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One-dimensional symmetric rectangular well: from bound to resonance via self-orthogonal virtual state

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Abstract

As a one-dimensional symmetric rectangular well becomes shallower, the bound states move up to the threshold and eventually disappear, but not without leaving a trace. Shortly after a bound state has ceased to exist, a new resonance state appears above the well. In the interim a virtual state is formed at the threshold which then coalesces on its way down with another virtual state that is moving up towards it, giving rise to a pair of complex states inside the well, which move all the way up to become the resonance above the well and its conjugate virtual state. All this is readily deduced from the work of H M Nussenzveig (1959 *Nucl. Phys.* **11** 499), which may be rightfully considered a quite exhaustive though rather intricate treatment of the problem. In contrast to it the current quasi-analytical study is distinguished by extraordinary simplicity, offering an excellent visualization and a thorough grasp of the subject. Moreover, a startling phenomenon is revealed by going beyond the energy plane considerations and looking into the behaviour of the wavefunctions. Namely, when exterior complex scaling is deployed for normalization of exponentially divergent states, all divergent states turn out to be orthogonal between themselves with self-orthogonality at the point of coalescence of two virtual states and consequent abnormality in the amplitudes of the resonances when just formed inside the well.

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1. Introduction

There are two different sets of boundary conditions that give rise to all the possible discrete states of a symmetric well. The first one called outgoing waves is responsible for the bound states (real eigenvalues inside the well) and for the resonance states (complex eigenvalues mostly above the well). The states obtained when the second set of boundary conditions called incoming waves is imposed are the virtual states. They may have real eigenvalues when inside the well (also known as antibound states) or they may be the complex conjugates of the corresponding resonances when not limited to the real axis. In the case of real eigenvalues both for the outgoing and for the incoming waves an analytical representation can be constructed to follow their behaviour as a function of the well depth. The complex eigenvalues for either of the boundary conditions are followed numerically (for the method to solve transcendental equations of complex variable see [3]).

A one-dimensional symmetric rectangular potential well is defined by

$$V(x) = \begin{cases} 0 & (x < 0 \text{ or } x > a) \\ -V_0 & (0 < x < a) \end{cases}$$

where V_0, the depth of the well, is a positive number. The corresponding time-independent Schrödinger equation is

$$\begin{cases} \Psi'' + k_0^2\Psi = 0 & k_0 = \sqrt{2mE}/\hbar & (x < 0 \text{ or } x > a) \\ \Psi'' + k^2\Psi = 0 & k = \sqrt{2m(E + V_0)}/\hbar & (0 < x < a) \end{cases}$$

and its general solution is given by

$$\begin{cases} \Psi = C\,\mathrm{e}^{\mathrm{i}k_0x} + C'\,\mathrm{e}^{-\mathrm{i}k_0x} & (x < 0) \\ \Psi = A\,\mathrm{e}^{\mathrm{i}kx} + B\,\mathrm{e}^{-\mathrm{i}kx} & (0 < x < a) \\ \Psi = D\,\mathrm{e}^{\mathrm{i}k_0x} + D'\,\mathrm{e}^{-\mathrm{i}k_0x} & (a < x) \end{cases}$$

where A, B, C, C', D and D' are some integration constants, and the functions $\mathrm{e}^{\mathrm{i}k_0x}$ and $\mathrm{e}^{-\mathrm{i}k_0x}$ represent the waves moving towards the right and the left respectively. By requiring $C = D' = 0$ (or, alternatively, $C' = D = 0$) together with the continuity of Ψ and Ψ' transcendental equation for the outgoing (incoming) waves is obtained.

2. Outgoing boundary conditions

As the name implies, outgoing boundary conditions represent an outward flow from inside the well. For real $E > 0$, k_0 would be real, thus outgoing waves are represented by $\mathrm{e}^{\mathrm{i}k_0x}$ to the right of the well and by $\mathrm{e}^{-\mathrm{i}k_0x}$ to the left of it. However, real solutions of the transcendental equation are possible only for $E < 0$, when k_0 is pure imaginary, in which case the outgoing waves become decaying exponents pertaining to the bound states. In general, the transcendental equation for the outgoing waves is

$$2\cot ka = \frac{\mathrm{i}\left(k^2 + k_0^2\right)}{kk_0} \tag{1}$$

and, in particular, for $k_0 = \mathrm{i}\kappa$ ($\kappa = \sqrt{-2mE}/\hbar$, $E < 0$) it becomes

$$2\cot ka = \frac{k^2 - \kappa^2}{k\kappa}. \tag{2}$$

Whereas the complex equation (1) can be dealt with numerically only, a graphical solution of equation (2) exists (see [2]) by means of which behaviour of the bound states as a function of the well depth can be derived in an elegant manner.

