A quantum pipette

1995 J. Phys. A: Math. Gen. 28 5323

(http://iopscience.iop.org/0305-4470/28/18/021)

J. Phys. A: Math. Gen. 28 (1995) 5323–5330. Printed in the UK

A quantum pipette

Pavel Exner†

Nuclear Physics Institute, Academy of Sciences, 25068 Řež near Prague, Czech Republic
and
Doppler Institute, Czech Technical University, Břehová 7, 11519 Prague, Czech Republic

Received 6 April 1995

Abstract. 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 up to the spin degeneracy.

1. Introduction

Though numerous quantum phenomena can be explained by the usual semiclassical concepts, a complete theory—even in the case of non-relativistic quantum mechanics—would certainly be more fundamental. A recent illustration was provided by the 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 from the obvious zero-measure set) in their classical counterparts.

These bound states and the related resonance effects in scattering [4] have attracted considerable interest—a list of references can be found in the review paper [3]. The interest is motivated not only by the mentioned theoretical reason, but also by the fact that curved tubes (and more complicated regions constructed from 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 crystalline 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 half-line 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. A more detailed discussion of this approximation together with references to the corresponding physical literature can be found in [3].

There are other motivations to study the Schrödinger equation in hard-wall tubes. A very recent one comes from the proposal to use *hollow optical fibres* as waveguides for the 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 the last few years, many questions remain to be answered. This concerns, in particular, the effects of external fields. Most attention has been paid to magnetic fields, either perpendicular to the waveguide

† E-mail address: exner@ujf.cas.cz

plane (cf [6, 12] for further references) or threaded through the tube [5], or the quantum Hall effect; however, the influence of an electric field alone remains mostly untreated.

One of our aims is to draw attention to the fact that the Stark effect in non-straight tubes has a rich structure coming from a 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 a general discussion, here we shall concentrate on 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 in 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 non-zero charge q. We also assume that it is under the 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 $F \geqslant 0$. Neglecting the spin of the particles (apart from the Pauli principle which we shall need in the following) we therefore describe a single fermion in the tube by the 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, section XIII.15]; for the sake of simplicity we put $\hbar = 2m^* = 1$. The same operator can be used to treat a family of confined fermions if we make another idealization and neglect their mutual interaction.

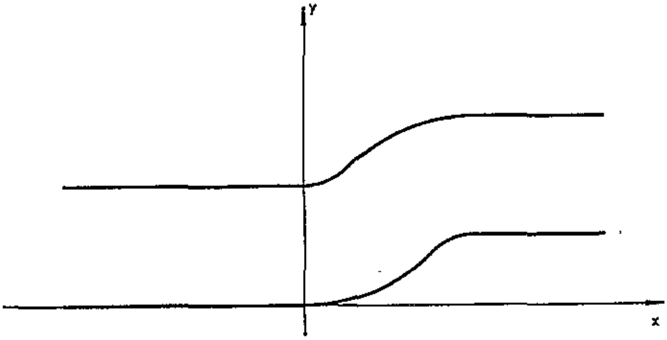

Figure 1. The model: a curved strip in an electric field.

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 is perpendicular to the field direction. Moreover, we shall assume that the 'tilt' of Ω is one sided so that there are no field-induced bound states in the corresponding classical system.

We have to put these assumptions in 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

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

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

$$\xi(s) = \int_0^s \cos\beta(s_1)\,\mathrm{d}s_1 \qquad \eta(s) = \int_0^s \sin\beta(s_1)\,\mathrm{d}s_1 \tag{4}$$

where $\beta(s_2, s_1) := -\int_{s_1}^{s_2} \gamma(s)\,\mathrm{d}s$ is the bending angle of Γ between the points s_1 and s_2 (in contrast to [6, 7] we choose the bending angle 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) $\gamma \in L^1_{\mathrm{loc}}(\mathbb{R})$;

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

(r3) Ω is not self-intersecting; and

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

Assumption (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 $L^2(\mathbb{R} \times [0, d], g^{1/2}\,\mathrm{d}s\,\mathrm{d}u)$, 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 assumption (r4) is also valid, one can remove the Jacobian, i.e. to use the unitary operator $U : L^2(\Omega) \to L^2(\mathbb{R} \times [0, d])$ 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 form

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

where

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

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

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

(s2) $\int_0^{s_0} \gamma(s)\,\mathrm{d}s = 0$; and

(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 $H_\Omega(F) \geqslant H_\Omega(F')$ obviously holds for $F \geqslant F'$, all eigenvalues are, by the minimax principle, non-decreasing functions of F. *This does not automatically mean, however, that $N(\cdot)$ is monotonic, because we count the* eigenvalues below $\inf \sigma_{\text{ess}}(H_\Omega(F)) = \inf \sigma(h_u(F))$, 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) $N(0) \geqslant 1$. 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 $F \geqslant F_0$.

