Addendum to: “Periodic quantum wires and their quasi-one-dimensional nature”

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The discussion of bound states in section 2.2 of our paper [J. Phys. D **26**, 798-803 (1993)] was incorrect. A proper treatment is presented here.

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I. INTRODUCTION

Our paper [1] concerned a simple framework for understanding the properties of a periodic two-dimensional quantum wire. By periodic we mean a system consisting of straight leads of uniform width connecting a finite number of equally spaced (separation ℓ) cavities of arbitrary shape. The external leads are infinite. In the low-energy regime, one can make the (one-dimensional) approximation of considering only a single mode of transmission in the leads connecting the cavities. The scattering properties of a single cavity are expressed through the transmission $t(k)$ and reflection $r(k)$ amplitudes of this mode from which the transfer matrix is constructed (assuming time-reversal symmetry) in the form [2]

$$\mathbf{M} = \begin{pmatrix} \frac{1}{t(k)} & \frac{r(-k)}{t(-k)} \\ \frac{r(k)}{t(k)} & \frac{1}{t(-k)} \end{pmatrix} \tag{1}$$

Here, the wave function is represented in terms of right and left moving waves on each side of the cavity,

$$\Psi(x) = f_1(k,x)e^{ik(x-x_\alpha)} + f_2(k,x)e^{-ik(x-x_\alpha)} \tag{2}$$

and the amplitudes on opposite boundaries of a cell at $x_\alpha = x_L, x_R$, are related by

$$\begin{pmatrix} f_1 \\ f_2 \end{pmatrix}_L = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} \begin{pmatrix} f_1 \\ f_2 \end{pmatrix}_R \tag{3}$$

A cell consists of one cavity and a length ℓ of connecting lead in which the potential is zero. For a system of N-cells, the transfer matrix is simply the product $\mathbf{M}^N$. Unitarity implies that $\det(\mathbf{M}) = 1$, and therefore it satisfies the equation

$$\mathbf{M}^2 = (2\cos\phi)\mathbf{M} - \mathbf{I} \tag{4}$$

where we have defined the Bloch phase by $2\cos\phi = Tr(\mathbf{M})$. By induction one proves that

$$\mathbf{M}^N = \frac{\sin N\phi}{\sin\phi}\mathbf{M} - \frac{\sin(N-1)\phi}{\sin\phi}\mathbf{I} \tag{5}$$

From this, it is clear that the transfer matrix for a single cell plus the Bloch phase directly determines the scattering properties of an N-cell system.

II. BOUND STATES

Bound states may be considered as a special case where there is no incoming wave on either side of the system:

$$\begin{pmatrix} 0 \\ f_2 \end{pmatrix}_L = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix}^N \begin{pmatrix} f_1 \\ 0 \end{pmatrix}_R \tag{6}$$

and occur when $M_{11}^N = 0$. (Matrix elements of $\mathbf{M}^N$ are denoted by a superscript N.)

Above threshold, the physical transmission and reflection amplitudes for k real are boundary values of analytic functions, with the property $t(-z) = t(z^*)$, $r(-z) = r(z^*)$, relating points reflected in the imaginary axis. There is a cut along the real axis, and the values of the amplitudes on opposite sides of the cut are complex conjugates of each other. This makes $t(k^*) = t^*(k)$, when k is taken on the upper side of the cut. Hence, from eq. 1 we have $\cos\phi = ReM_{11}$.

Below threshold, the channel wave number becomes complex: $k \to i\kappa$, so incoming/outgoing waves become exponentially increasing/decreasing waves (as one moves away from the cell). When we analytically continue the elements of $\mathbf{M}$ onto the imaginary axis, they become real numbers, but this does *not* mean that the diagonal elements of M become equal. Rather, since $k = i\kappa$, one has $-k = k^*$, and the relation $t(-k) = t(k^*)$ just relates the amplitude to itself. The matrix elements of M involve $t(\pm\kappa)$ and $r(\pm\kappa)$ (see eq.16 below for an example). The symmetry which is preserved is time-reversal: one can exchange the labels 1 and 2 while $\kappa \to -\kappa$.

Below threshold, $\cos\phi$ must be computed from its definition as half the trace. So the statement, eq. 29 of [1] that bound states occur when $\cos N\phi = 0$, was wrong. However, we will see here that in most cases the bound states are not far from these positions.