The graphical solution is done by introducing two new variables

$$\alpha = \sqrt{1 + \frac{E}{V_0}} \qquad \text{and} \qquad \gamma = \sqrt{\frac{2mV_0a^2}{\hbar^2}}$$

in terms of which equation (2) is expressed as

$$\gamma\alpha = (n-1)\pi + 2\cos^{-1}\alpha \qquad (n = 1, 2, \ldots) \tag{3}$$

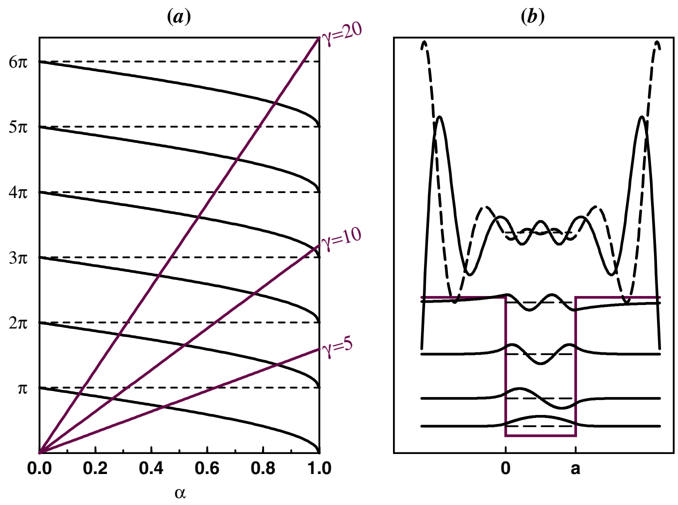

Figure 1. (*a*) Graphical solution of equation (3). (*b*) Wavefunctions of the five lowest outgoing wave states for $V_0 = 8$, $a = 2.5$, $m = 1$, $\hbar = 1$ ($\gamma = 10$). The real part of the resonance above the well is depicted by a solid line and the imaginary part is depicted by a dashed line.

(see appendix A) and both sides of it are then plotted as a function of α. Since the right-hand side of equation (3) is independent of γ, varying the depth of the well leaves it unaltered while the slope of the straight line on the left changes. In figure 1(*a*) the graphical solution is plotted for three different γ. Values of α at the points of intersection of the straight line with the branches of $2\cos^{-1}\alpha$ give the energies of the corresponding bound states according to the formula

$$E = -V_0(1-\alpha^2).$$

It is immediately evident from the graph that as the well becomes shallower, the bound states move towards the threshold where they eventually disappear with the exclusion of the first bound state which always remains inside the well. The number of the bound states for a given well depth is clearly the greatest integer contained in the quantity $(\gamma/\pi + 1)$.

Wavefunctions of the five lowest outgoing wave states for a certain well are shown in figure 1(*b*). Four of them are bound states and the fifth is the first resonance above the well. The resonance wavefunction is normalized using ECS to be discussed in section 5.

3. Incoming boundary conditions

Incoming boundary conditions stand for an inward flow and therefore are represented by e^{-ik_0x} to the right of the well and by e^{ik_0x} to the left of it. The transcendental equation for the incoming waves is

$$2\cot ka = \frac{-i\left(k^2+k_0^2\right)}{kk_0} \tag{4}$$

the solutions of which are obviously the complex conjugates of those of equation (1) unless k_0 is pure imaginary, $k_0 = i\kappa$, and equation (4) takes the form

