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MVBerry [1] &KieronBurke [2]

[1]HHWillsPhysicsLaboratory,TyndallAvenue,BristolBS81TL,UK
(asymptotico@bristol.ac.uk,OrcidID:0000 -0001-7921-2468)

[2] DepartmentofChemistry,1102 NaturalSciences2,UniversityofCalifornia,
Irvine,California92697,USA(kieron@uci.edu),

Abstract

Aninfinitepotentialwell,truncatedatfiniteheight,providesasimplemodelfor studyingtheeffectof nonanalyticityonsemiclassicalapproximations.Anexact quantizationconditionfortheboundstatesseparatestheeffectsassociatedwith theuntruncatedwellfromthoseofthetruncation.Becausethetruncation occursbeyondtheclassicalturningpoint s,ithasnoeffecttoanyfiniteorderin powers of Planck's constant. The truncation contribution is exponentially smallanddependsonthepotentialintheclassicallyforbiddenregion.The contributionassociatedwiththewell,whenconsistentlyappr oximatedbeyond allsemiclassicalorders,alsoleadstoasmallexponential,dependingonthe potentialintheclassicallyallowedregion.Bothexponentiallysmall contributionscanbeextractedbyasymptoticanalysis,withexplicitresultsin thesimple caseofalinearwell.Thiscombinationofseveraldifferent semiclassicaltechniquescouldbepedagogicallyusefulasanexercisein teachingphysicalasymptoticsatthepostgraduatelevel.

Keywords:asymptotics,singularities,smallexponentials ,diver gentseries

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1. Introduction

The quantization of energies in a one-dimensional potential well is a familiar vehicle for introducing and illustrating semiclassical (small $\hbar$) approximation techniques, especially the WKB method [1, 2]. Here we describe a slightly more sophisticated variant, requiring the understanding of two different kinds of small exponential, with the pedagogical advantage that it combines several different kinds of asymptotics while being precisely solvable.

The variant is that the potential $V(x)$ (chosen even for convenience) is truncated at $x=\pm L$ as illustrated in figure 1. Thus

$$V(x) = \begin{cases} V_{\text{well}}(x) & (|x| < L) \\ V_L = V_{\text{well}}(L) & (|x| > L) \end{cases}. \tag{1.1}$$

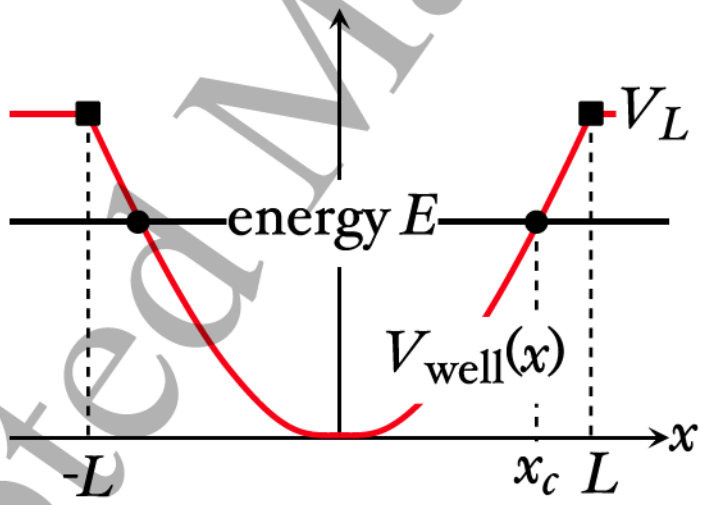

Figure 1. Truncated potential, with energy less than the truncation.

The aim is to understand how the truncation affects the energy levels of the bound states $E<V_L$, in the semiclassical regime of small $\hbar$. The interest lies in the fact that the discontinuity of slope means that the potential is nonanalytic, while standard semiclassical asymptotics works for analytic potentials. The classical turning point x_c, defined by $E=V_{\text{well}}(x_c)$, separates the classically

allowed region $|x|\leq x_c(E)$ from the classically forbidden region $|x|>x_c(E)$. Since the truncation at $x=L$ occurs in the classically forbidden region, and semiclassical asymptotics for the energy levels depends on the potential and its derivatives in the classically allowed region, the truncation is invisible to all orders $\hbar^n$, i.e. all orders of semiclassical approximation. The semiclassical influence of truncation on the spectrum is exponentially small in $\hbar$, and can be understood only by going beyond all orders.