The condition for a bound state of an N-cell system, $M_{11}^N = 0$ can be rewritten in several forms. To start,

$$\begin{aligned} M_{11}^N \sin\phi &= M_{11}\sin N\phi - \sin(N-1)\phi \\ &= \sin N\phi(M_{11} - \cos\phi) + \cos N\phi \sin\phi \\ &\equiv A(k)\sin(N\phi + \delta) \end{aligned} \tag{7}$$

where the phase δ is defined (between 0 and π) by

$$\begin{aligned} \tan\delta &= \frac{\sin\phi}{M_{11} - \cos\phi} \quad \text{and} \\ A^2(k) &= (M_{11})^2 - 2\cos\phi M_{11} + 1 \\ &= 1 - M_{11}M_{22} = -M_{12}M_{21} \end{aligned} \tag{8}$$

Note that M_{11}^N is independent of the sign of ϕ, because it involves the ratio of two sine-functions. In the physical region above threshold, ϕ starts at some initial value, say zero, and increases from there to π in the first allowed band, to 2π in the second, and so on. The sign of the cosine plays a vital role in all this, but it would change nothing if $-\phi$ were used everywhere. On the other hand, the *relative sign* of δ and ϕ is important, and this is set by the sign of the denominator in the first line of eq. 8. See also eq. 13 below.

The amplitude $A(k)$ can vanish only when we are dealing with a diagonal M matrix, with $M_{11} = e^{\pm i\phi}$. At a bound state of the single cell system, $M_{11} = 0$, and $A^2 = 1$. If $A(k)$ were to vanish in the allowed band, then that energy would give a bound state for all N including $N = 1$, in contradiction to the last statement. Hence, using eq. 7, the condition for a bound state of the N-cell system becomes

$$\chi_N \equiv N\phi + \delta = j\pi \quad , \quad j = 1, 2, ... \tag{9}$$

To understand the possibilities we examine the hypothetical situation in which $M_{11} = M_{22} = \cos\phi$, which makes $\delta = \pi/2$, and the bound-state condition becomes

$$\cos N\phi = 0 \tag{10}$$

with N solutions at $\phi_j = (j - 1/2)\pi/N$, $j = 1, 2, ...N$. This is the case discussed in the original article [1], but we now see that the bound states can occur anywhere within a strip of width π/N about these particular points. When N is large the strips are narrow, and that is why we found numerically that the average positions ϕ_j were a good approximation. However, we have assumed here that δ is constant, which is clearly not true, so this example does not give the whole story.

In the above, we have assumed that ϕ is a real angle. Below threshold, M_{ij} are real, but there is nothing to prevent $|\cos\phi| > 1$. This is a "forbidden zone", in which $\phi \to i\theta + s\pi$, with $s = 0$ when $\cos\phi > 1$ and $s = 1$ when $\cos\phi < -1$ [2]. Repeating the above arguments, and setting $\tan\delta = i\tanh\eta$, we have

$$M_{11}^N \sinh\theta = (-)^s A(k)\sinh(N\theta + \eta) \tag{11}$$

where

$$\begin{aligned} \tanh\eta &= \frac{\sinh\theta}{(-)^s M_{11} - \cosh\theta} \quad \text{and} \\ A^2(k) &= (M_{11})^2 - 2(-)^s\cosh\theta M_{11} + 1 = -M_{12}M_{21} \end{aligned} \tag{12}$$

As before, the amplitude can vanish only when we are dealing with a diagonal M matrix, with $M_{11} = (-)^s e^{\pm\theta}$. Because $\cosh\theta$ is always positive, the parameter s has been introduced to take care of the sign. For the same reasons discussed earlier, the relative sign of θ and η is determined by the sign of the denominator. The only way to have a zero of M_{11}^N is for there to be a cancellation between $N\theta$ and η in the argument of the hyperbolic sine in eq.11. It requires *opposite* signs of θ and η for this to occur.

To shed some further light, note that eq. 7 can also be written in the forms

$$\begin{aligned} M_{11}^N &= \cos N\phi + \frac{\sin N\phi}{\tan\delta} \\ &= \frac{1}{\sin\delta}\sin(N\phi + \delta) \\ &= (-)^s\big(\cosh N\theta + \frac{\sinh N\theta}{\tanh\eta}\big) \\ &= (-)^s\frac{1}{\sinh\eta}\sinh(N\theta + \eta) \end{aligned} \tag{13}$$

depending on whether one deals with the real or the imaginary case.