$$2\cot ka = \frac{\kappa^2-k^2}{k\kappa}. \tag{5}$$

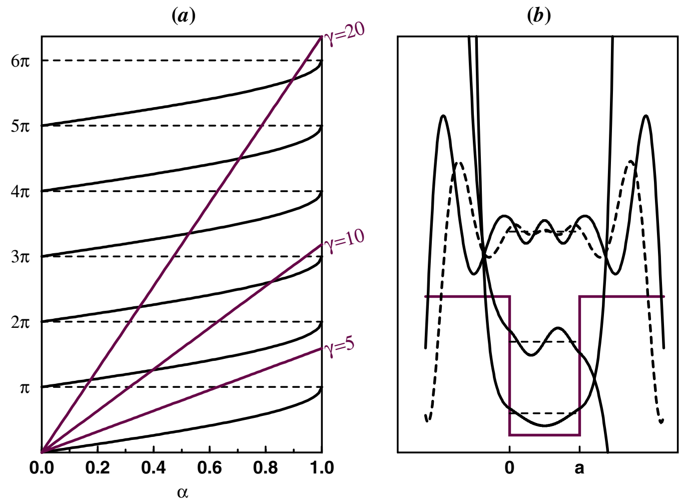

Figure 2. (*a*) Graphical solution of equation (6), (*b*) wavefunctions of the three lowest incoming wave states for $V_0 = 8, a = 2.5, m = 1, \hbar = 1$ ($\gamma = 10$). The real part of the complex virtual state above the well is depicted by a solid line and the imaginary part is depicted by a dashed line.

A graphical solution for the real virtual states described by equation (5) can be done in analogy with bound states. Using the same definition for α and γ the transcendental equation for the real virtual states is transformed into

$$\gamma\alpha = (n-1)\pi + 2\cos^{-1}\sqrt{1-\alpha^2} \qquad (n = 1, 2, \ldots) \tag{6}$$

(see appendix B). The graphical solution of this equation is shown in figure 2 together with a plot of ECS normalized virtual states' wavefunctions. It should be noted that the parity of the real virtual states corresponding to the consecutive branches of the right-hand side of equation (6) is in reversed order to that of the bound states. The real part of the complex virtual state is, of course, identical to the real part of the corresponding conjugate resonance state and the imaginary part has a phase equal to π relative to the resonance.

4. Varying the depth of the well

To get an insight into what happens as the depth of the well is varied, the graphical solutions for the bound and the real virtual states are combined in one diagram (see figure 3). By inspecting the diagram it can be readily concluded that every time nth bound state with $n \geqslant 3$ reaches the threshold as a result of diminishing the depth of the well, a new $n-1$ virtual state is formed there, in addition to already existing $n-1$ virtual state, and as the depth of the well is diminished further, these two virtual states move towards each other, coalesce and disappear. Solving simultaneously the complex transcendental equation for the incoming waves, it is found that right after the two real solutions merge into one, subsequent decrease in the depth of the well makes this solution complex. First the new complex virtual state sits inside the well, but as the bottom of the well is continuously pushed up, it eventually crosses the threshold. Of course, the moment a new complex incoming wave state is formed its complex conjugate appears as a new solution for the outgoing wave transcendental equation. Thus a disappearing bound state is turned into a resonance via a virtual state collision. This is true for any $n \geqslant 3$. Figure 4 shows these transitions for the $n = 3$ bound state. The $n = 2$ bound state never

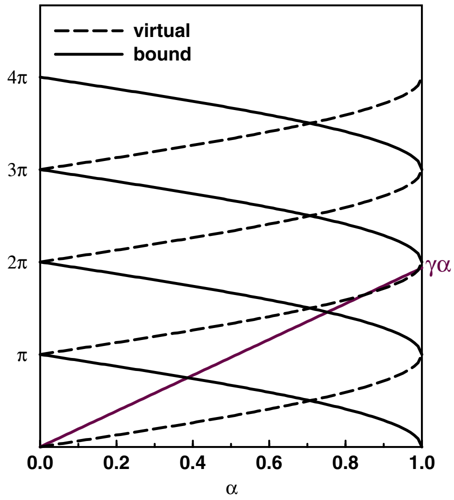

Figure 3. Graphical solutions for bound and real virtual states of a symmetric rectangular well combined in one diagram.

