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2006 J. Phys. A: Math. Gen. 39 7341

(http://iopscience.iop.org/0305-4470/39/23/012)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND GENERAL

J. Phys. A: Math. Gen. **39** (2006) 7341–7348 doi:10.1088/0305-4470/39/23/012

Reflectionlessness, kurtosis and top curvature of potential barriers

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Received 15 February 2006, in final form 28 April 2006
Published 23 May 2006
Online at stacks.iop.org/JPhysA/39/7341

Abstract
Apart from the rectangular barrier, other barriers having a single maximum generally display reflectivity, $R(E)$, as a smoothly decreasing function of energy. We conjecture that symmetric potential barriers with a single maximum entail zeros or sharp minima in $R(E)$ provided they have either their coefficient of kurtosis lying in the range (1.8, 3.0), or their top curvature as zero, or both.

PACS number: 03.65.Nk

1. Introduction

Generally, a rectangular potential barrier is thought to be an exceptional model of quantal reflection (transmission) from a one-dimensional potential barrier entailing multiple zeros in the reflection coefficient, $R(E)$, at energies above the barrier. On the other hand, the well-known analytically solvable potential barriers do not show reflectivity zeros at all whatever the values of E, V_0 (height) and a (slope) may be. By a single top potential barrier we mean the positive definite potentials ($V(x) \geqslant 0$) having a single maximum. The exactly and the analytically solvable (quantal and WKB) instances are the Eckart barrier [1], the parabolic barrier [1], the exponential barrier [2], the Morse barrier [3], the asymmetric parabolic barrier [4] and one more [5] which interpolates between the Morse and the Eckart barriers. The Ginocchio barrier [6] is the most recent addition to this class. Other useful instances of potential barriers which are not analytically solvable are the Lorentzian and the Gaussian barriers. We shall refer to these potential barriers as type-I.

The type-I potential barriers have one common interesting feature that at energies above the barrier they strictly entail only two complex conjugate turning points (roots of $E = V(x)$). The conventional WKB formula for the reflection coefficient is essentially limited only to two complex conjugate turning points and this gives rise to the smooth (non-oscillatory) variation of $R(E)$. See figure 1 and inset of figure 2. These barriers have non-zero top curvature (i.e., $V''(0) \neq 0$). The coefficient of kurtosis (β_2, see below equation (1)) for these profiles is more than 3.

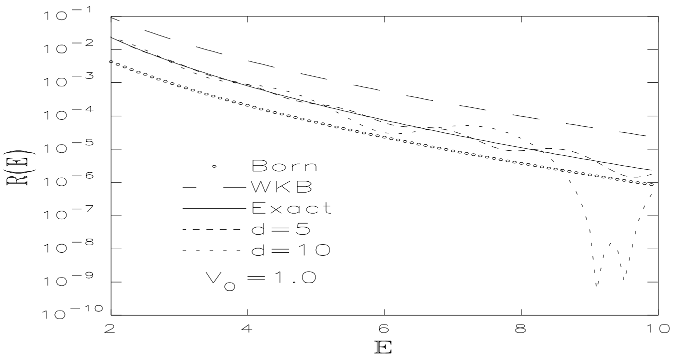

Figure 1. $R(E)$ for the truncated and untruncated Lorentzian (type-I) barriers. When the cut-off length d approaches 100 the oscillations disappear. The WKB formula (3*a*) overestimates (though there is only one pair of complex conjugate turning points at over-the-barrier energies). The Born approximation underestimates and gives smooth reflectivity.

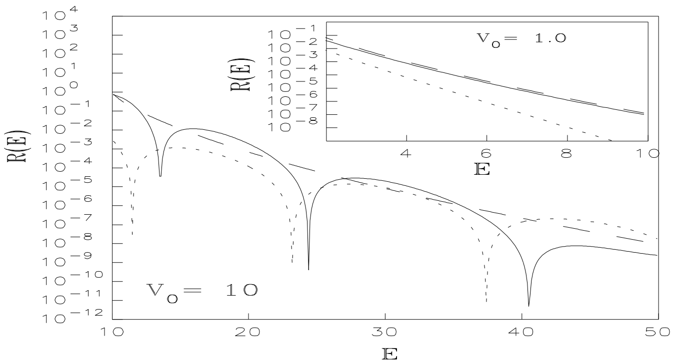

Figure 2. $R(E)$ for a type-II barrier: $V(x) = V_0\,\mathrm{e}^{-x^4}$ and (in the inset) for a type-I barrier: $V(x) = V_0\,\mathrm{e}^{-x^2}$ potential barriers. Solid lines are exact quantal (2) results, dotted lines are due to the Born approximation and the long dashed lines represent the WKB (using two turning points) results. Note that the type-II barriers yield oscillatory reflectivity wherein the WKB (using two turning points) methods fail and the Born approximation works only qualitatively.

