Bound states in open-coupled asymmetrical waveguides and quantum wires

Paolo Amore\textsuperscript{1}, Martin Rodriguez\textsuperscript{2} and César A Terrero-Escalante\textsuperscript{1}

\textsuperscript{1} Facultad de Ciencias, CUICBAS, Universidad de Colima, Bernal Díaz del Castillo 340, Colima, Colima, Mexico
\textsuperscript{2} Facultad de Ciencias, Universidad de Colima, Bernal Díaz del Castillo 340, Colima, Colima, Mexico

Received 17 October 2011, in final form 11 January 2012
Published 21 February 2012
Online at stacks.iop.org/JPhysA/45/105303

Abstract
The behaviour of bound states in asymmetric cross, T- and L-shaped configurations is considered. Because of the symmetries of the wavefunctions, the analysis can be reduced to the case of an electron localized at the intersection of two orthogonal crossed wires of different width. For different values of the ratio of the widths we prove the existence and non-existence of bound states in each symmetry class. Our arguments yield that for the even–even case the bound state of the cross configuration persists as one of the arms becomes infinitesimally narrow. In the case of odd–odd states, we find that the lowest mode is bounded when the width of the two arms is the same and stays bound up to a critical value of the ratio between the widths; in the case of the even–odd states we find that the lowest mode is unbound up to a critical value of the ratio of the widths. Numerical calculations are used to support those results and to determine precisely the critical values of the ratio of the widths.

PACS numbers: 03.65.Ge, 73.21.Hb, 73.20.–r
(Some figures may appear in colour only in the online journal)

1. Introduction

Trapped waves in open geometries have been known for 60 years now [1]. Ursell [2], in a theoretical and experimental study of ‘beach’ waves in a particular semi-infinite canal, found that the system has discrete, continuous and mixed spectra, and predicted the existence of a confined resonance at a discrete frequency, while at a cutoff frequency the resonance extends a long way down the canal. These waves can be described by the Helmholtz equation subject to Dirichlet boundary conditions, and therefore similar confinement properties are expected in the solutions of analogous acoustic or electromagnetic problems. Indeed, about 15 years after Ursell, long-lived resonance modes in open laser systems were reported [3]. Even more, since this setup is equivalent to that of electrons in open configurations described...
by the time-independent Schrödinger equation, by 1984, several studies already suggested that confinement is also a feature of the two-dimensional transport of charge carriers in ultra-fine metal and semiconductor devices [4]. From then on, many theoretical and experimental studies have shown that, generally, by bending and crossing waveguides and quantum wires, bound (confined, trapped) states can be obtained with energies below the continuous spectrum [5–7]. Moreover, many similar quantum wire systems have been found with bound states embedded into the continuum [8]. For a full mathematical treatment of the spectra of open quantum waveguides we refer the reader to chapter 16 of the book by Blank et al [9].

Bound states just below the continuum may strongly influence the scattering of waves and charge carriers. This allows them to be detected and it is also the source of new phenomena and applications. For instance, mesoscopic systems with similar geometries are common in nanoelectronics, and it has been shown experimentally that they exhibit suppression (quenching) of the Hall resistance [10], and enhanced bend resistance [11]. On the other hand, if the above-mentioned bound states exist only due to a particular geometry, when this geometry is modified, resonances could be expected to arise. Therefore, the confinement of electromagnetic radiation at the intersection of coupled waveguides opens a window for a new kind of resonator, which combines a very simplified spectrum with high performances [12]. Similar phenomena should be also relevant for the performance of novel kinds of (cold) atom [13], phonon [14] and laser waveguides [15]. Moreover, the possibility of geometrically inducing confined states allows for the design of unused ways to create a Bose–Einstein condensate in a quasi-one-dimensional Bose gas [16]. Last but not least, besides the possible practical applications, it should be noted that such systems constitute a very interesting theoretical framework for studying the correspondence between classical and quantum dynamics. Note that, in this kind of arrangement, the classical motion of point particles with finite energy is typically unbound because there are no forbidden regions along the wires. Therefore, a phase-space semiclassical approximation to dynamics seems not to be valid here, and this is particularly relevant if the corresponding classical motion exhibits chaos [17].

A relevant question, from both the theoretical and experimental points of view, is how strongly the properties of the bound states depend on the perturbation of the structure and, this way, on the mechanical imperfections. Amongst other factors, it is perhaps the geometry of the configuration that plays the fundamental role since it controls the coupling with the propagating modes. Some studies suggested that the isolated bounded modes are not affected by the level of geometrical symmetry and thus they can exist under very general conditions [18]. For theoretical and experimental reasons it is often convenient to consider geometries with coupled arms of equal widths. Obviously, such ideal configurations are hardly technically available. Nevertheless, for certain geometries an analysis of the impact on the discrete spectrum of a perturbation of this kind of symmetry is still lacking.