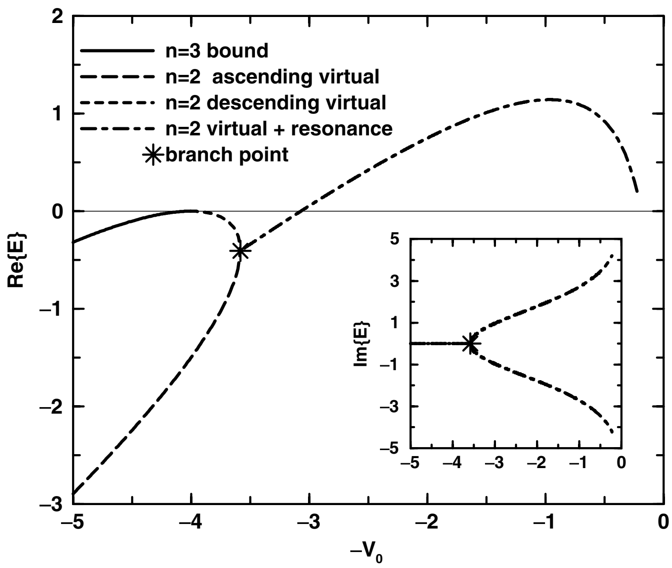

Figure 4. Disappearing of the $n = 3$ bound state and formation of a new resonance as a result of diminishing the depth of the well. The calculations were made with $\hbar = 1$, $m = \frac{1}{2}$, $a = 3.14$.

becomes a resonance consistently with the fact that the $n = 1$ real virtual state is essentially different from those above it, as is apparent from the graphical solution.

The values of the potential depths at which branch points, the points of coalescence of two virtual states, occur can be determined by demanding the two sides of equation (6) to be tangent to each other at the point of their intersection. The tangency requirement alone yields that the energy of the branch point's virtual state is independent of n and is given by

$$E_{\mathrm{bp}} = -\frac{2\hbar^2}{ma^2}.$$

The transcendental equation obtained when the intersection is also taken into account is

$$\sqrt{\gamma^2 - 4} = (n-1)\pi + 2\cos^{-1}\frac{2}{\gamma}.$$

For $n = 1$ this equation is very easy to solve ($\gamma = 2$) and it corresponds to $-V_0 = E_{\mathrm{bp}}$, which means that after $n = 2$ bound state is turned into $n = 1$ virtual state it moves down towards the bottom of the well until it collides with it and disappears.

It also may be interesting to note from figure 3 that for certain well depths some nth bound state will have the same energy as the nth virtual state. The relation that must hold between V_0 and n for this to happen is

$$V_0 = \frac{\left(n - \frac{1}{2}\right)^2 \pi^2 \hbar^2}{ma^2}$$

and the energy of the nth bound and virtual states will then be

$$E = -\tfrac{1}{2} V_0.$$

5. Using exterior complex scaling

Resonances and virtual states cannot be normalized in the usual sense by virtue of being exponentially divergent. To overcome this difficulty in the case of resonances (or Gamow functions, as this type of resonances is commonly known) Zeldovich [4] introduced a convergence factor $\mathrm{e}^{-\varepsilon x^2}$ defining the 'norm' by: $(\Psi|\Psi) \equiv \lim_{\varepsilon\to 0}\int_{-\infty}^{\infty} \mathrm{e}^{-\varepsilon x^2}\Psi^2\,\mathrm{d}x = 1$. Although this definition can be successfully extended to the bound states yielding the usual norm [5], it fails for the virtual states. Instead ECS [6–9] can be used.

In ECS the x coordinate is rotated to the complex plane through an angle θ from the point at which the potential $V(x)$ becomes zero. For the symmetric rectangular well this means

$$x \to \begin{cases} x\,\mathrm{e}^{\mathrm{i}\theta} & (x < 0) \\ x & (0 \leqslant x \leqslant a) \\ a + (x-a)\,\mathrm{e}^{\mathrm{i}\theta} & (x > a) \end{cases}$$

with the time-independent Schrödinger equation in the scaled region being transformed into

$$\mathrm{e}^{-2\mathrm{i}\theta}\Psi'' + k_0^2\Psi = 0$$

and the matching conditions for Ψ' at $x = 0$ and $x = a$ becoming

$$\begin{cases} \mathrm{e}^{-\mathrm{i}\theta}\Psi'_{x<0}\,(x=0) = \Psi'_{0<x<a}\,(x=0) \\ \Psi'_{0<x<a}\,(x=a) = \mathrm{e}^{-\mathrm{i}\theta}\Psi'_{x>a}\,(x=a). \end{cases}$$