For explicit calculations, we choose the untruncated potential V_{well} to be linear, so

$$V_{\text{linear}}(x) = \begin{pmatrix} |x| & (|x| < L) \\ L & ((|x| > L)) \end{pmatrix}. \qquad (1.2)$$

Figure 2 shows the spectrum, calculated as explained in the next section. As L increases, the binding increases and more levels are sucked down from the continuum. After its birth, the influence of the truncation on each level diminishes: the energies approach those of the untruncated potential. This is the behaviour we aim to understand.

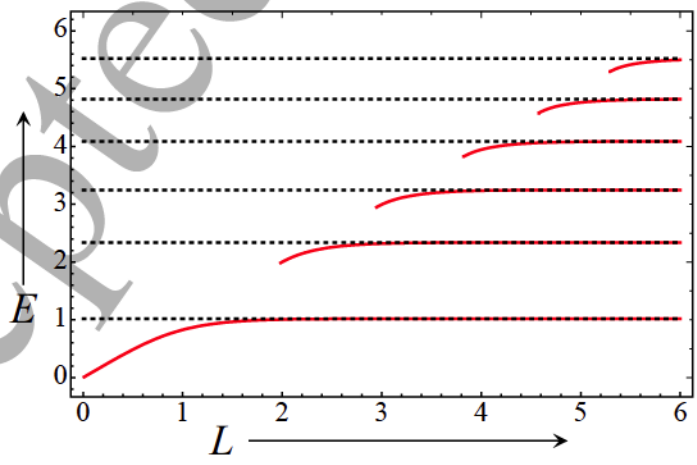

Figure 2. Red curves: even and odd energy levels in the truncated potential (1.2), for increasing truncation distance L; dotted lines: levels of the untruncated linear potential, i.e. zeros of Ai′ (even levels) and Ai (odd levels).

Insection2wederiveanexact quantizationcondition,inaformwhere theinfluenceofthetruncationisseparatedfromtheconditonforthelevelsof theuntruncatedpotential.Section3calculatestheasymptoticsofthetruncation terminthequantizationcondition. Awayfromthe birthsofeachlevelatthetop ofthewell,thetruncationtermisexponentiallyweak.Thusforsemiclassical consistencythequantizationoftheuntruncatedwellshouldalsobe approximatedtoincludeexponentiallysmallterms;thisisdescribedinsection 4,andthetwoexponentialsarecompared ,andpossibleextensionsdiscussed,in theconcludingsection5 . Werecognisethatsomeoftheasymptoticanalysis (especiallyinsection4) ischallengingandunfamiliarinmanygraduate curricula,butwehave triedtomakei t assimpleaspossible(thoughnot simpler,asEinsteinisreputedtohaveadvised).

2.Exactquanti zationcondition

Theenergylevelsareeigenvaluesdeterminedbytheone -dimensionaltime - independentSchrödingerequation,whichwewrite inconvenientunitswhere themassis1/2,andofcourseretainingthesemiclassicalparameter $\hbar$;thus

$$\hbar^2\psi''(x)+\big(E-V(x)\big)\psi(x)=0\ . \tag{2.1}$$

Forevenpotentials,successiveeigenstatesareevenandodd,soitis necessarytoconsideronly $x\geq 0$. For $x<L$,thesolutionsarelinearcombinations ofthoseoftheuntruncatedpotential V_{well}. It is convenient to choose these as the unique exact solution $\psi_-(x;E)$ that decays exponentially in the classically forbidden region $x_c<x<L$, and any exact solution $\psi_+(x;E)$ that grows exponentially. The linear combinations are fixed by symmetry: at $x=0$, $\psi=0$ for the odd states, and the derivative $\psi'=0$ for the even states. For $x>L$, the solution

in the constant potential V_L is a decaying exponential. Thus the even states can be written as

$$\psi'_{\text{even}}(0;E)=0$$
$$\psi_{\text{even}}(x;E)=\begin{cases}\psi'_{+}(0;E)\psi_{-}(x;E)-\psi'_{-}(0;E)\psi_{+}(x;E) & (x<L)\\ C\exp\left(-\dfrac{x\sqrt{V_L-E}}{\hbar}\right) & (x>L)\end{cases}, \tag{2.2}$$

and the odd states as

$$\psi_{\text{odd}}(0;E)=0.$$
$$\psi_{\text{odd}}(x;E)=\begin{cases}\psi_{+}(0;E)\psi_{-}(x;E)-\psi_{-}(0;E)\psi_{+}(x;E) & (x<L)\\ C\exp\left(-\dfrac{x\sqrt{V_L-E}}{\hbar}\right) & (x>L)\end{cases}. \tag{2.3}$$

