eigenvalues of H_1 below π^2, i.e., in this case the wave guide has no one-particle bound states.*

On the other hand, we consider a system of two bosons of mass $m = \frac{1}{2}$, which interact via a harmonic potential. The corresponding Hamiltonian is

$$H_2 = -\partial_{x_1}^2 - \partial_{y_1}^2 - \partial_{x_2}^2 - \partial_{y_2}^2 + \alpha(x_1 - x_2)^2 + \alpha(y_1 - y_2)^2$$

in $L^2(\Omega \times \Omega)$, where x_i and y_i are the particle coordinates and $\alpha > 0$ is the interaction strength. Again we impose Dirichlet conditions on the boundary of Ω.

Lemma 2.2.
a) For any choice of L , h and ϵ one has

$$\sigma_{\text{ess}}(H_2) \subset [\sqrt{2\alpha} + 2\pi^2, \infty).$$

b) There is a choice of the constants L and h with $L^{-2} + h^{-2} > 1$ such that

$$\inf \sigma(H_2) < \sqrt{2\alpha} + 2\pi^2$$

for every $\epsilon > 0$, i.e., the operator H_2 has a bound state.

From the above lemmata we conclude that a wave guide exists that has no bound state for one particle, but does have a geometrically induced bound state for two interacting particles.

A remark on the physical interpretation of this effect is in order. As mentioned above, the argument of two particles acting like one of the double mass doesn't apply to geometrically induced bound states, since their existence is mass-independent. To gain a physical intuition for our results anyway, we note that a bound state in a wave guide with bulges can be seen as a trade-off between reduced kinetic energy in the transverse direction (due to the enlarged cross-section) and increased kinetic energy in the longitudinal direction (due to the localization of the particle). Consider now two particles that attract each other and that would in free space form a 'molecule' with an average distance d between them. Assume for the case of our wave guide Ω that d is considerably bigger than the cavity width h, but considerably smaller than the cavity length L. This means that in their transverse movement the two particles act rather as if they were independent of each other, thus receiving twice the energy decrease from the enlarged cross-section. In longitudinal direction, on the other hand, the two particles in the cavity behave like one particle of the double mass, such that the energy increase due to longitudinal localization is only half of what it would be for one particle alone. It follows that the energy trade-off is more 'favorable' for the system of two interacting particles than for a single one.

3. Two-particle bound states caused by Neumann boundary conditions

If one introduces Neumann boundary conditions, an effect similar to the one described above happens even for particles in only one dimension: Be $H_3 = -\partial_x^2$ in $L^2(\mathbb{R}^+)$ with a Neumann condition at $x = 0$. Then it is clear that $\sigma_{ess}(H_3) = \mathbb{R}^+$ and H_3 has no eigenvalues. The corresponding two-particle Hamiltonian though turns out to have a bound state, if the interaction potential is purely attractive:

Lemma 3.1. *Let $V : \mathbb{R}^+ \to \mathbb{R}$ be a strictly increasing function. Then the operator*

$$H_4 = -\partial_{x_1}^2 - \partial_{x_2}^2 + V(|x_1 - x_2|)$$

on $L^2(\mathbb{R}^+ \times \mathbb{R}^+)$ with Neumann boundary conditions at $x_1 = 0$ and at $x_2 = 0$ has a bound state, i.e., an eigenvalue below the lower threshold of the essential spectrum.

In view of Lemma 3.1 it is no surprise that wave guides exist which have no one-particle bound states, but which do have a two-particle bound state induced by mixed boundary conditions. Omitting the proof, we only mention the simple example of a straight tube with Dirichlet boundary conditions on the edge and an additional Neumann condition imposed on one cross-section.

4. Proofs of the results

Proof of Lemma 2.1. We introduce the operator $\tilde{H}_1$, which we define to be the Laplace operator on Ω with Dirichlet conditions on $\partial\Omega$ and additional Neumann conditions on the set

$$\{(x, y) : x = \pm L/2 \text{ and } |y| < |\epsilon|\}.$$

To prove Lemma 2.1 it is then sufficient to show that $\tilde{H}_1$ has no spectrum below π^2. With the introduction of the new boundary conditions we have cut Ω into three separate domains Ω^+/Ω^- (the semi-strip in positive / negative x-direction) and Ω^0 (the rectangle $(-\frac{L}{2}, \frac{L}{2}) \times (-\frac{h}{2}, \frac{h}{2})$). Thus $\tilde{H}_1$ is the orthogonal sum of the Laplace operators on Ω^+, Ω^- and Ω^0 (subject to appropriate boundary conditions), and

$$\sigma(\tilde{H}_1) = \sigma(-\Delta_{\Omega^+}) \cap \sigma(-\Delta_{\Omega^-}) \cap \sigma(-\Delta_{\Omega^0}).$$