These transformations, apparently, leave the transcendental equations for the outgoing and incoming waves unaltered. Finally, the 'norm' is defined by $(\Psi|\Psi) \equiv \mathrm{e}^{\mathrm{i}\theta}\int_{-\infty}^{\infty}(\Psi^{\mathrm{ECS}})^2\,\mathrm{d}x = 1$. It should be emphasized that this 'norm', of course, is not what is usually understood as a norm in an inner product space (it would be advisable to see [10] for the description of the c-product and for the properties of the 'norm' induced by it). Additionally, as is apparent from its definition the 'normalization' integral is θ independent: the θ's job is to provide convergence at infinity. Accordingly, normalization of resonances by ECS is completely equivalent to using Zeldovich' convergence factor, though ECS is absolutely indispensable for normalization of virtual wavefunctions. It is obvious that the only way to force the real virtual states to converge is by choosing $\theta > \frac{\pi}{2}$ and for the complex virtual states θ should be made even larger. But to ensure convergence of all the virtual states up to infinity it looks like $\theta = \pi$ is the only option

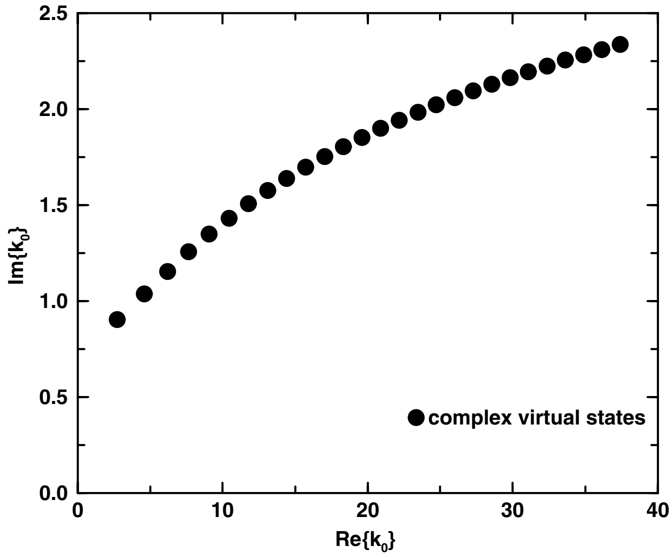

Figure 5. The free space wave vectors of the complex virtual states for $\hbar = 1, m = 1$, $a = 2.5$, $V_0 = 8.5$.

(see figure 5). Thus all exponentially divergent states, namely, resonances, complex virtual states and real virtual states become square integrable under ECS by $\theta = \pi$. Of course, such ECS makes bound states divergent; however, they are also orthogonal to all the other discrete states when disregarding the 'upper limits' of the overlap integrals.

Besides furnishing the normalization tool for exponentially divergent states ECS' 'inner product' definition $\left((\Psi_1|\Psi_2) \equiv \mathrm{e}^{\mathrm{i}\theta} \int_{-\infty}^{\infty} \Psi_1^{\mathrm{ECS}} \Psi_2^{\mathrm{ECS}}\, \mathrm{d}x\right)$ provides orthogonality between all the virtual and resonance states. This is a highly remarkable result, since it means that the two colliding virtual states are mutually orthogonal and, hence, the virtual state at the branch point is self-orthogonal. The self-orthogonality at the branch point can be tracked by calculating the normalization integral of a single wavefunction of the appropriate virtual and resonance states as is shown in figure 6. Additionally, since the normalization integral of the freshly formed resonance vanishes in the vicinity of the branch point, it has a huge norm there, so one may suggest that such a resonance ought to affect significantly the transmission probabilities above the well. However, it turns out not to be the case as shown in the next section.

6. Transmission probabilities above the well

The transmission probability above a symmetric rectangular well is given by (see [2])

$$|T|^2 = \frac{4\mu^2}{(1+\mu^2)^2 \sin^2 ka + 4\mu^2 \cos^2 ka}$$

where $\mu = k/k_0$. The total transmission occurs each time ka assumes the value of an integer times π. As the well becomes shallower the condition for $ka = n\pi$ can be fulfilled for smaller and smaller n. For a given potential depth the smallest possible value of n is given by