The constant C can be eliminated by the requirement that the value and slope of the solutions of (2.1) must be continuous at $x=L$. This gives the quantization condition for the energies E, in the form of a function $Q(E)$ that vanishes at the eigenvalues. After some elementary manipulations, this can be expressed in the convenient form

$$Q(E)=Q_w(E)+Q_t(E)=0, \tag{2.4}$$

in which Q_w alone generates the levels of the untruncated well and Q_t is the effect of the truncation. The two terms are

$$Q_{w,\mathrm{even}}(E)=\frac{\psi'_-(0;E)}{\psi'_+(0;E)},\quad Q_{w,\mathrm{odd}}(E)=\frac{\psi_-(0;E)}{\psi_+(0;E)}$$

$$Q_t=-\frac{\left(\psi_-(L;E)+\dfrac{\hbar}{\sqrt{V_L-E}}\psi'_-(L;E)\right)}{\psi_+(L;E)+\dfrac{\hbar}{\sqrt{V_L-E}}\psi'_+(L;E)}. \tag{2.5}$$

Note that the well contribution Q_w is different for the even and odd states, while the Q_t is independent of the symmetry.

For the model well V_{linear} (1.2), the decaying and growing solutions of (2.1) are the standard Airy functions [3, 4]

$$\psi_-(x)=\mathrm{Ai}\left(\frac{x-E}{\hbar^{2/3}}\right),\quad \psi_+(x)=\mathrm{Bi}\left(\frac{x-E}{\hbar^{2/3}}\right). \tag{2.6}$$

The turning point is $x_c=E$, and the truncation value of the potential is $V_L=L$. An immediate simplification is that $\hbar$ can be scaled away by redefining

$$\frac{E}{\hbar^{2/3}}\Rightarrow E,\quad \frac{L}{\hbar^{2/3}}\Rightarrow L, \tag{2.7}$$

so the semiclassical regime is $E>>1$, $L>>1$. (Similar rescaling eliminates $\hbar$ for any power-law potential $V_{\mathrm{well}}=|x|^n$.) The two contributions (2.5) to the quantization condition can now be written explicitly:

$$Q_{w,\mathrm{even}}(E)=\frac{\mathrm{Ai}'(-E)}{\mathrm{Bi}'(-E)},\quad Q_{w,\mathrm{odd}}(E)=\frac{\mathrm{Ai}(-E)}{\mathrm{Bi}(-E)}$$

$$Q_t(X)=-\frac{\left(\mathrm{Ai}(X)+\dfrac{1}{\sqrt{X}}\mathrm{Ai}'(X)\right)}{\mathrm{Bi}(X)+\dfrac{1}{\sqrt{X}}\mathrm{Bi}'(X)},\quad \text{where } X\equiv L-E. \tag{2.8}$$

For the untruncated well, the energies are zeros of the Airy functions: Ai(–*E*)=0 for the odd states and Ai′(–*E*)=0 for the even states. It is easy to calculate the zeros of the full *Q(E)* numerically (e.g. using the FindRoot function in Mathematica), and that is how figure 2 was calculated.

The truncations L_{birth} at which levels are born can also be calculated. These correspond to $L=E$, i.e. $X=0$ in Q_t. From

$$Q_t(0) = \frac{1}{\sqrt{3}}, \tag{2.9}$$

the truncations are given by

$$\begin{aligned} \text{Ai}'(L_{\text{birth}}) &= -\frac{\text{Bi}'(L_{\text{birth}})}{\sqrt{3}}, \quad L_{\text{birth}} = 2.948689,\ 4.578055,\ldots \quad (\text{even}) \\ \text{Ai}(L_{\text{birth}}) &= -\frac{\text{Bi}(L_{\text{birth}})}{\sqrt{3}}, \quad L_{\text{birth}} = 1.986352,\ 3.825339,\ldots \quad (\text{odd}) \end{aligned} \tag{2.10}$$

For the even levels, the first value of L_{birth} corresponds to the first excited even state, not the lowest, denoted $E_{1,\text{even}}$, because this is the ground state and exists for all purely attractive one-dimensional potential wells, however weakly binding [5, 6]. Thus this state exists for all L, as illustrated in figure 2.