Proof. (a) Cf [8] and [3, sections 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, i.e. $\inf \sigma_{\text{ess}}(H_\Omega(F)) = \inf \sigma_{\text{ess}}(\tilde{H}(F))$. In this case $N(F) \leqslant \tilde{N}(F) := N(\tilde{H}(F))$ so it is sufficient to choose $\tilde{H}(F)$ which would have $\tilde{N}(F) = 0$ for F large enough.

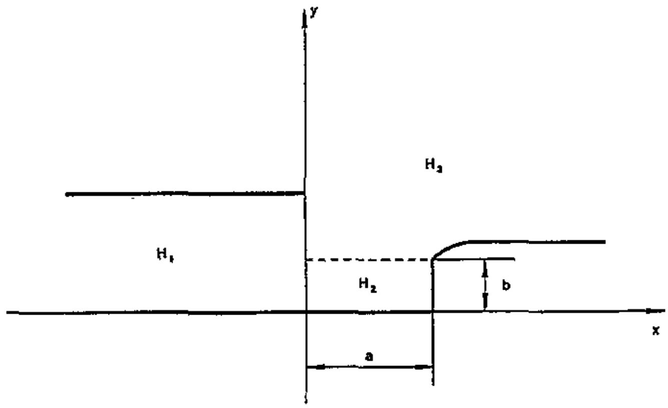

Figure 2. The definition of $\tilde{H}(F)$. The full and broken lines represent Dirichlet and Neumann boundaries, respectively.

The estimating operator is constructed in the way sketched in figure 2. We cut the straight tube in the left half-plane 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 half-plane is not important; we may remove it completely. 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, section XIII.15], $H_\Omega(F) \geqslant \tilde{H}(F)$, so it remains for us to check that $\tilde{H}(F)$ has the other required properties. Obviously, $\inf \sigma(H_3(F)) \geqslant Fb$. 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

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

and the spectral conditions read

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

in the first and 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 the asymptotic properties of the Airy functions [1], we find from (8) and (9) that the lowest eigenvalue is, in the first case, given by

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

where $c_1 := -\mathrm{Bi}(a_1)/2\mathrm{Ai}'(a_1) \approx 0.325$. 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

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

Hence, for all F large enough, $\lambda_1(F) \leqslant \min\{\mu_1(F), Fb\}$, 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, in this section we shall discuss, 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 then be reduced to a discussion of the one-dimensional Schrödinger operator

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

on $L^2(\mathbb{R})$, 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, section 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

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

The estimate certainly makes 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 $F \neq 0$ when the asymptotics on the two sides are different.

The right-hand side of 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.

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

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 $N(0) \approx N\beta/\pi$ and the estimate can be used as long as the number of bends $N \gg \pi/\beta$. Using the parametrization (2), we easily find that

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

Hence, $y(\cdot)$ is a sum of two functions, one linear and one periodic. 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 obtain

$$N(F) \approx \begin{cases} \dfrac{\beta}{24\pi F R^3 \sin^2\beta/2} \\ \quad \times[1-(1-16NFR^3\sin^2\beta/2)^{3/2}] & 0 < F \leqslant (16NR^3\sin^2\beta/2)^{-1} \\ \dfrac{\beta}{24\pi F R^3 \sin^2\beta/2} & F \geqslant (16NR^3\sin^2\beta/2)^{-1}. \end{cases} \tag{14}$$

The result is shown in figure 4. Using this result we can estimate the field values at which the number of 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