In contrast to this, we propose to study the potential barriers which yield non-smooth oscillatory reflectivity entailing multiple zeros/minima at energies above the barrier (the super-barrier energies).

The query raised here also receives significance from the following phenomenon. The suppression of localization wherein the appearance of extended states [7] requires the vanishing of reflectivity from a single scatterer at a discrete set of electron energies. In nucleus–nucleus fusion at energy near the Coulomb barrier, the fusion rates $\sigma(E)$ for the systems like ${}^{12}C + {}^{12}C$ and ${}^{16}O$ + ${}^{16}O$ display oscillations as a function of energy. And in the barrier penetration model fusion (see [4]) it is the penetrability factor (transmission coefficient), $T(E)$, which is required to be oscillatory. In anti-de Sitter cosmologies the universe is required to pass over a potential barrier reflectionlessly [8]. More recently, the PT-symmetric origin of reflectionlessness of potential barriers has been revealed [9]. According to this work, for the potential barriers of the type $V(x) = -x^{2K+2}$, $K = 1, 2, 3, \ldots,$ reflectionlessness is the result of the imposition of the PT-symmetric boundary condition on the wavefunction.

By PT-symmetry, we mean the invariance under the joint action of parity ($x \to -x$) and time-reversal ($i \to -i$) transformations. These instances bring into contention the potential barriers other than type-I as discussed above.

2. Existing conditions on potentials for reflectivity with minima/zeros

Usually, in textbooks the reflectivity zeros of the rectangular barrier are passed off as artificial or exceptional. Else, one tends to attribute the reflectivity zeros of the rectangular barrier to the strict finite support of the potential. The above-mentioned type-I barriers if truncated on both the sides of the barrier do give rise to oscillatory behaviour of $R(E)$ or $T(E)$ [10]. But more often the reflectivity zeros of the rectangular barrier are intuitively conceived to be arising from the sharp edges (points of non-differentiability) of the barrier in analogy with Fabry–Perot interferometry. The question arising here is whether there can be a class of *smooth* (single piece and single maximum) potential barrier which can give rise to a discrete energy spectrum of reflectivity zeros or minima. It needs to be emphasized that when a potential is truncated (e.g. at $x = \pm d$) on both the sides it becomes a three-piece potential and it is a piecewise continuous profile. However, the truncation of a potential barrier provides us with a condition on the potential for observing oscillatory reflectivity. We shall refer to it as the first condition ($\mathbf{C}_1$).

In a very interesting paper on semiclassically weak reflections above analytic and non-analytic potential barriers, Berry [11] has attributed the oscillatory reflectivity to the non-analyticity of the potential and the rectangular barrier has been acknowledged as a kind of non-generic. For a specially tailored potential barrier $V_{\mathrm{Berry}}(x) = V_0(1 - \mathrm{e}^{-1/|x|})$, $R(E)$ has been found to be oscillatory [11]. This work provides us with another condition ($\mathbf{C}_2$) for the super-barrier reflectionlessness.

Later potential profiles like $V_{\mathrm{Ch}}(x) = V_0/(1 + x^4)$ [12] have been considered as a new variety in semi-classical WKB analysis. The new feature is that this potential unlike the above-mentioned type-I potentials entails *two pairs* of complex conjugate turning points at super-barrier energies ($E > V_0$). Using the interesting asymptotic properties of the Schrödinger equation arising from the Eckart potential ($-\mathrm{sech}^2 x$) a new WKB formula for reflectivity has been proposed [12]. It is found that $R(E)$ for $V_{\mathrm{Ch}}(x)$ entails a discrete spectrum of reflectivity zeros. Here we encounter the third condition ($\mathbf{C}_3$).