In a classical paper written more than 20 years ago Schult, Ravenhall and Wyld [19] studied the problem of an electron which can freely move in a two-dimensional symmetric region of orthogonally crossed wires of finite and equal width and infinite length. They showed that the ground state of this system corresponds to a state where the electron is confined in the region of the crossing, with an energy which falls below the threshold of the continuum, \( E_{\text{TH}} \). Using two different numerical approaches (finite differences and a mode expansion) they estimated the ratio between the ground-state energy and the threshold energy, \( E_1/E_{\text{TH}} \approx 0.66 \). They also identified a second bound state, with odd–odd symmetry, corresponding to a ratio \( E_2/E_{\text{TH}} \approx 3.72 \). The energy of this second state falls below the threshold of the continuum for odd–odd states, confirming the result in [20] for an L-shaped waveguide. These results were later supported by Avishai et al [21]. More recently, Amore, Fernández and Rodríguez [22], have used the conformal collocation method (CCM) [23] to obtain a precise value for the ground
state of the infinite cross, using a non-uniform grid. They obtained \( E_1/E_{TH} \approx 0.659611 \). Trefethen and Betcke [24], on the other hand, have obtained a precise value for the second bound state, \( E_2/E_{TH} \approx 3.71648 \) (note that these authors report the value of \( E_2 \), from which the ratio can be obtained).

Different geometries are closely related to the symmetric cross. Bulgakov and collaborators have studied the properties of a configuration of non-orthogonal (scissor-shaped) crossed wires, observing the emergence of multiple bound states below the continuum as the angle between the arms is reduced [25]. Bound states have also been found in a waveguide with straight segments and a rectangular bending [26].

A particular case of T-shaped waveguide is obtained from the symmetric cross by desymmetrizing the region for even–odd modes, although this particular system does not support bound states. Nazarov [27] analysed the bound states of a similar configuration, but with arms of different widths.

Moreover, a L-shaped waveguide is obtained by desymmetrizing the region for the odd–odd modes and, as was mentioned above, the existence of a bound state in the corresponding symmetric configuration was shown in [19–21].

Therefore, in all these cases the relative width of the coupled arms may be relevant for the spectrum. By an asymmetric configuration, here we will understand different widths of the orthogonal arms. Taking that into account, in this paper, we study asymmetric variations of the above-mentioned geometries. Starting with the symmetric cross discussed by Schult et al [19], our goal is to investigate the behaviour of the bound states of this system, as one of the arms is enlarged, and the possibility of the disappearance of these states or the appearance of new bound states. The related L- and T-shaped configurations are also analysed. We will focus on planar waveguides: we expect the qualitative analysis of three-dimensional configurations to be a generalization of those carried out here (see, for instance, [28] where a similar problem is solved in a conical layer), nevertheless, confirming the corresponding results with numerical calculations is beyond our current computational capabilities.

The paper is organized as follows: in section 2, we describe the system of the asymmetric cross and study the behaviour of the bound states as one of the arms is enlarged; in section 3, we present the numerical results, which have been obtained using a collocation method; finally, in section 4, we draw our conclusions.

2. The asymmetric cross

As we have mentioned in the introduction, Schult, Ravenhall and Wyld [19] have proved that an electron which moves freely in an infinite symmetric cross is localized in the central region of the cross when it finds itself in the ground state. They also discovered a second localized state, which is the lowest energy state with odd–odd symmetry.

The goal of our paper is to investigate the behaviour of these modes (as well as the possible appearance of further localized states), as the width of one of the two arms is changed, thus obtaining the asymmetric cross. An extremal case with \( w_x \ll w_y \) is shown in figure 1.

In particular, we ask ourselves whether the localized modes of the symmetric cross can survive to arbitrary perturbations of this kind: what happens when one of the arms is much smaller than the other? Would we still have bound states? What does this imply for the L- and T-shaped configurations?

To answer our questions we need to solve the scalar Helmholtz equation

\[
-\frac{1}{2}\Delta \Psi_n(x, y) = E_n \Psi_n(x, y),
\]  

(1)
where \((x, y) \in \Omega = \{|x| < w_x/2, |y| < w_y/2\}\), and we are using \(\hbar/m = 1\). The wavefunctions obey Dirichlet boundary conditions on \(\partial \Omega\). We have called the widths of the two arms \(w_x\) and \(w_y\), defining \(\beta = w_y/w_x\). In all our calculations, we will consider only configurations with \(\beta \geq 1\), since the case with \(\beta < 1\) corresponds just to a rotation of the domain. For \(\beta = 1\) one recovers the symmetric cross.

Before trying to answer our question in a quantitative way, we may attack the problem qualitatively. First of all, note that for \(\beta > 1\) the vertical arms of the cross can be regarded as an outward local deformation of the horizontal strip. In this case, an effective attraction arises. Following closely \(29\), we can simply assume that there is such a \(b > 0\) that the triangle spanned by the points \((-w_x/2, w_y/2), (w_x/2, w_y/2), (0, w_y/2 + b)\) is in the upper arm, while another spanned by the points \((-w_x/2, -w_y/2), (w_x/2, -w_y/2), (0, -w_y/2 - b)\) is in the lower arm. We note that, since \(\beta \geq 1\), the threshold for the continuum is determined by the horizontal band. We may use a variational argument to obtain an upper bound for the energy of the fundamental mode; define the following trial function:

\[
\hat{\psi}_{\alpha \delta}(x, y) = \begin{cases} 
\sin \left( \frac{\pi (y + w_y)}{w_y} \right) e^{-\delta |x - \frac{w_x}{2}|}, & |x| > \frac{w_x}{2}, |y| < \frac{w_y}{2}, \\
\sin \left( \frac{\pi [y + w_y + \alpha (1 - \frac{2|x|}{w_x})]}{w_y + 2\alpha (1 - \frac{2|x|}{w_x})} \right), & |x| \leq \frac{w_x}{2}, |y| < \frac{w_y}{2} + \alpha \left( 1 - \frac{2|x|}{w_x} \right), \\
0, & \text{otherwise},
\end{cases}
\]

where \(0 < \alpha < b\) and \(\delta > 0\). We then obtain

\[
E(\hat{\psi}_{\alpha \delta}) = \frac{||\nabla \hat{\psi}_{\alpha \delta}||^2}{2||\hat{\psi}_{\alpha \delta}||^2},
\]

\[
= 6\alpha (\pi^2 + \delta^2 \beta^2 w_y^2) - \delta \beta (4\alpha^2 (6 + \pi^2) + 3\pi^2 w_x^2) \log \left( \frac{\beta w_x}{2\alpha + \beta w_y} \right).
\]

As \(\beta\) grows, the minimum of \(E\) is reached for smaller values of \(\alpha\) and \(\delta\). This corresponds to a wavefunction which decays slowly in the wider arm, away from the crossing, and which extends itself just in a reduced portion of the narrower arm. Thus, for \(\beta \gg 1\) we can expand in series and obtain

\[
E(\hat{\psi}_{\alpha \delta}) = \frac{\pi^2}{2w_y^2} \left( 1 - \frac{2\alpha \delta}{\beta} \right) + O(\alpha^2 \delta) + O(\delta^2) < \frac{\pi^2}{2w_y^2},
\]
where for the inequality we used that $\alpha$ and $\delta$ can be chosen small enough. Therefore, for the cross configuration there will be a bound state below the continuum as long as the width of the vertical arms remains finite.

We can also study the remaining lowest modes in each symmetry class. In figures 2, 3 and 4 we display the desymmetrized regions corresponding to the symmetry classes of modes with even–odd, odd–even and odd–odd respectively.
First of all, the even–odd case of figure 2 is analogous to that of figure 1. Recalling that now the width of the horizontal arm is taken to be \( w_y / 2 \) and the corresponding threshold is \( 2\pi^2 / w_y^2 \), then the existence of a bound state for \( \beta > 2 \) can be proved using the volume enlarging argument with a triangle \((-w_x / 2, w_x / 2), (w_x / 2, w_y / 2) \) and \((0, w_y / 2 + b)\) in the semi-infinite arm.

For \( \beta < 2 \), the continuous dependence of discrete eigenvalues on deformations of domains with Dirichlet conditions [30] implies that this bound state persists, but it must be localized in the semi-infinite arm (which is now the wider arm).

Thus, for \( 1 < \beta < 2 \), we consider two triangular bumps in the horizontal arms of figure 2 and use the following trial function:

\[
\hat{\Psi}_{a0}(x, y) = \begin{cases} 
\frac{w_y}{2} \sin \left( \frac{\pi}{w_x} \left( x + \frac{w_x}{2} \right) \right) e^{-\delta \left| y - \frac{w_y}{2} \right|}, & |x| < \frac{w_x}{2}, |y| > \frac{w_y}{2}, \\
y \sin \left( \frac{\pi}{w_x} \left( x + \frac{w_x}{2} + \alpha \left( 1 - \frac{2|x|}{w_y} \right) \right) \right), & |x| < \frac{w_x}{2} + \alpha \left( 1 - \frac{2|x|}{w_y} \right), |y| \leq \frac{w_y}{2}, \\
0, & \text{otherwise.}
\end{cases}
\]

Applying the variational method, we obtained an explicit expression for the variational energy, which we do not report here because it is lengthy and not very informational; expanding this expression in series for \( \alpha \) and \( \delta \) we obtain

\[
E(\tilde{\Psi}_{a0}) = \frac{\pi^2}{2w_x^2} \left[ 1 + \delta \left( \frac{4w_x}{\pi^2 \beta - \alpha \beta^2 / 3} \right) \right] + O(\delta^2) + O(\delta^3).
\]

For a given \( \beta \), we minimized the full variational energy over \( \alpha \) and \( \delta \) and found that there is a critical value \( \beta_* \approx 1.828 \) above which there is a bound state localized in the semi-infinite strip. In section 3, we will obtain a more precise value of \( \beta_* \) by means of numerical calculations.