For the imaginary case, line four is most helpful. In some cases, $\tanh\eta$ passes through ± 1 at a particular energy, causing $\eta \to \pm\infty$ over a very narrow energy interval. This is associated with a vanishing amplitude $A = 1/\sinh\eta$ at this energy. Near this point, $\sinh\eta$ is exponentially large, but so is the numerator. Their ratio is of order $e^{-N|\theta|}$ which is small but non-zero (assuming that θ and η have opposite signs). Then, given that η is varying extremely rapidly, there may well be a point close by at which the argument of the $\sinh(N\theta + \eta)$ in line four, is zero. Because θ is varying slowly compared to η, the position will depend very little on the number of cells N. Such a bound state might even occur for the single-cell case, and if so it would persist in the many-cell situation at almost the same energy. When $|\theta| < |\eta|$, it may require more than one or two cells before the bound state can occur, but for large enough N it will. By this mechanism, bound states can occur in a forbidden zone.

It would also be possible for $\tanh\eta \to \pm 1$ asymptotically as the energy goes to ∞. In this case the bound states for different N could be more spread out in energy. Finally, one can also consider the cases where only one of ϕ, δ becomes imaginary, in eq. 13. M_{11}^N then is a complex number, so there would be two conditions to make it vanish, and one soon sees that they cannot both be satisfied.

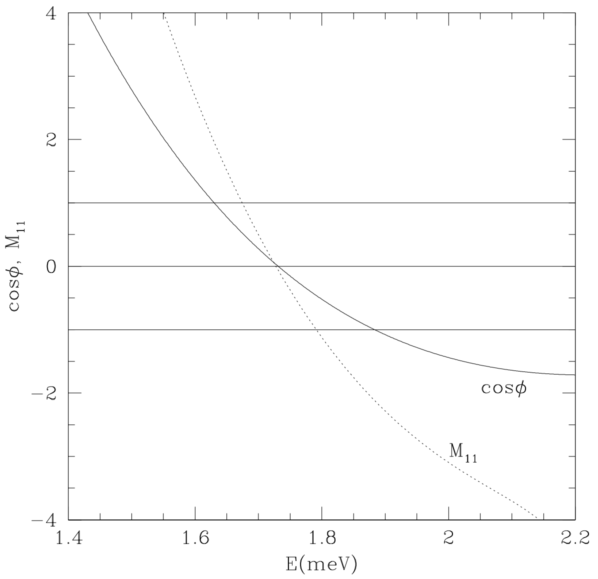

FIG. 1. Behaviour of M_{11} (dashed line) and $\cos\phi$ (solid line) in the below-threshold energy region.

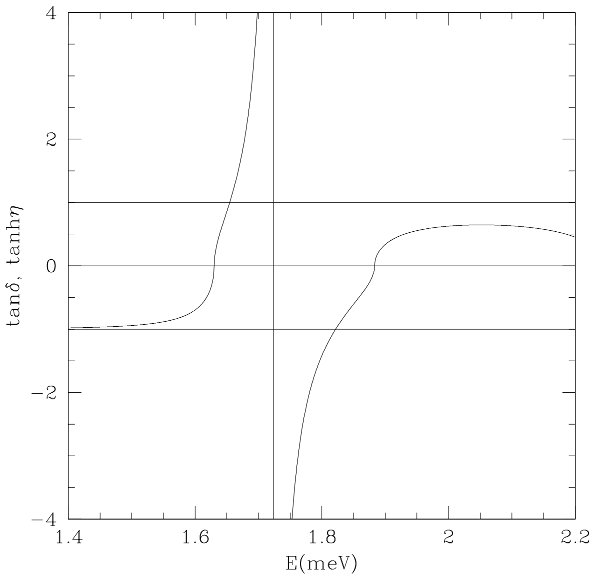

FIG. 2. Behaviour of $\tan\delta$ ($\tanh\eta$) in the below threshold energy region. The allowed zone ends where $\tan\delta = 0$. Note that $\tanh\eta$ never reaches ± 1.

III. A NUMERICAL EXAMPLE

We computed the bound state positions, in the single-mode approximation, for the system considered by Brum [3]. This was the main example in our original paper [1]. For brevity we discuss here only the transverse-symmetric cavity states. From Fig. 3 of reference [1], the threshold is at 2.7 meV. The behaviour of $\cos\phi$ and M_{11} is shown in Fig. 1. One sees that there is a sub-threshold allowed zone between 1.63 and 1.89 meV in which ϕ is a real angle, flanked by two forbidden zones. Fig. 2 shows the behaviour of $\tan\delta$ ($\tanh\eta$). In the allowed zone, δ increases from zero to π, along with ϕ.