3. The coefficient of kurtosis and top curvature of profiles: two new proposals

The rise and fall of the rectangular barrier is sharp (most rapid) and that is the limit. We utilize this as a crucial feature of the barriers for displaying reflectionlessness at discrete energies. Hence, we look out for potential barriers which rise and fall more and more rapidly. Consequently, the potential would get flattened around its top. Interestingly, in statistical data analysis [13] we have one such measure that enables the determination of the flatness of a (distribution) function, $V(x)$. It is called the coefficient of kurtosis, denoted as β_2 and defined as

$$\beta_2 = \frac{\mu_0 \mu_4}{\mu_2^2}, \qquad \mu_n = \langle (x - \bar{x})^n \rangle = \int_{-\infty}^{\infty} (x - \bar{x})^n V(x)\, \mathrm{d}x, \qquad \bar{x} = \int_{-\infty}^{\infty} x V(x)\, \mathrm{d}x. \quad (1)$$

Here $\bar{x}$ is the mean value of x which for a symmetric profile coincides with, $x = 0$, the position of the top of the barrier. If the profile is normalized, μ_0 is unity. Note that β_2 is dimensionless, scaling free (independent of a) and also independent of the absolute value of the function. Usually, in statistical analysis β_2 is compared against a value of 3 which corresponds to a normal (the Gaussian) distribution function, and various profiles are categorized as platykurtic (when $\beta_2 < 3$) or mesokurtic (when $\beta_2 > 3$).

The values of β_2 for the Lorentzian, $V_L(x) = V_0/(1+x^2)$, the exponential, $V_e(x) = V_0\,\mathrm{e}^{-|x|}$ [2], the Eckart, $V_E(x) = V_0\,\mathrm{sech}^2 x$ [1] and the Gaussian, $V_G(x) = V_0\,\mathrm{e}^{-x^2}$, barriers are indeterminate, 6, 4.2, 3, respectively. A more general potential of type-I is $V_1(\nu, x) = \frac{V_0}{(1+x^2)^\nu}$; it has $\beta_2(V_1, \nu) = 3\frac{2\nu-3}{2\nu-5} > 3$, for $\nu > 5/2$.

We find that β_2 for $V_{\mathrm{Berry}}(x)$ is indeterminate. It may be good to note that $V_{\mathrm{Berry}}(x)$ and its first derivative are continuous for $x \in [-\infty, \infty]$. However, we find that this potential is flat at the top from another point of view wherein we have $V''(0) = 0$. We know that if $V''(0) = 0$ (where $x = 0$ is strictly the position of the top of the barrier, i.e., $V'(x=0) = 0$), the function $V(x)$ will be flatter around the barrier top (infinite radius of curvature) and hence rectangular type. This motivates us to analyse the top curvature of the barriers which have oscillatory reflectivity. We claim that these potential barriers will not possess reflectivity zeros. The reflectivity, $R(E)$, for $V_e(x)$ and $V_G(x)$ and $V_C(x) = V_0\,\mathrm{e}^{-|x|^3}$ has been found to be non-oscillatory [11]. Moreover, it can be readily checked that all these well-known type-I potentials have $V''(0) \neq 0$. Also note that $V_1''(\nu, 0) = -2\nu V_0$.

Here we propose two new conditions on a barrier to possess such a reflectivity. We find that when either the coefficient of kurtosis (β_2, see (1)) of a barrier lies in the interval (1.8, 3.0) ($\mathbf{C}_4$), or its top curvature is zero ($\mathbf{C}_5$), or both, the reflectivity entails multiple zeros/minima. Barriers satisfying both or either of these conditions shall be referred here as type-II barriers.

We remark that $V_{\mathrm{Berry}}(x)$ and $V_{\mathrm{Ch}}(x)$ do possess oscillatory reflectivity, however, due to mutually exclusive characteristics of the potential. The former has a non-analyticity built in but does not have more than one pair of complex conjugate turning points at super-barrier energies. On the other hand, $V_{\mathrm{Ch}}(x)$ has two pairs of such turning points yet it does not possess any non-analyticity. Also these are (non-truncated) smooth single-piece potentials. Thus the conditions $\mathbf{C}_1$, $\mathbf{C}_2$, $\mathbf{C}_3$ can be adjudged to be at most sufficient and not necessary.

The two new criteria/conditions presented here may or may not be mutually exclusive in telling whether there will be reflectivity zeros. Our conclusions shall be based on the exact extraction of the reflection coefficient by numerical integration of the Schrödinger equation as outlined below.