Although not part of the semiclassical analysis, we can understand the behaviour of the ground state for small L by expanding the even Q_w in (2.8) for small E, and Q_t for small X, and solving for E. This is an elementary exercise involving known small-argument formulas for the Airy functions [3], leading to

$$E_{1,\text{even}}(L) = L - \tfrac{1}{4}L^4 + O(L^7). \tag{2.11}$$

Figure 3 illustrates the accuracy of this formula as L increases from zero.

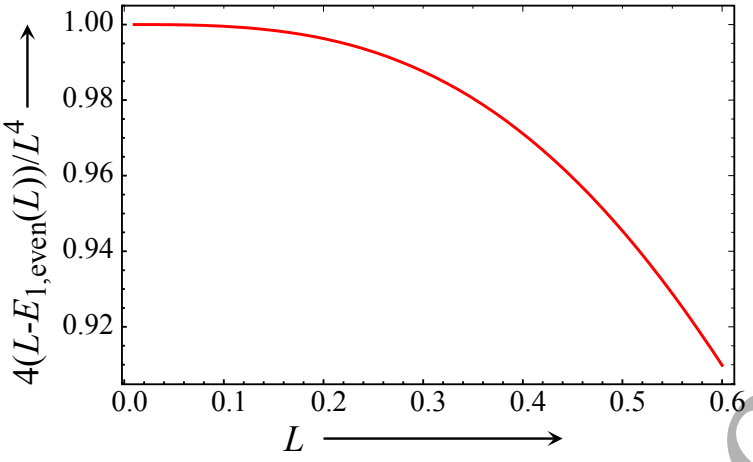

Figure3 .Testofthesmallwelllimitingform(2.11)fortheground -stateenergy $E_{1,\mathrm{even}}$.

3.Asymptotictruncationexponential

Themainaimofthissectionistocalculatethesemiclassicalapproximationto Q_t, inordertocaptureitssmallexponential.Thenextsectionwillconcernthe correspondingexpo nentialin Q_w. Since $x=L$ liesintheclassicallyforbidden region, werequiretheleadingWKBapproximationsto thegrowingand decayingsolutionsof(2.1) ;we choosetheuniquegrowingsolutionthat containsnosmallexponential itscompleteasymptoticexpansion . Thesemust connectwiththecorrespondingoscillatorysolutionsintheclassicallyallowed region;itisconvenienttochooseth osesolutionswhose sinusoidal oscillations havethesame prefactor. ThisisthecelebratedWKBconnectionproblem, whoseanalysisleadsto [7-9]

$$\psi_{+}(x;E)\approx\frac{\exp\left(+\frac{1}{\hbar}\int_{x_c(E)}^{x}\mathrm{d}x'\sqrt{V_{\mathrm{well}}(x')-E}\right)}{\left(V_{\mathrm{well}}(x)-E\right)^{1/4}}$$
$$\psi_{-}(x;E)\approx\frac{\exp\left(-\frac{1}{\hbar}\int_{x_c(E)}^{x}\mathrm{d}x'\sqrt{V_{\mathrm{well}}(x')-E}\right)}{2\left(V_{\mathrm{well}}(x)-E\right)^{1/4}}. \qquad (3.1)$$

From the quotient form of Q_t in (2.5), the exponentially growing solution in the denominator dominates the exponentially decaying solution in the numerator. In the denominator, the two terms add when calculated from (3.1) to leading order in $\hbar$, that is, by differentiating just the exponential. But when the same procedure is applied to the numerator in (2.5), the two terms cancel. Therefore it is necessary to go one stage further, to include the derivative of the prefactor in the second term of the numerator in (3.1). (It is not necessary to include the first WKB correction to the approximation (3.1) for ψ_-, because its contributions to the two terms in the numerator of (2.5) cancel.) Thus the leading semiclassical approximation to the truncation term in the quantization condition is found, after a short calculation, to be

$$Q_t(E) \approx \frac{\hbar V'_{\text{well}}(L)}{16\left(V_L - E\right)^{3/2}} \exp\left(-\frac{2}{\hbar} \int_{x_c(E)}^{L} \mathrm{d}x' \sqrt{V_{\text{well}}(x') - E} \right). \tag{3.2}$$

This is the first of our two small exponentials.