Let us now rotate our system 90° and consider a T configuration like that in figure 3. We denote this domain by \( \Omega \) and its area measure by \( dA \). Next, we decouple the infinite and semi-infinite arms by considering just the Dirichlet conditions \( \Psi(0, y) = 0 \) in the infinite arm (\( \Omega_1 = \{0 \leq x \leq w_x / 2, -\infty < y < \infty\} \)) and \( \Psi(x, -w_y / 2) = \Psi(x, w_y / 2) = 0 \) in the semi-infinite one (\( \Omega_2 = \{w_x / 2 \leq x \leq \infty, -w_y / 2 \leq y \leq w_y / 2\} \)). With such conditions we can now estimate

\[
\int_{\Omega} |\nabla \Psi|^2 \, dA \geq \int_{\Omega_1} \left| \frac{\partial \Psi}{\partial x} \right|^2 \, dA + \int_{\Omega_2} \left| \frac{\partial \Psi}{\partial y} \right|^2 \, dA
\]

\[
= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left| \frac{\partial \Psi}{\partial x} \right|^2 \, dx \, dy + \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left| \frac{\partial \Psi}{\partial y} \right|^2 \, dx \, dy
\]

\[
\geq \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{\pi^2}{w_x^2} |\Psi|^2 \, dx \, dy + \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{\pi^2}{w_y^2} |\Psi|^2 \, dx \, dy
\]

\[
= \pi^2 \int_{\Omega_1} |\Psi|^2 \, dA + \pi^2 \int_{\Omega_2} |\Psi|^2 \, dA \geq \frac{\pi^2}{w_x^2} \int_{\Omega_1} |\Psi|^2 \, dA + \frac{\pi^2}{w_y^2} \int_{\Omega_2} |\Psi|^2 \, dA,
\]

where in the third line we used Poincaré inequalities corresponding to each type of Dirichlet condition, and for the last inequality we take into account that \( \beta \geq 1 \). Thus,

\[
\frac{1}{2} ||\nabla \Psi||^2 - \frac{\pi^2}{2w_y^2} ||\Psi||^2 \geq 0,
\]

and for the odd–even case there is no spectrum below the threshold of the continuum if \( \beta \geq 1 \), implying (after rotating our system back) that there is no bound state for the even–odd case when \( \beta \leq 1 \).
Finally, for the L-shaped configuration in figure 4, as we have already mentioned, it is known that there is a discrete eigenvalue for $\beta = 1$ [19–21]. Because of the continuous dependence of discrete eigenvalues on domain deformations [30], this bound state will persist for certain $\beta > 1$ as well. Nevertheless, we have performed a similar calculation as in equation (2) by decoupling the horizontal and vertical arms and using the corresponding Poincaré inequalities, and have found out that there is no bound state for any $\beta \geq 2$. As for the even–odd case, we could use the variational method to estimate the corresponding critical value where the state gets unbounded but, looking for accuracy, we will rather obtain this value numerically in section 3.

3. Numerical results

The arguments given in the previous section were useful to establish the existence of bound states in the analysed configurations, however, they do not give precise quantitative information about the critical values of $\beta$ for the existence of the different bound states. Thus, here we verify, by numerically solving equation (1), that the results obtained in the previous section are correct, and look for accurate predictions for the critical values of $\beta$.

We now illustrate the method that we have used in our calculations. Upon a simple rescaling of the $y$-axis, defining $y' = y/\beta$ ($x' = x$), we write equation (1) in the form of a modified Helmholtz equation

$$\frac{1}{2} \left( \frac{\partial^2}{\partial x'^2} + \frac{1}{\beta^2} \frac{\partial^2}{\partial y'^2} \right) \psi_n(x', y') = E_n \psi_n(x', y'),$$

(4)

which allows us to work on an infinite symmetric cross of width $w_x$, with $\beta$ playing the role of a parameter.

As we are interested in the bound states of equation (4), we may ‘cut’ the cross at some large but finite distances $L_x$ and $L_y$ by imposing Dirichlet boundary conditions at $x = \pm L_x$ and $y = \pm L_y$. If $L_x$ and $L_y$ are large enough the wavefunctions of the bound states are exponentially small at larger distances and the error introduced by this approximation is negligible compared to the error due to the discretization. In general, for $\beta \gg 1$, one may choose $L_x \gg L_y$, as the probability density is mostly concentrated on the wider arm. The maximum size of $L_x$ and $L_y$ is essentially dictated by the total number of collocation points corresponding to this choice.

On the other hand, excessively large values of $L_x$ and $L_y$ should be avoided, since they increase the number of collocation points and therefore the computational power needed in the calculation.

To discretize equation (4), we use a collocation approach based on ‘tent functions’ (TF): on the interval $|x| \leq L$ we define the uniform grid, whose $N - 1$ points are $x_k = 2Lk/N$, where $N$ is an even integer and $k = -N/2 + 1, -N/2 + 2, \ldots, N/2 - 1$. The tent function peaked at the point $x_k$ is defined as

$$\phi_k(x) = \begin{cases} \frac{x - x_{k-1}}{x_k - x_{k-1}}, & x_{k-1} \leq x \leq x_k \\ \frac{x_{k+1} - x}{x_{k+1} - x_k}, & x_k \leq x \leq x_{k+1} \\ 0, & x < x_{k-1}, x > x_{k+1} \end{cases}$$

(5)

A function $f(x)$ obeying Dirichlet boundary conditions at $x = \pm L$ ($f(\pm L) = 0$) can be interpolated using the TF as

$$f^{(\text{TF})}(x) = \sum_{k=-N/2+1}^{N/2-1} f(x_k) \phi_k(x) \approx f(x).$$

(6)
Figure 5. Ratio $E^{(ee)}/E_{TH}$ as a function of $\beta$ for the asymmetric cross; the solid line is the least-squares fit $E_1/E_{TH} = 1.003 - 0.505\beta^{-3.23725} + 0.165\beta^{-6.475}$.

