A quantum pipette

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Curved quantum waveguides are known to bind particles. We show that a number of charged fermions in such a trap can be tuned by an external electrostatic field; if the latter is slowly increased, the bent duct can serve as a single particle ejector.

1 Introduction

Though numerous quantum phenomena can be explained by usual semiclassical concepts, a complete theory — even in the case of the nonrelativistic quantum mechanics — is certainly deeper. A recent illustration was provided by properties of particles within bent tubes or other infinitely extended regions with Dirichlet boundaries (*i.e.*, hard walls). It was demonstrated that such systems exhibit isolated energy eigenvalues [7, 8, 11] despite the absence of closed trajectories (apart of the obvious zero–measure set) in their classical counterparts.

These bound states and related resonance effects in scattering [4] have attracted a considerable interest — a list of references can be found in the review paper [3]. It is motivated not only by the mentioned theoretical reason, but rather by the fact that curved tubes (and more complicated regions constructed of them) can model some real physical systems.

The most prominent among them are *quantum wires, i.e.*, tiny strips of a very pure semiconductor material. Due to the purity and crystalic structure, an electron within the conductivity band can be regarded as a free particle of a certain effective mass. To replace the band by a halfline and to neglect the effective–mass dependence on the electron momentum is certainly a crude approximation; nevertheless, it is good enough to reproduce some properties of real quantum wires.

There are other motivations to study Schrödinger equation in hard–wall tubes. A very recent one comes from the proposal to use *hollow optical fibres* as waveguides for transport of atoms or ions [10]; in view of the achievable widths of such ducts, quantum effects must again be taken into account.

Despite numerous investigations of quantum waveguides during last few years, many questions remain to be answered. This concerns, in particular, effects of external fields. Most attention has been paid to magnetic fields, either perpendicular to the waveguide plane (*cf.* [6, 12] for further references) or threaded through the tube [5], or to the quantum Hall effect, while the influence of an electric field alone remained mostly untreated.

One of our aims is to draw attention to the fact that Stark effect in non–straight tubes has a rich structure coming from combination of the curvature–induced attractive interaction and the electrostatic potential which is nonlinear along the tube even if the field is homogeneous. Instead of discussing it generally, however, we shall concentrate here on discussion of an interesting particular case.

2 Description of the model

We consider a particle whose motion is confined to a curved planar strip Ω of a constant width d as sketched on Figure 1. Though we have in mind the systems mentioned in the introduction, in general we shall suppose only that the particle is a fermion of a nonzero charge q. We also assume that it is under influence of a homogeneous electric field of an intensity E ; we denote $F := qE$. Without loss of generality we shall suppose in the following that $F \geq 0$. The operator to study is the corresponding Hamiltonian,

$$H_\Omega(F) := -\Delta_D^\Omega + Fy\,, \tag{1}$$

where $-\Delta_D^\Omega$ is the Dirichlet Laplacian on $L^2(\Omega)$ defined conventionally as in [9, Sec.XIII.15]; for the sake of simplicity we put $\hbar = 2m = 1$. If the electric field is absent, $F = 0$, the essential spectrum of $H_\Omega(F)$ starts at $\lambda_1 := (\pi/d)^2$ which is the lowest eigenvalue of the transverse Dirichlet problem. In addition, it has at least one eigenvalue below λ_1 whenever Ω is non–straight; a more precise formulation will be given below.

What happens with these eigenvalues when the field is switched on depends, of course, substantially on the shape of Ω. We restrict our attention here to the case when Ω is curved within a bounded region only, and outside it is perpendicular to the field direction. Moreover, we shall assume that the "tilt" of Ω is one–sided, so there are no field-induced bound states in the corresponding classical system.

We have to put these assumptions on more mathematical terms. Following the standard procedure [3, 7] we choose the "lower" boundary of Ω as a reference curve; we call it Γ. We also introduce the usual curvilinear coordinates: s is the arc length of Γ and u is the distance from Γ (for points "above" the curve; it runs through the interval $[0, d]$). The Cartesian coordinates of the strip points are then given by

$$x = \xi(s) - u\dot{\eta}(s)\,, \quad y = \eta(s) + u\dot{\xi}(s)\,, \tag{2}$$

where the functions ξ, η satisfy the normalization condition $\dot{\xi}(s)^2 + \dot{\eta}(s)^2 = 1$. One can use them to define the signed curvature of the reference curve,

$$\gamma(s) := \dot{\eta}(s)\ddot{\xi}(s) - \dot{\xi}(s)\ddot{\eta}(s)\,. \tag{3}$$