One can convince oneself easily that

$$\sigma(-\Delta_{\Omega^+}) = \sigma(-\Delta_{\Omega^-}) = [\pi^2, \infty).$$

The spectrum of $-\Delta_{\Omega^0}$ is purely discrete and if we call $\lambda(\epsilon)$ its lowest eigenvalue then

$$\lambda(0) = \pi^2(h^{-2} + L^{-2}) > \pi^2.$$

We can now apply a theorem of Gadyl'shin [9] to see that $\lambda(\epsilon) - \lambda(0)$ is of order ϵ^2, i.e., for small enough $\epsilon > 0$ we have $\inf \sigma(-\Delta_{\Omega^0}) > \pi^2$. Altogether this means that

$$\inf \sigma(H_1) \geq \inf \sigma(\tilde{H}_1) = \pi^2 \quad \text{for small } \epsilon.$$

□

Proof of Lemma 2.2, part a). Using the center of mass coordinates

$$u = \frac{1}{2}(x_2 + x_1) \quad \text{and} \quad w = \frac{1}{2}(x_2 - x_1) \tag{1}$$

we rewrite H_2 in the form

$$H_2 = -\frac{1}{2}\partial_u^2 - \frac{1}{2}\partial_w^2 + 4\alpha w^2 - \partial_{y_1}^2 - \partial_{y_2}^2 + \alpha(y_2 - y_1)^2. \tag{2}$$

To estimate the spectrum of H_2 from below we introduce Neumann boundary conditions on

$$\{(u, w, y_1, y_2) : |w| = \beta\} \quad \text{and} \quad \{(u, w, y_1, y_2) : |w| < \beta, |u| = \beta + \frac{L}{2}\},$$

for some $\beta > 0$, which turns H_2 into the orthogonal sum

$$\tilde{H}_2 = H_2|_{\{|w|>\beta\}} \oplus H_2|_{\{|w|<\beta, |u|<\beta+\frac{L}{2}\}} \oplus H_2|_{\{|w|<\beta, |u|>\beta+\frac{L}{2}\}}.$$

The spectrum of $H_2|_{\{|w|>\beta\}}$ can be estimated from below by $4\alpha\beta^2$ and the spectrum of $H_2|_{\{|w|<\beta,|u|<\beta+\frac{L}{2}\}}$ is discrete. By separation of variables the spectrum of $H_2|_{\{|w|<\beta,|u|>\beta+\frac{L}{2}\}}$ if found to be purely continuous and its lower threshold is equal to the lowest eigenvalue of the 'transversal' operator

$$H_t = -\frac{1}{2}\partial_w^2 + 4\alpha w^2 - \partial_{y_1}^2 - \partial_{y_2}^2 + \alpha(y_2 - y_1)^2$$

on $L^2((-\beta, \beta) \times (-1/2, 1/2)^2)$ with Neumann conditions at $|w| = \beta$ and Dirichlet conditions at $|y_1| = 1/2$ and $|y_2| = 1/2$. Neglecting the positive potential term $\alpha(y_2 - y_1)^2$, we see that the lowest eigenvalue of H_t converges to some number bigger than $\sqrt{2\alpha} + 2\pi^2$ for $\beta \to \infty$. Part a) of Lemma 2.2 now follows from the fact that $\tilde{H}_2 < H_2$ and the min-max principle. □

Proof of Lemma 2.2, part b). We choose to fix the relations

$$\alpha = L^{-2} \quad \text{and} \quad h^{-2} + L^{-2} =: M > 1 \tag{3}$$

between the parameters that describe our wave guide. We define the domain $\tilde{\Omega}$ as the set of all (x_1, y_1, x_2, y_2) that satisfy the conditions

$$u \in \left(-\frac{3L}{8}, \frac{3L}{8}\right), \quad w \in \left(-\frac{L}{8}, \frac{L}{8}\right), \quad y_1, y_2 \in \left(-\frac{h}{2}, \frac{h}{2}\right),$$

using the coordinates u and w as defined in (1). One can check that $\tilde{\Omega} \subset \Omega$. We now define the test function Ψ by

$$\Psi = \left(\cos\frac{4\pi u}{3L}\right) \cdot (\phi(w) - C) \cdot \left(\cos\frac{\pi y_1}{h}\right) \cdot \left(\cos\frac{\pi y_2}{h}\right)$$

on $\tilde{\Omega}$ and $\Psi = 0$ on $\Omega\backslash\tilde{\Omega}$, setting

$$\phi(w) = e^{-\sqrt{2\alpha}w^2} \quad \text{and} \quad C = \phi(L/8).$$

The function Ψ is continuous and differentiable and satisfies the boundary conditions of H_2. Using the form (2) of H_2 and the min-max principle [11] we have