For a higher dimensional problem, the same procedure may be followed, using multidimensional TFs which are the direct product of the TFs along each orthogonal direction:

$$\Phi_{i_1,i_2,\ldots,i_d}(x_1,x_2,\ldots,x_d) = \phi_{i_1}(x_1) \phi_{i_2}(x_2) \ldots \phi_{i_d}(x_d).$$

In principle, the interpolation of a $d$-dimensional function on a $d$-dimensional region $|x_i| \leq L_i$, requires $M = \prod_{i=1}^{d} (N_i - 1)$ points.

The eigenvalue equation (4) may then be converted to a matrix eigenvalue problem calculating the matrix elements of the Hamiltonian operator between all the functions of a set: the size of the matrix depends on the total number of functions used in the calculation, which rapidly grows with the dimensionality of the problem. A drastic reduction of the number of functions however can be achieved by considering only functions which are peaked at points internal to the cross.

A second observation concerns the choice of $N_i$, i.e. the number of collocation points in each orthogonal direction: although in principle, $N_i (i = 1,\ldots,d)$ can take any integer value, it is convenient to pick values of $N_i$, which allows us to sample exactly the border of the cross. The eigenvalues obtained for different grids sampling the border of the domain provide a monotonic sequence of values, which allows us to obtain a good approximation via extrapolation [31].

Before calculating the eigenvalues of the asymmetric cross, we have tested this collocation method on the symmetric cross, for which a precise result is available [22]. The method used in that case is the CCM [23]. Working with grids with $N = N_x = N_y = 80, 120, \ldots, 880$ we have calculated the lowest eigenvalue of the corresponding collocation matrix, obtaining a monotonic sequence of values: the most accurate value, corresponding to the finest grid, provides a ratio $E_1/E_{TH} = 0.66166$, which is just 0.3% above the value reported by Amore et al [22]. We have also performed a least-square fit of the monotonic sequence of values with the functional form $a_1 + a_2/N^\gamma + a_3/N^{2\gamma} + a_4/N^{3\gamma}$, obtaining $a_1 = 0.65955$, which differs just 0.1% from the value previously reported [22]. This test makes us confident that our results are precise.

We can now present the results obtained for the asymmetric cross, discussing separately the states with different symmetries. In all cases, we expect that the wavefunction of a bound state will decay exponentially as one moves far away from the centre of the cross; in particular, the variational approach in the previous section predicts $|\Psi(x, y)|_\text{fixed} \approx e^{-x/\ell_x}$ for $|x| \gg w_x/2$. 
in the limit $\beta \geq 1$. We have found that there is at most only one bound state in each symmetry class.

### 3.1. Even–even state

We first study the lowest energy state with even–even symmetry of the asymmetric cross. In the third column of table 1, we report the values of the ratio $E^{(ee)}/E_{TH}$, obtained for different values $\beta$. We used three different sets, corresponding to $L = 20$ and $N = 600$ (set I), $L = 40$ and $N = 800$ (set II) and $L = 100$ and $N = 1600$ (set III). The fourth and fifth column report the values of the decay lengths $\ell_x$ and $\ell_y$ obtained fitting the numerical eigenfunctions with
0.662 960 1.098 1.098
0.723 925 1.335 1.006
0.774 665 1.613 0.938
0.816 242 1.936 0.887
0.849 968 2.309 0.847
0.879 058 2.770 0.818
0.900 702 3.267 0.793
0.918 059 3.830 0.773
0.931 999 4.463 0.757
0.943 228 5.172 0.744
0.952 308 5.960 0.733
0.959 682 6.832 0.723
0.965 821 7.959 0.717
0.970 627 9.053 0.711
0.974 578 10.252 0.705
0.977 844 11.564 0.700
0.980 557 12.992 0.696
0.982 821 14.542 0.690
0.984 719 16.219 0.689
0.986 319 18.026 0.689
0.987 674 19.965 0.685

the asymptotic behaviour \( \Psi(x, 0) \approx e^{-x/\ell_x} \) and \( \Psi(0, y) \approx e^{-y/\ell_y} \), respectively for \( |x| \gg w_x/2 \) and \( |y| \gg w_y/2 \).

These values are plotted in figures 5 and 6. The dependence on \( \beta \) is described very accurately by simple least-square fits. In particular, within the accuracy of our calculations, the fit of \( E^{(ee)}/E_{TH} \) is consistent with the survival of the bound state for \( \beta \to \infty \).
Figure 9. Ratio $E^{(oo)}/E_{TH}$ as a function of $\beta$ for the asymmetric cross; the solid line is the least-squares fit $E^{(oo)}/E_{TH}^{\text{FIT}} = -15.61 - 15.56\beta^{1.974} + 34.88\beta^{0.9869}$.

Figure 10. $\ell_x$ and $\ell_y$ as a function of $\beta$ for the lowest odd–odd state of the asymmetric cross; the solid and dashed lines are the least-squares fits $\ell_x^{\text{FIT}} = 0.0108614/(1 - 0.992232\beta^{0.067332})$ and $\ell_y^{\text{FIT}} = 0.514767 + 0.81312\beta^{-12.3632}$. The vertical line corresponds to the critical value $\beta^{*} = 1.2279$, where $\ell_x^{\text{FIT}}$ is singular.