$$n = \mathrm{int}\left[\frac{\sqrt{2mV_0}a}{\pi\hbar}\right]$$

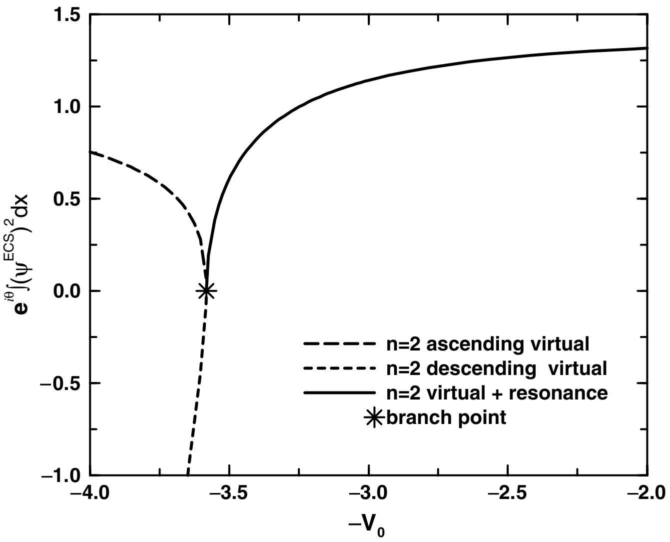

Figure 6. ECS normalization integrals of the $n = 2$ disappearing real virtual states and of the freshly formed $n = 2$ complex virtual and resonance states in the vicinity of the branch point. The calculations were made with $\hbar = 1, m = \frac{1}{2}, a = 3.14$. For the complex eigenvalues the absolute value of the integral is plotted.

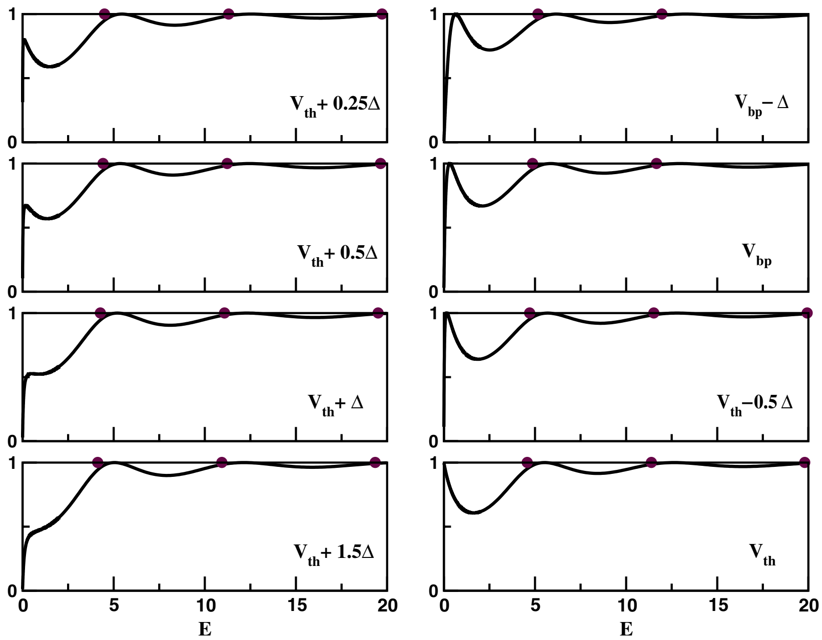

Figure 7. Transmission probability above a symmetric rectangular well for $m = 1, \hbar = 1$ and $a = 2.5$ as the $n = 4$ bound state disappears. V_{th} is the depth of the well corresponding to the $n = 4$ bound state at the threshold, V_{bp} the depth of the well corresponding to the $n = 3$ branch point, $\Delta = V_{th} - V_{bp}$. Filled circles stand for the resonance' positions.

so as the depth of the well is decreased a new peak for the transmission probability is formed at the threshold whenever the depth of the well becomes

$$V_0 = \frac{1}{2m}\left(\frac{n\pi\hbar}{a}\right)^2.$$

But this is exactly the V_0 at which the $n+1$ bound state arrives at the threshold. In figure 7, the formation of a new transmission probability peak is demonstrated as the $n = 4$ bound state disappears. After it has formed, the new peak moves smoothly to the higher energies without anything special happening around the branch point.