4. The method for the calculation of $R(E)$

First, we outline the method we adopt to calculate $R(E)$ when potential barriers converge asymptotically on both the sides of the barrier top. Let the barriers be symmetric and of arbitrary shape. We treat them as though they are truncated at a large distance, d. The truncated potential is then defined as $V(|x| > d) = 0, V(|x| < d) = V_0 f(x/a)$. The reflection coefficient $R(E)$ for such potentials can be obtained as

$$R(E) = \frac{[k^2a^2u(d/a)v(d/a) + u'(d/a)v'(d/a)]^2}{[k^2a^2u(d/a)v(d/a) + u'(d/a)v'(d/a)]^2 + k^2a^2}, \tag{2}$$

where $k = \sqrt{2mE}/\hbar$. The orthogonal functions $u(x), v(x)$ are the even and odd linearly independent solutions of the Schrödinger equation such that $u(0) = 1, u'(0) = 0$ and $v(0) = 0, v'(0) = 1$. The numerical integration of Schrödinger equation is to be carried out with these initial values from $x = 0$ to $x = d$ and the end values are to be retained for equation (2). The end values should yield the value of the Wronskian ($=uv' - u'v$) as unity for every energy; this serves as a test of goodness for the integration method. Note that a finite value of d indicates the finite support which otherwise is infinity, if the potential converges asymptotically on both the sides. We have used the Runge–Kutta method for numerical integration.

5. Type-II potential barriers

We have employed many analytic potential barrier profiles to demonstrate the claimed criterion for the occurrence of reflectivity minima. Some of these models are $V_2(n, x) = \frac{V_0}{1+(x/a)^{2n}}$, with $\beta_2(V_2, n > 2) = \frac{\sin^2(3\pi\eta)}{\sin(\pi\eta)\sin(5\pi\eta)}$; and $V_3(n, x) = V_0 \exp(-(x/a)^{2n})$, with $\beta_2(V_3, n) = \frac{\Gamma(\eta)\Gamma(5\eta)}{\Gamma^2(3\eta)}$, where $\eta = \frac{1}{2n}$. These two coefficients of kurtosis yield $9/5(=1.8)$ in the limit when $n \to \infty$, so we *a priori* infer that these two potentials are rectangular like and hence these will support reflectivity zeros as n increases (see figure 2). Note that $\beta_2(V_3, n = 1) = 3$, which is the well-known value of the coefficient of kurtosis for the Gaussian function and the reflectivity for the Gaussian barrier (type-I) as displayed in figure 2 (solid line) is non-oscillatory. We must remember to check that for type-II potentials, e.g., V_2 $(n > 1, x)$ and V_3 $(n > 1, x)$, the second derivative at $x = 0$ vanishes as we have $V''(0) = -2V_0\delta_{n,1}$.

6. Calculations and discussions

Using equation (2) we calculate the reflectivity, $R(E)$, for the truncated Lorentzian potential: $V(|x| \leqslant d) = \frac{V_0}{1+(x/a)^2}$, $V(|x| > d) = 0$. We assume that $2m = 1 = \hbar^2$, $V_0 = 1$ and $a = 1$. These results are presented in figure 1. As the truncation distance, d, increases the oscillations in $R(E)$ reduce and disappear when $d = 100$ (see the solid line in figure 1). For the Lorentzian ($V_L(x)$, i.e., $V_1(1, x)$), the reflectivity resulting from the simple WKB and the Born approximations works to

$$R_{\mathrm{WKB}}(E) = \exp(-4\sqrt{V_0}[\mathcal{E}(\beta) - \alpha^2\mathcal{K}(\beta)]/\beta), \qquad \alpha = \sqrt{V_0/E}, \qquad \beta = \sqrt{1-\alpha^2}. \tag{3a}$$

$$R_{\mathrm{Born}}(E) = \frac{\pi^2 V_0^2}{4E} \exp(-4\sqrt{E}\Delta). \tag{3b}$$

Here $\mathcal{E}$ and $\mathcal{K}$ are elliptic integrals. These reflectivities are found to be non-oscillatory wherein the WKB approximation (long dashed line) overestimates and the the Born approximation (open circles) underestimates. The exact quantal $R(E)$ from equation (2) for almost untruncated case ($d = 100$) is given by the solid line.