Note that $\ell_x$ grows roughly cubically in $\beta$ for $\beta \gg 1$, limiting the range of values of $\beta$ where the numerical calculation can be performed. As an example, in figures 7 and 8 we show different representations of our numerical results for the wavefunction of the lowest even–even state for $\beta = 2$ (in these figures, as well in the other figures representing the wavefunctions, the region of the plot is smaller than the actual region where the numerical calculations were performed).

3.2. Odd–odd state

As was found previously [19, 20], the symmetric cross ($\beta = 1$) has a second bound state, which has odd–odd symmetry and therefore it is also an eigenstate of an infinite $L$. According to our results in the previous section, we expect that this state becomes unbound at some finite $\beta$.

In table 2, we report the results for the ratio $E^{(oo)}/E_{TH}$ (second column) and for the longitudinal and transverse length scales, $\ell_x$ and $\ell_y$ (third and fourth columns). In this case
Figure 11. Wavefunction of the lowest odd–odd state for $\beta = 1.1$.

Table 2. The ratio $E^{(oo)}/E_{TH}$ for the lowest odd–odd state of the asymmetric cross. All the results are obtained using $L = 100$ and $N = 1600$.

| $\beta$ | $E^{(oo)}/E_{TH}$ | $\ell_x$ | $\ell_y$ |
|---------|-------------------|----------|----------|
| 1.00    | 3.720 42          | 1.332    | 1.332    |
| 1.01    | 3.756 11          | 1.465    | 1.232    |
| 1.02    | 3.788 77          | 1.623    | 1.148    |
| 1.03    | 3.818 39          | 1.816    | 1.076    |
| 1.04    | 3.844 99          | 2.055    | 1.014    |
| 1.05    | 3.868 55          | 2.359    | 0.960    |
| 1.06    | 3.889 09          | 2.760    | 0.912    |
| 1.07    | 3.906 59          | 3.313    | 0.870    |
| 1.08    | 3.921 07          | 4.125    | 0.832    |
| 1.09    | 3.932 52          | 5.429    | 0.797    |
| 1.10    | 3.940 95          | 7.875    | 0.766    |
| 1.11    | 3.946 35          | 14.119   | 0.739    |
| 1.111   | 3.946 73          | 15.322   | 0.735    |
| 1.112   | 3.947 07          | 16.745   | 0.733    |
| 1.113   | 3.947 39          | 18.456   | 0.730    |
| 1.114   | 3.947 67          | 20.549   | 0.728    |
| 1.115   | 3.947 92          | 23.167   | 0.726    |
| 1.116   | 3.948 15          | 26.528   | 0.722    |

the length scales are obtained fitting the asymptotic behaviour of the wavefunction with

$\Psi(x, w_x/3) \approx e^{-x/\ell_x}$ and $\Psi(w_y/3, y) \approx e^{-y/\ell_y}$, respectively for $|x| \gg w_x/2$ and $|y| \gg w_y/2$, since the wavefunction vanishes for $x = 0$ or $y = 0$.

In figure 9, we report the results for $E^{(oo)}/E_{TH}$ of table 2 and compare them with the least-squares fit

$$E_1^{(oo)}/E_{TH}^{\text{FIT}} = -15.61 - 15.56\beta^{1.974} + 34.88\beta^{0.9869}.$$ 

Note that the fit has a maximum corresponding to $\beta = 1.12288$. 

12
Figure 12. Wavefunction of the lowest odd–odd state for $\beta = 1.1$.

Figure 13. Wavefunction of the lowest even–odd state for $\beta = 1.55$.

In figure 10, we display the length scales $\ell_x$ and $\ell_y$ as functions of $\beta$, and compare them with the fits

$$\ell_x|_{\text{FIT}} = \frac{0.0108614}{1 - 0.992232\beta^{0.0673327}},$$

and

$$\ell_y|_{\text{FIT}} = 0.514767 + \frac{0.81312}{\beta^{12.3632}}.$$
Table 3. The ratio $E^{(oo)} / E_{TH}$ for the lowest odd–odd state of the asymmetric cross. All the results are obtained using $L = 100$ and $N = 1600.$