$$\begin{aligned} \inf\sigma(H_2) &\leq \frac{\langle \Psi, H_2\Psi\rangle_{L^2(\tilde{\Omega})}}{||\Psi||^2} \\ &= \frac{8\pi^2}{9L^2} + \frac{2\pi^2}{h^2} + \frac{\pi^2-6}{6\pi^2}\alpha h^2 \\ &\quad + \frac{\int_{-L/8}^{L/8}(\frac{1}{2}\phi'(w)^2 + 4\alpha w^2(\phi(w)-C)^2)\,\mathrm{d}w}{\int_{-L/8}^{L/8}(\phi(w)-C)^2\,\mathrm{d}w}. \end{aligned} \tag{4}$$

The last term can be estimated from above by

$$\begin{aligned} \frac{\int_{-L/8}^{L/8}(\frac{1}{2}\phi'(w)^2 + 4\alpha w^2\phi(w)^2)\,\mathrm{d}w}{\int_{-L/8}^{L/8}(\phi^2(w) - 2C\phi(w))\,\mathrm{d}w} &= \frac{\sqrt{2\alpha}}{1 - 2C||\phi||^{-2}_{[-L/8,L/8]}\int_{-L/8}^{L/8}\phi(w)\,\mathrm{d}w} \\ &= \sqrt{2\alpha} + \mathcal{O}(e^{-\sqrt{2}L/64}) \end{aligned} \tag{5}$$

for large L, where in the last step we have used that $\alpha = L^{-2}$ and thus $C = e^{-\sqrt{2}L^2/64}$. Putting (5) into (4) and using (3) yields

$$\inf\sigma(H_2) < \sqrt{2\alpha} + 2M\pi^2 - \frac{10\pi^2}{9L^2} + \frac{\pi^2-6}{9\pi^2(L^2-1)} + \mathcal{O}(e^{-\sqrt{2}L/64}).$$

If we chose L sufficiently large and M sufficiently close to one, we get for any $\epsilon > 0$

$$\inf\sigma(H_2) < \sqrt{2\alpha} + 2\pi^2,$$

proving part b) of Lemma 2.2. □

Proof of Lemma 3.1. Using the center of mass coordinates from (1) and a similar argument as in the proof of Lemma 2.2, part a), one can show that

$$\sigma_{ess}(H_3) = [\lambda, \infty),$$

where λ is the lowest eigenvalue of the operator $h = -\frac{1}{2}\partial_w^2 + V(|2w|)$ on $L^2(\mathbb{R})$. It remains to show that H_3 has an eigenvalue below λ.

Consider the potential $V(|x_1 - x_2|)$ as a function in the first quadrant of the cartesian (x_1, x_2) coordinate system. Let $\tilde{V}(x_1, x_2)$ be the potential defined on the whole x_1-x_2-plane that can be obtained by reflecting $V(|x_1 - x_2|)$ first on the x_1-axis and then the resulting function on the x_2-axis. Because V is a strictly increasing function, we have

$$\tilde{V}(x_1, y_1) \leq V(|x_1 - x_2|) \tag{6}$$

on the whole plane with equality only in the first and in the third quadrant. Let

$$\tilde{H}_3 = -\partial^2_{x_1} - \partial^2_{x_2} + \tilde{V}(x_1, x_2)$$

in $L^2(\mathbb{R}^2)$. Then, by symmetry of $\tilde{V}$ and by the boundary conditions of H_3, the lowest eigenvalue of $\tilde{H}_3$ is also the lowest eigenvalue of H_3.

In the center of mass coordinates (1) one has

$$\tilde{H}_3 = -\frac{1}{2}\partial^2_u - \frac{1}{2}\partial^2_w + V(|2w|) + D(u, w)$$

with $D(x_1, x_2) = \tilde{V}(x_1, y_1) - V(|x_1 - x_2|)$. Because of (6) the function D is zero in the first and third quadrant and negative in the second and fourth. We call $\phi(w)$ the (normalized) lowest eigenfunction of h and define the test function

$$\Psi = \phi(w)e^{-\epsilon|u|} \quad (\text{with}\, \epsilon > 0).$$

Then the min-max principle [11] tells us that

$$\inf \sigma(\tilde{H}_3) \quad \leq \quad \epsilon^2 + \lambda + \epsilon \int \Psi^2 D \, \mathrm{d}x_1 \, \mathrm{d}x_2.$$

The integral in the last summand is negative and its absolute value increases when ϵ goes to zero. Consequently, for some small enough ϵ we have $\inf \sigma(\tilde{H}_3) < \lambda$, which proves Lemma 3.1. □

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