The latter determines in turn the curve Γ uniquely up to Euclidean transformations of the plane: we have

$$\xi(s) \;=\; \int_0^s \cos\beta(s_1)\, ds_1\,, \quad \eta(s) \;=\; \int_0^s \sin\beta(s_1)\, ds_1\,, \tag{4}$$

where $\beta(s_2,s_1) := -\int_{s_1}^{s_2} \gamma(s)\, ds$ is the bending angle of Γ between the points s_1 and s_2 (in distinction to [6, 7] we choose it to be anticlockwise positive), and $\beta(s) := \beta(s,0)$; the non–uniqueness has been removed by choosing the reference frame in such a way that $\xi(0)=\eta(0)=\dot\eta(0)=0$ and $\dot\xi(0)=1$.

We adopt several general regularity assumptions, namely

(r1) $\gamma \in L^1_{loc}(I\!R)$,

(r2) $a\|\gamma\|_\infty < 1$,

(r3) Ω is not self–intersecting,

(r4) γ is piecewise C^2 with $\dot\gamma$, $\ddot\gamma$ bounded.

Among them, *(r2)* is needed to ensure that the other boundary of the strip is also smooth, while *(r4)* represents a strengthening of *(r1)*. Under *(r1)*–*(r3)*, one can rewrite $H_\Omega(0)$ as the Laplace–Beltrami operator on $L^2(I\!R\times[0,d],\, g^{1/2} ds\, du)$, where $g^{1/2}(s,u) := 1+u\gamma(s)$ [3, 7]; the potential part of (1) can be easily expressed in terms of the curvilinear coordinates by means of (2) and (4). If the assumption *(r4)* is also valid, one can remove the Jacobian, *i.e.*, to use the unitary operator $U:\; L^2(\Omega)\to L^2(I\!R\times[0,d])$ defined by

$$(U\psi)(s,u) \;:=\; (1+u\gamma(s))^{1/2}\psi(x,y)\,. \tag{5}$$

The operator resulting from this transformation, which by abuse of notation we will also denote as $H_\Omega(F)$, has the following form:

$$H_\Omega(F) \;=\; -\partial_s\,(1+u\gamma(s))^{-2}\,\partial_s \;-\; \partial_u^2 \;+\; V_F(s,u)\,, \tag{6}$$

where

$$\begin{aligned} V_F(s,u) \;&=\; V_0(s,u) \;+\; F\int_0^s \sin\beta(s_1)\, ds_1 \;+\; Fu\,\cos\beta(s) \\ V_0(s,u) \;&=\; -\,\frac{\gamma(s)^2}{4(1+u\gamma(s))^2} \;+\; \frac{u\ddot\gamma(s)}{2(1+u\gamma(s))^3} \;-\; \frac{5}{4}\,\frac{u^2\dot\gamma(s)^2}{(1+u\gamma(s))^4}\,. \end{aligned} \tag{7}$$

After this preliminary, we can formulate the special assumptions of our model which we have sketched above:

(s1) $\gamma\ne 0$ with $\operatorname{supp}\gamma \in [0,s_0]$ for some $s_0>0$,

(s2) $\int_0^{s_0} \gamma(s)\, ds = 0$,

(s3) $\beta(s)\in[0,\pi]$ for $s\in[0,s_0]$.

3 Existence of bound states

Let $N(F) := N(H_\Omega(F))$ be the number of bound states of $H_\Omega(F)$, *i.e.*, the number of its isolated eigenvalues counting their multiplicity. Since $H_\Omega(F) \geq H_\Omega(F')$ holds obviously for $F \geq F'$, all eigenvalues are by the minimax principle nondecreasing functions of F. This does not mean automatically, however, that $N(\cdot)$ is monotonous, because we count the eigenvalues below $\inf \sigma_{ess}(H_\Omega(F)) = \inf \sigma(h_u(F))$, where $h_u(F) := -\partial_u^2 + Fu$ with the Dirichlet condition at $u = 0, d$, and the latter is also increasing. On the other hand, a strong enough field destroys all bound states.

Theorem: Assume *(r1)–(r3)* and *(s1)–(s3)*. Then

(a) $N(0) \geq 1$. If, in addition *(r4)* is valid and $\int_0^{s_0} |\gamma(s)|\, ds$ is small enough, $H_\Omega(0)$ has just one bound state, $N(0) = 1$.

(b) There is a positive F_0 such that $N(F) = 0$ for all $F \geq F_0$.