| $\beta$ | $E^{(oo)} / E_{TH}$ | $\ell_x$ | $\ell_y$ |
|-------|---------------------|---------|---------|
| 1.530 | 2.332 33            | 0.767   | 29.993  |
| 1.531 | 2.335 26            | 0.768   | 28.322  |
| 1.532 | 2.338 17            | 0.769   | 26.830  |
| 1.533 | 2.341 08            | 0.771   | 25.490  |
| 1.534 | 2.343 99            | 0.772   | 24.279  |
| 1.535 | 2.346 89            | 0.773   | 23.179  |
| 1.536 | 2.349 78            | 0.774   | 22.176  |
| 1.537 | 2.352 67            | 0.775   | 21.258  |
| 1.538 | 2.355 55            | 0.777   | 20.415  |
| 1.539 | 2.358 43            | 0.778   | 19.637  |
| 1.54  | 2.361 30            | 0.779   | 18.917  |
| 1.55  | 2.389 74            | 0.791   | 13.879  |
| 1.56  | 2.417 64            | 0.803   | 10.999  |
| 1.57  | 2.445 02            | 0.816   | 9.136   |
| 1.58  | 2.471 90            | 0.828   | 7.832   |
| 1.59  | 2.498 27            | 0.841   | 6.869   |
| 1.6   | 2.524 15            | 0.854   | 6.127   |
| 1.7   | 2.757 75            | 0.992   | 3.087   |
| 1.8   | 2.951 02            | 1.148   | 2.172   |
| 1.9   | 3.110 87            | 1.322   | 1.734   |
| 2.0   | 3.243 15            | 1.516   | 1.478   |
| 2.1   | 3.552 74            | 1.732   | 1.311   |
| 2.2   | 3.443 67            | 1.971   | 1.195   |
| 2.3   | 3.519 29            | 2.235   | 1.109   |
| 2.4   | 3.582 33            | 2.525   | 1.043   |
| 2.5   | 3.635 03            | 2.842   | 0.992   |
| 2.6   | 3.679 22            | 3.189   | 0.951   |
| 2.7   | 3.716 38            | 3.567   | 0.917   |
| 2.8   | 3.747 74            | 3.977   | 0.890   |
| 2.9   | 3.774 30            | 4.421   | 0.866   |
| 3.0   | 3.796 85            | 4.902   | 0.847   |
| 4.0   | 3.904 24            | 12.077  | 0.747   |
| 5.0   | 3.932 52            | 24.947  | 0.717   |

We believe that this plot offers convincing evidence of the existence of a singularity in $\ell_y$ close to $\beta_{\text{oo}}^\text{\star} = 1.2279$: for $\beta \geq \beta_{\text{oo}}^\text{\star}$ the wavefunction becomes unbound, in agreement with our earlier result. As an example, in figures 11 and 12 we show different representations of our numerical output for the wavefunction of the lowest odd–odd state for $\beta = 1.1.$

3.3. Even–odd state

In table 3, we report the results for $E^{(oo)} / E_{TH}, \ell_x$ and $\ell_y$ of this state, calculated using $L = 100$ and $N = 1600.$ The behaviour of the lowest even–odd state is rich and it is characterized by three different types of behaviour: a first region, below a critical value of $\beta$, where the wavefunction is unbound; a second region, where the wavefunction is bound, but mainly localized in the vertical arm (see, for instance, figures 13 and 14), and a third region, where the wavefunction is still bound, but mainly localized in the horizontal arm (see, for instance, figures 15 and 16).

The ratio $E_{TH}^{(oo)} / E_{TH}$ is plotted in figure 17 and compared with the fit

$$E_{1}^{(oo)} / E_{TH} \bigg|_{\text{FIT}} = 3.96521 + \frac{11.0968}{\beta^{2.38923}} - \frac{10.156}{\beta^{3.69462}}.$$
As for the even–even state, this behaviour is consistent with the survival of the bound state for $\beta \to \infty$.

In figure 18, we plot $\ell_x$ and $\ell_y$ and compare with them the fits

$$\ell_{x,y}^{\text{FIT}} = 0.129087\beta^{3.26312} + 0.258401$$
Figure 16. Wavefunction of the lowest even–odd state for $\beta = 3$.

Figure 17. Ratio $E^{(eo)} / E_{TH}$ as a function of $\beta$ for the asymmetric cross; the solid line is the least-squares fit $E^{(eo)} / E_{TH}^{\text{FIT}} = 3.96521 + \frac{11.0968}{\beta^2} - \frac{10.156}{\beta^4}$. 

and

$$\ell_y^{(\text{FIT})} = \frac{0.604788}{1 - \frac{2164.67}{\beta^2}}.$$  

The singularity of $\ell_y^{(\text{FIT})}$ is located at $\beta_{\star}^{(eo)} = 1.513$ (the vertical line in the plot) and represents the critical value where the bound state appears. Note also that $\ell_y^{(\text{FIT})} \approx \ell_y^{(\text{FIT})}$ for $\beta = 2$.

### 3.4. Odd–even state

In the case of the odd–even states we have not been able to find a bound solution for any of the $\beta \geq 1$ values considered. Once again this behaviour is consistent with our earlier results.
4. Conclusions

For years now, it has been verified theoretically as well as experimentally that the spectra of waves or quantum particles moving in several open two-dimensional systems can exhibit bound states.

For numerical and experimental reasons it is often convenient to consider domains with some degree of symmetry, for instance, waveguides and wires coupled in cross, T- and L-shaped configurations with a ratio of the widths of the crossing branches ($\beta$) equal to unity. However, for applications it is important to find out how the corresponding spectra are modified when $\beta \neq 1$.