For the linear model potential, this formula (or, equivalently, standard Airy asymptotics [3] gives

$$Q_t(X) \gg \frac{\exp\left(-\frac{4}{3}X^{3/2}\right)}{16X^{3/2}} \circ Q_{t,\,\text{large}}(X). \tag{3.3}$$

Although this approaches the exact $Q_t(X)$ as X increases, it fails to describe the behaviour for small X, which is necessary to understand the energy levels near the top of the potential, where the influence of the truncation is strongest. For this we need the small X behaviour in the first order beyond (2.9), namely

$$Q_t(X) \approx \frac{1}{\sqrt{3}} - \frac{2\Gamma(1/3)}{3^{5/6}\Gamma(2/3)} X^{1/2} = 0.57735 - 1.58393X^{1/2} \qquad (3.4)$$
$$\circ\ a - bX^{1/2} \circ Q_{t,\,\mathrm{small}}(X).$$

A useful fit to the two extremes is

$$Q_{t,\,\mathrm{combined}}(X) \approx \frac{a\exp\left(-\frac{4}{3}X^{3/2}\right)}{1+(b/a)X^{1/2}+16aX^{3/2}}. \qquad (3.5)$$

Figure 4 illustrates the accuracy of this fit to $Q_t(X)$. Using a more sophisticated interpolation, and higher-order approximations for large and small X, it would be possible to obtain a closer fit, but as figure 5 shows this is unnecessary, because the quantization condition based on (3.5) gives an accurate description of the levels close to their appearance at L_{birth}.

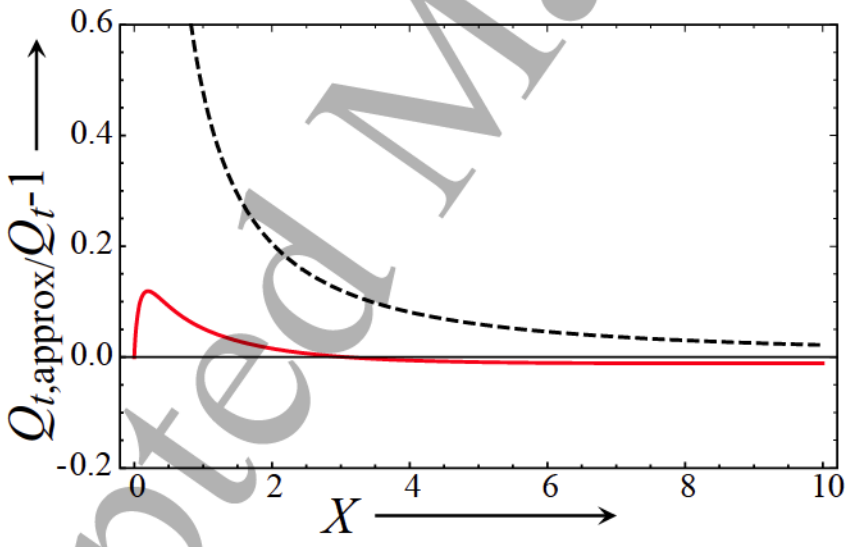

Figure 4. Errors in approximations to the truncation function Q_t. Dashed curve: large X approximation $Q_{t,\,\mathrm{large}}$ (3.3); red curve: approximation $Q_{t,\,\mathrm{combined}}$ (3.5) fitting the large and small X limits.