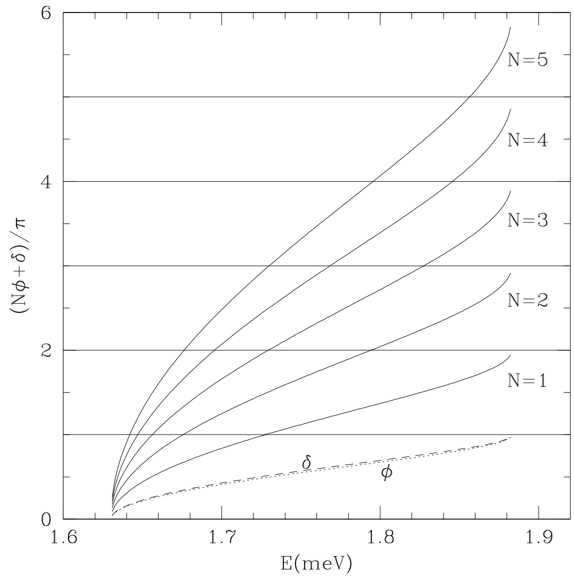

FIG. 3. Behaviour of χ_N/π for $N = 1$ to 5 (solid lines). The intersections with the horizontal lines give the bound state positions for each N. Below them are shown ϕ/π (dashed line) and δ/π (dash-dot line), all of these restricted to the allowed zone.

As a result, the argument $\chi_N \equiv N\phi + \delta$ starts at zero and ends at $(N+1)\pi$. The sine-function will vanish at the interior places where $\chi_N = j\pi$, with $j = 1, 2, 3, ...N$, giving the expected N bound states. This situation is illustrated in Fig. 3, for $N = 1$ to 5 cells. In the lowest part of the drawing, ϕ/π and δ/π are plotted. Above them we plot χ_N/π for $N = 1$ to 5. The intersections of χ_N/π with the horizontal lines at integers j give the bound states for each N.

In this example, one has approximately $\delta \approx \phi$, so the bound states are given more or less as the solutions of $\sin(N+1)\phi = 0$. The reason is that the cells are rather far apart, and this makes $|M_{11}| \approx 2\cos\phi >> |M_{22}|$. Then from eq. 8 we see that $\tan\delta \approx \tan\phi$. It would require the opposite situation, $|M_{11}| << |M_{22}|$, to have $\tan\delta \approx -\tan\phi$, giving $\delta = \pi - \phi$ to have fewer than N bound states in the allowed zone. Only then would some of the bound states be pushed into the forbidden zone.

To summarize, we have found N bound states for the N-cell system, of which (in this example) all N are in the sub-threshold allowed region.

For the case of $N = 10$ cells considered previously [1], Fig. 4 compares the positions from the proper result and the approximation $\cos N\phi = 0$. In the centre of the allowed zone, the two methods agree rather well, due to the phase δ being not too far from $\pi/2$ over much of the energy range. It is only near the boundaries where δ is close to zero or π that the zeros are noticeably displaced. In the paper of Brum [3], the bound states show up only as a clump in his figure 4, so one cannot say much about the detailed agreement.

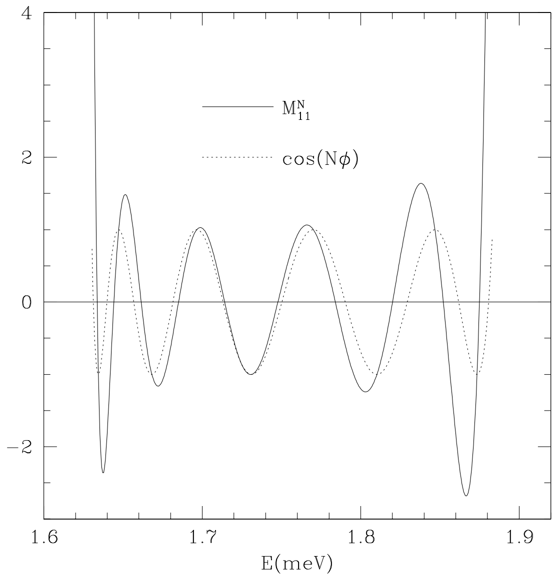

FIG. 4. Behaviour of M_{11}^N (solid line) and $\cos N\phi$ (dashed line) for $N = 10$ in the below threshold energy region. The dashed line ends at the boundary of the allowed zone. In the middle of the zone the bound states lie quite close to the points where the cosine vanishes.

IV. ANALYTICAL EXAMPLE

The simplest model to explore bound state properties is the Dirac comb, a line of delta-function potentials. The basic cell is defined on $0 \le x \le d$ with

$$V(x) = -C_0 \delta(x - d/2) \quad . \tag{14}$$

Here we assume $C_0 > 0$ so we have an attractive force. In the negative energy region where $k \to i\kappa$, we set

$$\kappa^2 = -\frac{2m}{\hbar^2} E$$
$$2\Omega = \frac{2m}{\hbar^2} C_0 \quad . \tag{15}$$

κd and Ωd are dimensionless parameters.