Proof: (a) *Cf.* [8] and [3, Secs.2, 4].
(b) The idea is to estimate $H_\Omega(F)$ from below by an operator $\tilde{H}(F)$ in such a way that the threshold of the essential spectrum is preserved, $\inf \sigma_{ess}(H_\Omega(F)) = \inf \sigma_{ess}(\tilde{H}(F))$. In that case $N(F) \leq \tilde{N}(F) := N(\tilde{H}(F))$ so it is sufficient to choose $\tilde{H}(F)$ which would have $\tilde{N}(F) = 0$ for F large enough.

The estimating operator is constructed in the way sketched on Figure 2. We cut the straight tube in left halfplane by an additional Neumann boundary. Furthermore, we deform Γ to the right of the origin and close the obtained region by another Neumann boundary to a rectangle of sides a, b; this is always possible under the assumptions *(s1)–(s3)*. Finally, the upper boundary in the right halfplane is not important; we may remove it at all. We denote the operators $-\Delta + Fy$ in these regions with the appropriate boundary conditions as $H_j(F)$, $j = 1, 2, 3$, and define $\tilde{H}(F) := H_1(F) \oplus H_2(F) \oplus H_2(F)$.

By the bracketing principle [9, Sec.XIII.15], $H_\Omega(F) \geq \tilde{H}(F)$, so it remains to check that $\tilde{H}(F)$ has the other required properties. Obviously, $\inf \sigma(H_3(F)) \geq Fb$. To estimate the bottom of the spectra of $H_1(F)$, $H_2(F)$, we need to solve the transverse (y–direction) problem. Its eigenfunctions are linear combinations of the fundamental solutions

$$u_\lambda(y) := \mathrm{Ai}\left(F^{1/3}\left(y - \frac{\lambda}{F}\right)\right), \quad v_\lambda(y) := \mathrm{Bi}\left(F^{1/3}\left(y - \frac{\lambda}{F}\right)\right), \tag{8}$$

and the spectral conditions read

$$u_\lambda(0)v_\lambda(d) - u_\lambda(d)v_\lambda(0) = 0, \quad u_\lambda(0)v'_\lambda(b) - u'_\lambda(b)v_\lambda(0) = 0 \tag{9}$$

in the first and the second region, respectively. Introducing the parameters $\eta := F^{-1/3}$ and $\delta := a_1 + \lambda F^{-2/3}$, where $a_1 \approx -2.33$ is the first zero of Ai and using asymptotic properties of the Airy functions [1], we find from (8) and (9) that the lowest eigenvalue is in the first case given by

$$\lambda_1(F) = F^{2/3}\left[-a_1 + c_1\, e^{-(4/3)d^{3/2}\sqrt{F}}(1 + \mathcal{O}(F^{-1/2}))\right], \tag{10}$$

where $c_1 := -\frac{\mathrm{Bi}(a_1)}{2\mathrm{Ai}'(a_1)} \approx 0.325$. The spectrum of $H_1(F)$ is then purely continuous and starts from $\lambda_1(F)$. On the other hand, the spectrum of $H_2(F)$ is purely discrete, the lowest eigenvalue being obtained in a similar way as

$$\mu_1(F) = \left(\frac{\pi}{2a}\right)^2 + F^{2/3}\left[-a_1 - c_1\, e^{-(4/3)b^{3/2}\sqrt{F}}(1+\mathcal{O}(F^{-1/2}))\right]. \tag{11}$$

Hence for all F large enough, $\lambda_1(F) \le \min\{\mu_1(F), Fb\}$, so the bottom of the spectrum of $\tilde{H}(F)$ is determined by that of $H_1(F)$. Since the latter has no eigenvalues, we arrive at the sought conclusion. ∎

4 Thin strips: a semiclassical estimate

The above general result yields only a very rough estimate of the critical field strength F_0 and it says nothing about the behaviour of the function $N(\cdot)$ in the interval $[0, F_0]$. To get a better idea, we shall discuss in this section on a heuristic level the case of a thin strip, $d\|\gamma\|_\infty \ll 1$. We shall suppose that the curvature γ is smooth enough, so that we can replace $H_\Omega(F)$ by the unitarily equivalent operator (6). If the strip is thin, the problem can be then reduced to discussion of the one–dimensional Schrödinger operator

$$H(F) := -\partial_s^2 + V_F(s) := -\partial_s^2 - \frac{1}{4}\gamma(s)^2 + F\int_0^s \sin\beta(s_1)\, ds_1 \tag{12}$$

on $L^2(I\!R)$, which is the leading term in the projection of the operator $H_\Omega(F)$ onto the lowest transverse mode with the corresponding contribution $\lambda_1 := (\pi/d)^2$ to the energy subtracted — for details see [3, Sec.5].