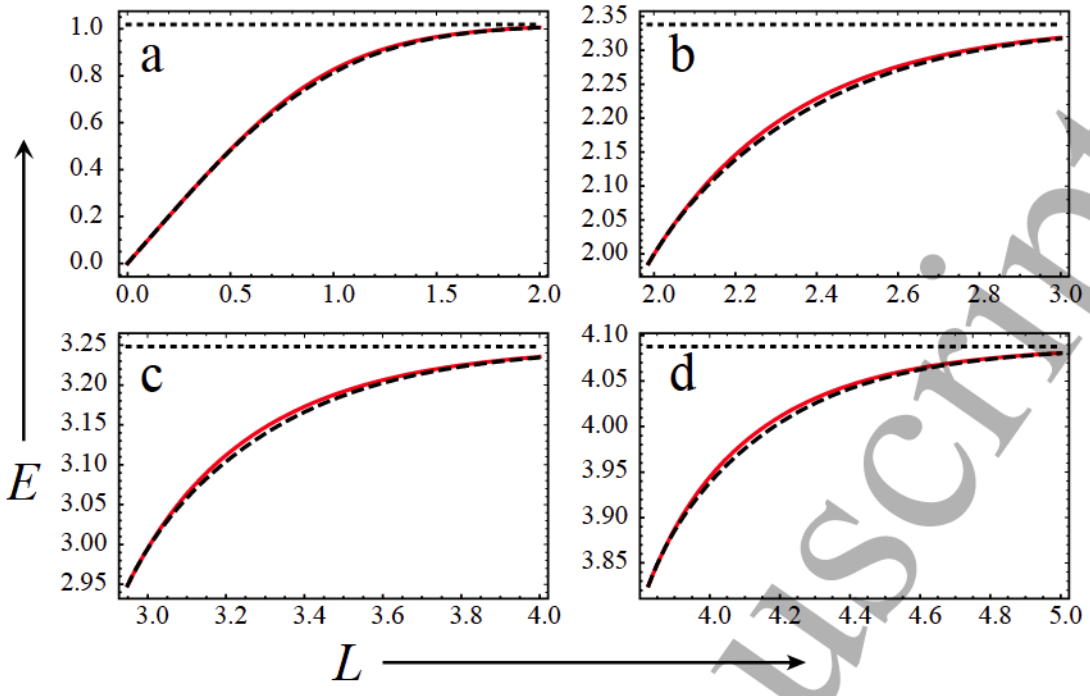

Figure 5. Lowest levels after their appearance when $L=L_{\text{birth}}(..)$ (magnification of part of figure 2): red curves: exact; dashed curves: using the approximation $Q_{t,\text{combined}}$ (3.5); dotted lines, levels of untruncated linear potential (1.2), i.e. zeros of Ai and Ai′. (a) Lowest even level (ground state); (b) lowest odd state; (c) first excited even state; (d) first excited odd state.

As L increases, the quantization sensitivity $\partial E/\partial L$ increases for states near the truncation, i.e. $X=L-E<<L$. From (2.8), and using the simple Bohr-Sommerfeld formula ((4.2) to follow) for Q_w, differentiation, and the fact that $Q_t(X)=O(1)$ near the truncation, leads to the estimate

$$\frac{\partial E}{\partial L} \gg \frac{1}{Q_t'(X)}\sqrt{L}\left(1+Q_t(X)^2\right) \sim \sqrt{L}\,. \tag{3.6}$$

Thus, the higher the truncation, the greater the sensitivity. Reinstating $\hbar$ from (2.7), the semiclassical sensitivity is $\partial E/\partial L \sim \hbar^{-1/3}$. This exponent is for the linear potential (1.2). If $V_{\text{well}}=x^n$, a similar calculation replaces the exponent –1/3 by $(n-2)/(n(n+2))$, so the asymptotic sensitivity increases for potentials increasing more slowly than quadratic, and decreases for potentials increasing faster.

4. Asymptotic semiclassical well exponential

Except near the birth of the levels at L_{birth}, the dominant contribution to the quantization condition Q_t in (2.4) is Q_w, associated with the untruncated well and defined in (2.5) for the even and odd states. In the WKB approximation, this arises from oscillatory solutions between the classical turning points, and in lowest order gives the familiar phase-corrected Bohr-Sommerfeld condition for the phase-space area associated with energy E:

$$\oint \mathrm{d}x\sqrt{E-V_{well}(x)} = 4\int_0^{x_c(E)} \mathrm{d}x\sqrt{E-V_{well}(x)} = \left(n+\tfrac{1}{2}\right)2\pi\hbar \qquad (4.1)$$
$$\left(n=0,1,2\cdots,\ \text{even states: } n \text{ even; odd states: } n \text{ odd:}\right).$$

Higher approximations involve increasing powers of $\hbar$ [8, 10]. But since the truncation term (3.2) is exponentially small in $\hbar$, approximating Q_w to comparable accuracy requires going beyond all orders in the semiclassical series. In fact, the semiclassical power series is divergent [8], and the small exponential originates in the resummation of its tail, as will now be explained.