The transfer matrix for this system is

$$\mathbf{M} = \begin{pmatrix} \frac{\kappa-\Omega}{\kappa} e^{\kappa d} & -\frac{\Omega}{\kappa} \\ \frac{\Omega}{\kappa} & \frac{\kappa+\Omega}{\kappa} e^{-\kappa d} \end{pmatrix} \tag{16}$$

Notice that as d increases, the ratio of M_{11}/M_{22} rises exponentially. It is immediately seen that the single-cell bound state occurs at $\kappa = \Omega$. (Had we taken a repulsive potential, it would have a virtual state at the same energy.) Also, we have

$$\cos(\phi) = \cosh \kappa d - \frac{\Omega}{\kappa} \sinh \kappa d$$
$$\frac{1}{2}(M_{11} - M_{22}) = \sinh \kappa d - \frac{\Omega}{\kappa} \cosh \kappa d \tag{17}$$

At threshold, $\cos\phi = 1 - \Omega d$. For large enough separation between the teeth of the comb, this will be less than -1, and we are in a forbidden zone. Then one replaces $\phi \to i\theta + \pi$.

There is an allowed zone surrounding the single-cell bound state, (at which $\cos\phi = e^{-\Omega d}$), and the forms listed in eq. 16-17 are appropriate. When $M_{11} = 0$, $\tan\delta = -\tan\phi$, so $\delta = \pi - \phi$, which satisfies the bound state condition in eq. 9. For large Ωd, this $\cos\phi$ will be very small, so ϕ will be $\pi/2 - \epsilon$. Starting from threshold, we enter the allowed zone with $\phi = \delta = \pi$ and we leave it at a point $\kappa > \Omega$ with both angles approaching zero. (At the high end of the band, $\cos\phi = 1$, which requires

$$\tanh \frac{1}{2}\kappa d = \frac{\Omega d}{\kappa d} \tag{18}$$

One can show that the band ends at a point where $\kappa d < 2\Omega d$.)

Looking at eq. 9, the phase $\chi_N = N\phi + \delta$ ranges from $(N+1)\pi$ to zero over the allowed zone. There will therefore be N bound states of the N-cell system at places where $\chi_N = j\pi$, $j = 1, 2, ...N$. For odd-N, one of these will lie very close to the single-cell bound state at $\kappa = \Omega$. In general they are distributed half above and half below this wave number.

This is the generic situation for the bound states of an N-cell system, when the inter-cell spacing becomes large. We see from eq. 16 that for large κd, $|M_{22}|$ is exponentially small compared to $|M_{11}|$. One is then in the situation where $M_{11} \approx 2\cos\phi$, which makes $\delta = \phi$. Then $\chi_N = (N+1)\phi$ and we get N bound states in the allowed band.

For small $\Omega d < 2$, the allowed band on the negative energy side is truncated, as it overlaps the threshold. Then ϕ begins at a value less than π, and the band may contain fewer than N bound states. Gasiorowicz discusses the example of $N = 2$ delta functions, and shows that the second bound state fails to exist when $\Omega d < 1$ [4].

V. CONCLUSION

In the single-mode approximation, a quantum wire connecting N cavities is equivalent to a one-dimensional N-cell system. Here we have found the bound states by the transfer matrix method. The important equation is eq. 13, which applies to any N and any potential. Once the phases ϕ and δ have been computed for the single cell, it is simply a matter of looking at $\chi_N = N\phi + \delta$

in the allowed zone, to locate the N-cell bound states, as in Fig. 3. In the generic case, there will be N bound states in the sub-threshold allowed band, for large enough inter-cell spacing. But in other cases, one or two of the bound states may be pushed into the forbidden zones, and some may even fail to be bound. Indeed, Sassoli de Bianchi and Di Ventra [5] have shown that all but one of the bound states may pass into the continuum as the wells are pushed closer together.

The numerical example, based on Brum's calculations of a two-dimensional wire, is a generic case. It was shown by Shockley [6] that you must have band crossing in order to have bound states outside the allowed zone, and this does not occur when the system is an array of square potentials.

The possible occurrences of bound states for an N-cell system are therefore much more interesting than the corresponding situation for the scattering regime [2]. The present formalism has the merit that it is independent of the shape of the single cell, and is well suited to either qualitative or quantitative discussion of the system both above and below threshold.

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