The multi-minima reflectivity found for $V_2(2, x) = \frac{V_0}{1+x^4}$ is not shown here. Notably, the coefficient of kurtosis of this profile is indeterminate; however, its top curvature is zero. In figure 2, $R(E)$ for the typical type-II barrier, $V_3(2, x)$, is given. The WKB (using two turning points) result fails to display the oscillatory behaviour whereas the Born approximated (short dashed line) result produces oscillations which agree with exact result (solid line) only qualitatively. The value of β_2 for this barrier is 2.18 and we also have $V''(0) = 0$. This is therefore an instance where both the criteria are met and the minima in the reflectivity are observed. We also find that a special branch of the Ginocchio [6] barrier constitutes an exactly solvable model of such a variety. In the inset of figure 2, $R(E)$ for another type-I barrier (the Gaussian) is given. The exact quantal result from equation (2) and the WKB approximated (long dashed line) results almost coincide here. This is generally true for type-I barriers with the Lorentzian barrier as an exceptional case. The Born approximation for the Gaussian, $V_3(1, x)$ or $V_G(x)$, case gives

$$R_{\mathrm{Born}}(E) = \frac{V_0^2\pi}{4E} \exp(-2E). \tag{4}$$

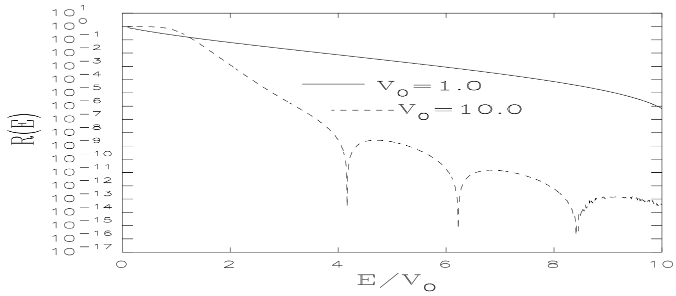

Figure 3. $R(E)$ for another type-II barrier: $V_\epsilon(x) = V_0\,\mathrm{e}^{-(\epsilon x^2+x^4)}$ when $\epsilon = 2.0$. For this case $\beta_2 = 2.60$, however, the barrier has got a finite curvature. The solid line is for $V_0 = 1.0$ and the dotted line for $V_0 = 10.0$. Note that the oscillatory reflectivity is observed when the barrier height is larger $V_0 = 10.0$. Else the reflectivity with multiple minima will be observed for $E \gg V_0$ when $V_0 = 1.0$.

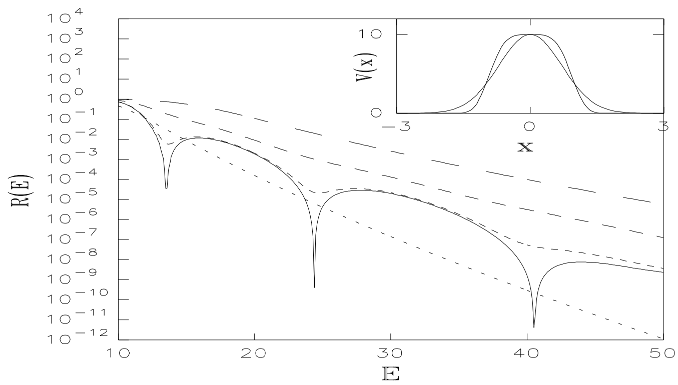

Figure 4. Exactly computed reflectivity, $R(E)$, for exponential potentials, $V_s(x) = V_0\,\mathrm{e}^{-x^4-sx}$. The dotted line displays the reflectivity for the Gaussian barrier and the solid line is for $V_{s=0}(x)$. The short-dashed, medium-dashed and long-dashed lines display the reflectivity when the asymmetry parameter s is 0.1, 0.5 and 1.0, respectively. Note that for the case of $s = 0.1$ feeble oscillations are still sustained. Here $V_0 = 10$ in arbitrary units. Note the flatness of the potential $V_{s=0}(x)$ (thick line) at the barrier top in comparison to the Gaussian barrier (thin line) in the inset. The value of the kurtosis parameter β_2 for the flat barrier is 2.18 ($s = 0$) and for the Gaussian it is 3. The values of the kurtosis parameter, β_2, for the case of $s = 0.1, 0.5, 1.0$ are 2.46, 2.76, 3.16, respectively. In the cases of $s = 0.5, 1.0$ an increased value of V_0 exhibits slightly more pronounced oscillations.

This is shown by a short dashed line underestimating the reflectivity. For the Gaussian barrier, we have $\beta_2 = 3$ and $V''(0) = -2V_0$.

In figure 3, we give the interesting example of $V_R(x) = V_0\,\mathrm{e}^{-(\epsilon x^2+x^4)}$, which has $\beta_2(\epsilon = 1) = 2.60$ and $\beta_2(\epsilon = 2) = 2.43$ and its reflectivity entails multiple minima when V_0 is large. The top curvature of the barrier being non-zero, this is an interesting example wherein the two criteria of top curvature and kurtosis are also mutually exclusive.