For simplicity, we do not carry out the resummation for a general V_{well} (we will return to the general case at the end of this section). Instead, we illustrate the procedure explicitly for the odd states of the linear potential (1.2), where the energies are the zeros of Ai($-E$). For this case, (4.1), or standard Airy asymptotics for negative argument [3], gives, for $Q_{w,\text{odd}}$ defined in (2.8), and consistent with (4.1),

$$Q_{w,\text{linear}}(E) \sim \tan\left(z(E)+\tfrac{1}{4}p\right) = 0, \text{ where } z(E) \circ \tfrac{2}{3}E^{3/2}. \qquad (4.2)$$

A convenient form for the *N*th order asymptotic approximations to the Airy functions of negative argument, that follows immediately from the separate series for Ai and Bi [3], is

$$\mathrm{Bi}_N\left(-E\right)+\mathrm{iAi}_N\left(-E\right)=\frac{\exp\left(\mathrm{i}\left(z\left(E\right)+\frac{1}{4}p\right)\right)}{\sqrt{p}\,E^{1/4}}S_N\left(z\left(E\right)\right), \tag{4.2}$$

where the series is

$$S_N\left(\zeta\right)=\sum_{m=0}^{N}\frac{\left(m-\frac{1}{6}\right)!\left(m-\frac{5}{6}\right)!}{\pi m!2^{m+1}}\left(\frac{-\mathrm{i}}{\zeta}\right)^m=1-\frac{5\mathrm{i}}{72\zeta}-\frac{385}{10368\zeta^2}+\cdots \tag{4.3}$$

In turn this gives the quotient for $Q_{w,\mathrm{odd}}$ in (2.8) as

$$Q_{w,\mathrm{linear},N}\left(E\right)=\tan\left(z\left(E\right)+\tfrac{1}{4}p+\mathrm{Im}\log S_N\left(z\left(E\right)\right)\right). \tag{4.4}$$

We cannot immediately extend the sum to $N=\infty$ because it is divergent. This follows from the large m limiting form of the cefficients

$$\frac{\left(m-\frac{1}{6}\right)!\left(m-\frac{5}{6}\right)!}{m!}\underset{m\to\infty}{\to}\left(m-1\right)! \tag{4.5}$$

(even for m=2 this is accurate to better than 90%). Therefore (as first observed in 1747 by Thomas Bayes for the related Stirling approximation [11, 12]), the increase of the coefficients in (4.3) will always dominate the decrease of the powers ζ^{-m}. The least term, representing optimal termination of the series, can be estimated from (4.3) and Stirling's formula for $(m-1)!$, as

$$N_{\mathrm{opt}}\left(z\right)=\left[2z\right], \tag{4.6}$$

where $\lfloor x \rceil$ denotes the integer nearest to x. The black dots in figure 6 illustrate, for values of $\zeta(E)$ corresponding to the lowest untruncated levels, how the error $S_N - S_\infty$ first gets smaller and then increases as N increases: the series diverges.