7. Conclusions

Transitions from a bound to a resonance state in a symmetric rectangular well are excellently visualized with the aid of the graphical solutions obtainable in the case of real outgoing and incoming wave states. All bound states with $n \geqslant 3$ exhibit similar behaviour as the depth of the well is decreased: they turn into $n-1$ virtual state at the threshold which then descends and collides with an additional $n-1$ ascending virtual state. The two real virtual states annihilate each other and give rise to a new pair of complex virtual and resonance states. The value of the energy at which this happens is the same for all n and the wavefunction of the branch point virtual states is orthogonal to itself under the ECS 'norm' definition. The ECS 'inner product' definition also makes all the divergent states orthogonal between themselves.

Finally, apart from providing a graceful way to illustrate the transitions from bound to resonance states the current treatment of the problem may also provide a wholesome tool for tackling different physical problems which can be approximated by a symmetric rectangular well with varying depth (see, for example, [11] in connection with modes of a slab waveguide).

Acknowledgments

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Appendix A. Graphical solution for the bound states

Using trigonometric identity

$$\cot 2\alpha = \frac{1}{2}\left(\cot\alpha - \frac{1}{\cot\alpha}\right)$$

equation (2) is transformed into

$$\cot(ka/2) - \frac{1}{\cot(ka/2)} = \frac{k}{\kappa} - \frac{\kappa}{k}$$

which can be split into two

$$\cot\frac{ka}{2} = \frac{k}{\kappa} \qquad \text{or} \qquad \cot\frac{ka}{2} = -\frac{\kappa}{k}.$$

The first one of the two equations corresponds to the even states (cosines inside the well) and the other one corresponds to the odd states (sines inside the well). These equations are further transformed into

$$\cos\frac{ka}{2} = \pm\sqrt{\frac{k^2}{\kappa^2 + k^2}} \qquad \text{or} \qquad \sin\frac{ka}{2} = \pm\sqrt{\frac{k^2}{\kappa^2 + k^2}}$$

each of which contains two spurious solutions, one for + and one for −, to be excluded so that $\cot(ka/2)$ will have positive values in the first equation and negative values in the second one.

From the definition of k and κ it can be readily seen that

$$\frac{k^2}{\kappa^2 + k^2} = \frac{E + V_0}{V_0} = 1 + \frac{E}{V_0}.$$

Therefore, by defining two new variables

$$\alpha = \sqrt{1 + \frac{E}{V_0}} \qquad \text{and} \qquad \gamma = \sqrt{\frac{2mV_0a^2}{\hbar^2}}$$

the above two equations can be written as

$$\cos\frac{\gamma\alpha}{2} = \pm\alpha \qquad \text{or} \qquad \sin\frac{\gamma\alpha}{2} = \pm\alpha$$

and after excluding the spurious solutions

$$\frac{\gamma\alpha}{2} = \cos^{-1}\alpha + n\pi \qquad \text{or} \qquad \frac{\gamma\alpha}{2} = \cos^{-1}\alpha + n\pi + \frac{\pi}{2}$$

where $n = 0, 1, 2, \ldots$.

Finally, the two equations can be combined into one

$$\gamma\alpha = (n-1)\pi + 2\cos^{-1}\alpha \qquad (n = 1, 2, \ldots).$$

Appendix B. Graphical solution for the real virtual states

To obtain the solutions for the real virtual states from the bound state equations the transformation $\kappa \to -\kappa$ should be performed, so that the even and the odd state equations become

$$\cot\frac{ka}{2} = -\frac{k}{\kappa} \qquad \text{or} \qquad \cot\frac{ka}{2} = \frac{\kappa}{k}.$$

Similarly to the bound states these can be written as

$$\sin\frac{ka}{2} = \pm\sqrt{\frac{\kappa^2}{\kappa^2 + k^2}} \qquad \text{or} \qquad \cos\frac{ka}{2} = \pm\sqrt{\frac{\kappa^2}{\kappa^2 + k^2}}$$

and since

$$\frac{\kappa^2}{\kappa^2 + k^2} = -\frac{E}{V_0} = 1 - \alpha^2$$

these equations can be rewritten as

$$\sin\frac{\gamma\alpha}{2} = \pm\sqrt{1 - \alpha^2} \qquad \text{or} \qquad \cos\frac{\gamma\alpha}{2} = \pm\sqrt{1 - \alpha^2}$$

and then combined into one

$$\gamma\alpha = (n-1)\pi + 2\cos^{-1}\sqrt{1 - \alpha^2} \qquad (n = 1, 2, \ldots).$$

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