Presently, we have discussed only asymptotically convergent potentials; the reflectionlessness of asymptotically divergent barriers, $V_K(x) = x^{2K+2}$, $K = 1, 2, 3, \ldots$, has been discussed in [9]. It is again worth remarking that $V_K(x)$ potentials have their β_2 indeterminate but they have the top curvature as zero.

We find that the symmetry of the barriers plays the most crucial role; a slight deviation from symmetry causes the weakening of the oscillations in the reflectivity. In figure 4, we present evidence for this as we compute the reflectivity for the potential $V(x) = V_0\,e^{-x^4-sx}$ when $s = 0.0, 0.1, 0.5, 1.0$ to find that the oscillations in $R(E)$ die out as we deviate from the symmetry of $V_s(x)$. It may be noted that here we have to perform the numerical integration on both the sides of the barrier and the end values of $u(x)$ and $v(x)$ at $x = \pm d$ will be used to determine $R(E)$; equation (2) has not been used here. However, once again the kurtosis of these barriers can be calculated using (1), where $\bar{x}$ will depend on the asymmetry parameter s. We find that β_2 increases as s increases; it is 2.18, 2.46, 2.76, 3.16 for $s = 0.0, 0.1, 0.5, 1.0$, respectively. Symmetry of the potential barriers is also behind the PT-symmetric origin of reflectionlessness [9].

7. Summary and conclusions

Having studied the question as to what type of potential barriers would entail reflectivity zeros/minima, we summarize our findings pointwise as follows.

- The symmetry of the single top barriers turns out to be most crucial.
- The reflectivity, $R(E)$, of a one-dimensional potential barrier having β_2 in the range $(1.8, \sim 3.0)$ is an oscillatory function of energy. When the value of β_2 is closer to 1.8 the barrier is rectangular type and the reflectivity minima are more pronounced. The barriers having β_2 closer to (or greater than) 3.0 are unlike rectangular barriers and the reflectivity is a smooth decreasing function of energy. The reflectivity for V_{Berry} and V_{Ch} is known to entail zeros; however, β_2 being indeterminate these two are the exceptions to this criterion/condition which we have referred to as $\mathbf{C}_4$.
- We find that the zero curvature at the top $(V''(0) = 0)$ is the most simple criterion/condition ($\mathbf{C}_5$) on the potential barriers for observing the oscillatory behaviour of $R(E)$. This criterion also includes the special potentials, $V_{\mathrm{Berry}}(x)$ and $V_{\mathrm{Ch}}(x)$.
- With an exception to $V_{\mathrm{Berry}}(x)$, we find that oscillatory reflectivity *mostly* implies or is implied by more than one pair of over-barrier complex conjugate classical turning points. Consequently, the conventional WKB formula based on the single pair of complex conjugate turning points fails as it essentially gives rise to smoothly decreasing reflectivity as a function of energy. We feel that the semi-classical derivation of reflectivity taking into account many (not just two, as in [12]) pairs of complex conjugate points is highly desirable.
- Interestingly, when there are reflectivity zeros or multiple minima in reflectivity the Born approximation which bypasses the use of classical turning points of the potentials works well qualitatively.
- Some potential barriers display oscillatory reflectivity only when the barrier height (V_0) is larger or when $E \gg V_0$ (see figure 3).

Both the criteria of kurtosis ($\mathbf{C}_4$) and top curvature ($\mathbf{C}_5$) favour flatter barriers which enable a potential to be more and more localized such that a bigger fraction of the area under the barrier remains within two points say $x = -a$ and $x = a$. This is the essence of the rectangular barrier which is well known for displaying the destructive interference of multiply reflected waves resulting in reflectivity zeros at discrete energies. The most familiar rectangular barrier is not an exception. It, in fact, is ironically both a paradigm (the first and the simplest) and an ultimate (the best) model of the barriers that can display reflectionlessness at super-barrier energies.

We end by concluding that the hitherto known five conditions/criteria on a potential barrier to have multiple minima/zeros in the reflectivity could at most be providing the sufficiency conditions. However, the intriguing question of the *necessary* condition(s) in this regard still remains open. We believe that the symmetry of the single top barriers could turn out to be one of the necessary conditions when a more rigorous treatment is available.

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