In particular, we have shown here, both analytically and numerically, that the bound state of the symmetric cross persists for any finite value of $\beta$. Richer behaviour is obtained for the T-shaped configuration as the width of the semi-infinite arm of the T tends to zero (i.e. $\beta \to \infty$): from $\beta = 1$ up to $\beta^{*}_{eo} = 1.513$ the wavefunction is unbound; above that critical value and up to 2 the wavefunction is localized on the semi-infinite arm of the T; if $\beta$ is still increased, the wavefunction gets localized on the infinite arm of the T. For this configuration no bound state arises when the width of the infinite arm is decreased from the symmetric case towards zero. Of course, in either of these two setups, when a bound state exists, it must disappear as soon as the width of the decreasing branch reaches zero. This implies that adding just a small perturbation on a very large two-dimensional quantum wire or waveguide may have a striking impact on the transport of charge carriers or waves along it. This is consistent with the known fact that any small bump in a waveguide leads to bound states.

Finally, for the L-shaped configuration, we have found that the bound state existing for the symmetric configuration becomes unbounded at the critical value $\beta^{*}_{lo} = 1.2279$ of the ratio of the width of the intersecting branches.

How strong these effects are, so as to be observable and applicable, will depend on how strong is the departure of the actual experimental setup from the ideal configurations considered. Nevertheless, if the results found here are confirmed by future experiments, then tuning the ratio of the widths of the coupled waveguides or wires could be used as a switch-like mechanism for trapping and untrapping waves and charge carriers. This would give rise to a number of important applications.
Acknowledgments

We acknowledge the detailed criticisms and suggestions of one of the anonymous reviewers which really helped us to improve the results reported in this paper. We thank R Sáenz for valuable discussions. This research was supported by the Sistema Nacional de Investigadores (México). The work of CAT-E was also partially funded by PROMEP (México) under grant PROMEP/103.5/10/4948.

References

[1] Ursell F 1951 Proc. Camb. Phil. Soc. 47 348
[2] Ursell F 1952 Proc. R. Soc. Lond. A 214 79–97
[3] Weinstein L A 1966 Open Resonators and Open Waveguides (Moscow: Sovetskoe Radio) (in Russian)
   Weinstein L A 1969 Open Resonators and Open Waveguides (Boulder, CO: Golem) (Engl. transl. by
   P Beckmann)
[4] Sakaki H 1984 Proc. Int. Symp. on Foundations of Quantum Mechanics in the Light of New Technology
   ed S Kamefuchi et al (J. Phys. Soc. Japan) pp 94–110
[5] Exner P and Seba P 1989 J. Math. Phys. 30 2574
[6] Goldstone J and Jaffe R L 1992 Phys. Rev. B 45 14100–7
[7] Carini J P, Londergan J T, Murdock D P, Trinkle D and Yung C S 1997 Phys. Rev. B 55 9842
[8] Londergan J T, Carini J P and Murdock D P 1999 Binding and Scattering in Two-dimensional Systems:
   Applications to Quantum Wires, Waveguides, and Photonic Crystals (Berlin: Springer)
[9] Blank J, Exner P and Havlek M 2008 Hilbert Space Operators in Quantum Physics (Berlin: Springer)
[10] Roukes M L, Scherer A, Allen S J Jr, Craighead H G, Ruthen R M, Beebe E D and Harbison J P 1987 Phys.
    Rev. Lett. 59 3011
[11] Timp G, Baranger H U, deVegvar P, Cunningham J E, Howard R E, Behringer R and Mankiewich P M 1988
    Phys. Rev. Lett. 60 2081
[12] Ammino G, Cassettari M and Martinelli M 2006 arXiv:physics/0603154
[13] Bromley M W J and Esry B D 2003 Phys. Rev. A 68 043609
[14] Ou S-X and Geller M R 2004 Phys. Rev. B 70 85414
[15] Hill Martin T et al 2007 Nature Photonics 1 589–94
[16] Exner P and Zagrebnov V A 2005 J. Phys. A: Math. Gen. 38 L463
[17] Exner P, Seba P, Tater M and Vank D 1996 J. Math. Phys. 37 4867
[18] Ammino G, Yashiro H, Cassettari M and Martinelli M 2006 Phys. Rev. B 73 125308
[19] Schult R L, Ravenhall D G and Wyld H W 1989 Phys. Rev. B 39 5476–9
[20] Exner P, Seba P and Stovicek P 1989 Czech. J. Phys. B 39
[21] Avishtai Y, Bessis D, Giraud B G and Mantica G 1991 Phys. Rev. B 44 8028–34
[22] Amore P, Fernández F M and Rodriguez M 2011 Variational collocation with non uniform grids Preprint
[23] Amore P 2008 J. Phys. A: Math. Theor. 41 265206
[24] Trefethen L N and Betcke T 2006 AMS Contemp. Math. 412 297
[25] Bulgakov E N, Exner P, Pichugin K N and Sadreev A F 2002 Phys. Rev. B 66 155109
[26] Sadurni E and Schleich W P 2010 arXiv:1011.0694
[27] Nazarov S A 2010 Acoust. Phys. 56 1004–15
[28] Exner P and Tater M 2010 arXiv:1006.0137
[29] Bulla W, Gesztesy F, Renger W and Simon B 1997 Proc. AMS 125 1487
[30] Freitas P and Krejcirik D 2007 Math. Res. Lett. 14 107–11
[31] Amore P and Chowell D 2010 J. Sound Vib. 329 1362–75