The number of bound states in the curved strip can be estimated semiclassically: denoting $\tilde{V}_F(s) := \min\{0, V_F(s)\}$ and $\tilde{p}_F(s) := \sqrt{-\tilde{V}_F(s)}$, we have

$$N(F) \approx \frac{1}{\pi}\int_0^{s_0} \tilde{p}(s)\, ds\,. \tag{13}$$

The estimate makes certainly sense as long as the phase space allowed for the classical motion is large enough. We know that it fails if the field is absent and the strip is only slightly curved, because then $N(0) = 1$ for an arbitrarily small non–zero γ. On the other hand, if $N(0) \gg 1$ we can still use it to assess the critical field value F_0, because the property of one–dimensional Schrödinger operators on which the above claim is based requires the potential to decay fast enough at infinity [2] which is certainly not true for $F \ne 0$ when the asymptotics on the two sides are different.

The right side of the relation (13) is a decreasing function of F and $\lim_{F\to\infty} N(F) = 0$ in accordance with the general result discussed above. As an illustration, consider the following particular case:

Example: Suppose that the waveguide has $2N$ bends of alternating orientation, each of them of radius R and angle β (*cf.* Figure 3). Then $s_0 = 2N\beta R$ and $V_0(s) = -(2R)^{-2}$, so $N(0) \approx \frac{N\beta}{\pi}$ and the estimate can be used as long as the number of bends $N \gg \frac{\pi}{\beta}$. Using the parametrization (2), we find easily

$$y(s) = \begin{cases} 2nR(1-\cos\beta) + R\left(1-\cos\left(\frac{s-2n\beta R}{R}\right)\right) & \ldots\quad s \in (2n\beta R, (2n+1)\beta R) \\ \\ 2(n+1)R(1-\cos\beta) - R\left(1-\cos\left(\frac{2(n+1)\beta R-s}{R}\right)\right) & \ldots\quad s \in ((2n+1)\beta R, (2n+2)\beta R) \end{cases}$$

Hence $y(\cdot)$ is a sum of two functions, a linear and a periodic one. For the purpose of an estimate we neglect the oscillating part; this yields

$$V_F(s) \;\approx\; \frac{2Fs}{\beta}\,\sin^2\frac{\beta}{2} - \frac{1}{4R^2}$$

so performing the integration in (13), we get

$$N(F) \;\approx\; \begin{cases} \frac{\beta}{24\pi F R^3 \sin^2\frac{\beta}{2}}\left[1-\left(1-16NFR^3\sin^2\frac{\beta}{2}\right)^{3/2}\right] & \ldots\quad 0 < F \le \left(16NR^3\sin^2\frac{\beta}{2}\right)^{-1} \\ \\ \frac{\beta}{24\pi F R^3 \sin^2\frac{\beta}{2}} & \ldots\quad F \ge \left(16NR^3\sin^2\frac{\beta}{2}\right)^{-1} \end{cases} \tag{14}$$

The result is shown on Figure 4. Using it, we can estimate the field values at which the number bound states in the trap changes by one. In particular, the critical value at which the last bound state is absorbed in the continuum is

$$F_0 \;\approx\; \frac{\beta}{24\pi R^3 \sin^2\frac{\beta}{2}}\,. \tag{15}$$

5 Conclusions

The existence of curvature–induced bound states means that bent quantum waveguides can serve as traps for particles which — as a result of a suitable cooling process — occupy these localized states. This is true anytime the waveguide model used here allows for a reasonable description of a quantum system, for instance, in the situations mentioned briefly in the introduction.

For the purpose of the present paper we disregard, of course, interactions between particles which should be taken into account if two or more states of the trap are occupied. In analogy with artificial atoms based on quantum dots [13] one expects the simple–minded semiclassical estimate of the preceding section should be in a more realistic treatment replaced by a sort of Thomas–Fermi theory.

The main conclusion of the above discussion is that an electrostatic field can be used to control the number of particles contained in the waveguide with a one–sided tilt. If all the states of the trap are occupied and the field intensity is changing adiabatically, at certain values the highest excited state disappears in the continuum and the particle which has occupied it is ejected into the "lower" straight duct. This mechanism may provide a possible source which would produce single particles at an experimentalist's will as indicated in the title.

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Figure captions

Figure 1 The model: a curved strip in an electric field

Figure 2 The definition of $\tilde{H}(F)$. The full and dotted lines represent Dirichlet and Neumann boundaries, respectively.

Figure 3 A strip with alternative bends for $\beta = \pi$ and $N = 2$.

Figure 4 The estimate of the bound state number, $\mathrm{Int}\, N(F)$, in the example for $\beta = \pi$, $R = 0.5$, and $N = 5$.