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

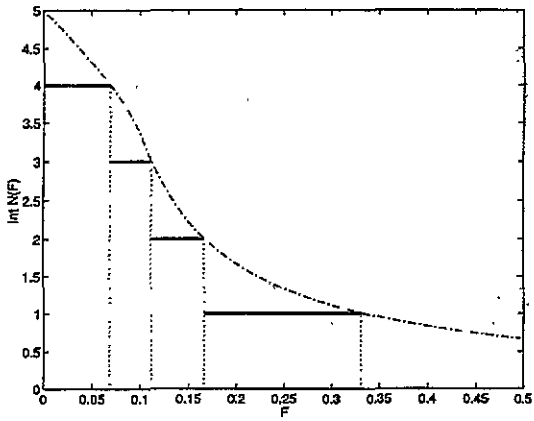

Figure 4. The estimate of the bound state number, Int $N(F)$, in the example for $\beta = \pi$, $R = 0.5$ and $N = 5$.

In a physical system of units the right-hand side has to be multiplied by $\hbar^2/2m^*$, where m^* is the reduced mass of the electron. A typical value is $m^* = 0.067m_e$ for GaAs quantum wires; choosing $\beta = \pi$ and R of the order of μm, we find the critical intensity E_0 of the order of μV. In a similar way, one can estimate the critical field value for other waveguide geometries and fermion types.

As mentioned above, we have taken the spin into account only through the Pauli principle. In reality each of the levels discussed here will be occupied by a pair of electronic states, or a $(2s + 1)$-tuple for fermions of spin s. Unless they are distinguished by an additional interaction, these states disappear in the continuum simultaneously as the field strength changes.

5. Conclusions

The existence of curvature-induced bound states means that bent quantum waveguides can serve as traps for particles which occupy these localized states. This is true any time that the waveguide model used here allows a reasonable description of a quantum system to be made; for instance, in the situations mentioned briefly in the introduction.

As we have said, for the purpose of the present paper we disregard 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 that the simple semiclassical estimate of the preceding section should be replaced by a sort of Thomas–Fermi theory in a more realistic treatment. A mathematical treatment of such a system would certainly be much more difficult; at the same time one expects that the interfermion interactions should not qualitatively change the dependence of the bound-state number on the applied field.

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—up to the spin degeneracy—at an experimentalist's will, as indicated in the title.

Acknowledgments

The author thanks the first referee for a useful comment. The work has been partially supported by the grants AS No 48409 and GA CR No 202-93-1314.

References

[1] Abramowitz M and Stegun I 1964 *Handbook of Mathematical Functions* (Washington, DC: National Bureau of Standards)

[2] Blanckenbecler R, Goldberger M L and Simon B 1977 The bound states of weakly coupled long-range one-dimensional quantum Hamiltonians *Ann. Phys.* **108** 89–78

[3] Duclos P and Exner P 1995 Curvature-induced bound states in quantum waveguides in two and three dimensions *Rev. Mod. Phys.* 7 73–102

[4] Duclos P, Exner P and Šťovíček P 1995 Curvature-induced resonances in a two-dimensional Dirichlet tube *Ann. Inst. H Poincaré* **62** 81–101

[5] Dunne G and Jaffe R L 1993 Bound states in twisted Aharonov–Bohm tubes *Ann. Phys.* **233** 180–196

[6] Exner P 1993 A twisted Landau gauge *Phys. Lett.* **178A** 236–8

[7] Exner P and Šeba P 1989 Bound states in curved quantum waveguides *J. Math. Phys.* **30** 2574–80

[8] Goldstone J and Jaffe R L 1992 Bound states in twisting tubes *Phys. Rev.* B **45** 14100–7

[9] Reed M and Simon B 1978 *Methods of Modern Mathematical Physics IV: Analysis of Operators* (New York: Academic)

[10] Savage C M, Markensteiner S and Zoller P 1993 Atomic waveguides and cavities from hollow optical fibres *Fundamentals of Quantum Optics III* ed S Eklotzky (Berlin: Springer)

[11] Schult R L, Ravenhall D G and Wyld H W 1989 Quantum bound state in classically unbound system of crossed wires *Phys. Rev.* B **39** 5476–9

[12] Vacek K, Okiji A and Kasai H 1993 Multichannel ballistic magnetotransport through quantum wires with double circular bends *Phys. Rev.* B **47** 3695–705

[13] Yngvason J 1994 Asymptotics of natural and artificial atoms in strong magnetic fields *XIth Congr. of IAMP (Paris)*