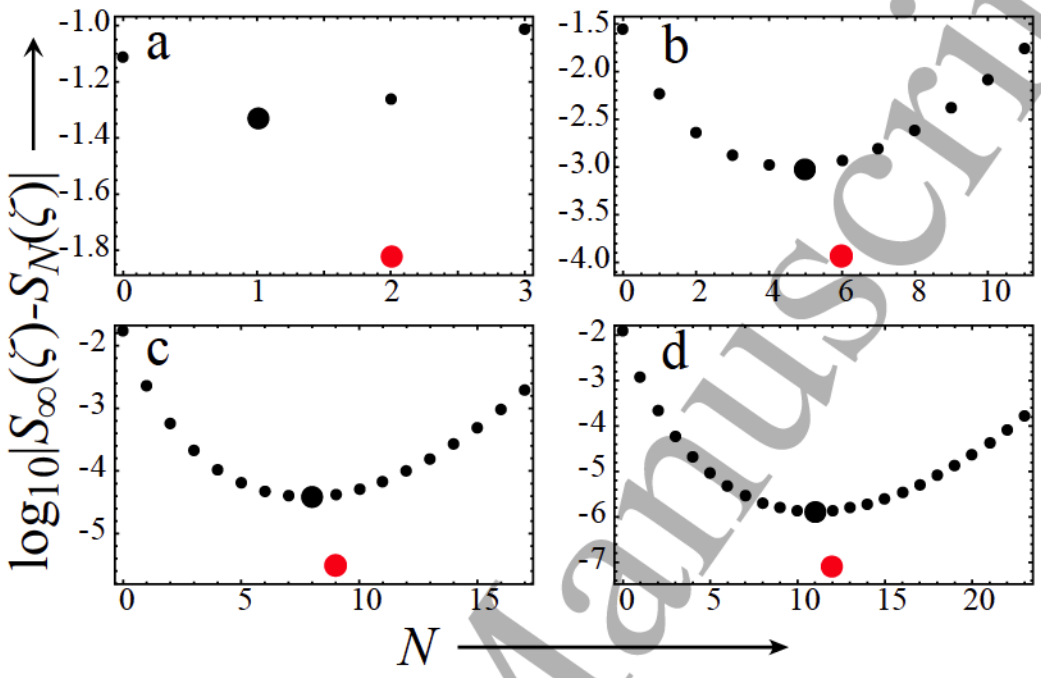

Figure 6. Black dots: errors in the approximations $S_N\left(z\left(E\right)\right)$ (4.3) to the sum $S_{¥}\left(z\left(E\right)\right)$ (4.7) for successive truncations N, showing the divergence of the series; the large dots indicate the smallest term: $N=N_{\rm opt}(E)$. Red dots: errors when the series optimally terminated at $N_{\rm opt}(E)$ is corrected by the resummed tail $R_{\rm summed}(E)$ (4.14), for energies E of the four lowest levels of the untruncated potential (1.2): (a) E=1.019 ($N_{\rm opt}$=1); (b) E=2.338 ($N_{\rm opt}$=5); (c) E=3.248 ($N_{\rm opt}$=9); (d) E=4.008 ($N_{\rm opt}$=12).

The formal infinite series can be defined exactly from (4.2) as

$$S_{¥}\left(z\left(E\right)\right) = \sqrt{\rho}\,E^{1/4}\left(\mathrm{Bi}\left(-E\right)+\mathrm{iAi}\left(-E\right)\right)\exp\left(-\mathrm{i}\left(z\left(E\right)+\tfrac{1}{4}\rho\right)\right), \qquad (4.7)$$

The small exponential that we seek is hidden in the remainder $R(\zeta)$ when the series is optimally terminated, defined formally by the divergent tail of the series:

$$R(z) \equiv S_\infty(z) - S_{N_{\rm opt}(z)}(z) = \sum_{m=N_{\rm opt}(z)+1}^{\infty} \frac{\left(m-\frac{1}{6}\right)!\left(m-\frac{5}{6}\right)!}{\rho\, m!\, 2^{m+1}} \left(\frac{-\mathrm{i}}{z}\right)^m . \qquad (4.8)$$

The main result will be the small exponential in (4.14) for this remainder. Readers interested only in this can skip the derivation that now follows.

We need only the leading order, and $N_{\rm opt}$ is large, so we can use the approximation (4.5). Thus, also using (4.6), we need to calculate

$$R(z) \approx \frac{1}{2\rho} \sum_{m=\lceil 2z \rceil+1}^{\infty} (m-1)! \left(\frac{-\mathrm{i}}{2z}\right)^m . \qquad (4.9)$$

In order to estimate this sum of a divergent series, it must be interpreted. There are several ways of doing this. The most general is to use Borel summation [8]: replacing $(m\text{-}1)!$ by its integral representation, summing the resulting geometric series, and then approximating the integral (e.g. by the saddle-point technique). But for the present purpose, of getting the lowest-order approximation, a simpler method will suffice. With the replacement

$$m = \lceil 2z \rceil + 1 + k, \qquad (4.10)$$

(4.9) becomes

$$R(z) \approx \frac{1}{2\rho} \left(\frac{-\mathrm{i}}{2z}\right)^{\lceil 2z \rceil+1} \sum_{k=0}^{\infty} \left(\lceil 2z \rceil + k\right)! \left(\frac{-\mathrm{i}}{2z}\right)^k . \qquad (4.11)$$

Next, we use the approximation

$$\left(\lceil 2z \rceil + k\right)! \gg \lceil 2z \rceil! \lceil 2z \rceil^k , \qquad (4.12)$$

based on the intuition that the value of the resummed series is determined by its behaviour near the least term, i.e. $k << \lfloor 2z \rfloor$. Thus (4.11) becomes

$$R(z) \approx \frac{1}{2p}\left(\frac{-\mathrm{i}}{2z}\right)^{\lfloor 2z \rfloor+1} \lfloor 2z \rfloor! \sum_{k=0}^{\infty}\left(-\mathrm{i}\frac{\lfloor 2z \rfloor}{2z}\right)^{k} . \tag{4.13}$$

Summing the geometric series (on the border of its domain of convergence), using $\lfloor 2z \rfloor \gg 2z$ for the large ζ we are concerned with here, and using Stirling's approximation for $\lfloor 2z \rfloor!$, we finally get the lowest approximation

$$R(z) \approx R_{\text{summed}}(z) = \frac{(-\mathrm{i})^{\lfloor 2z \rfloor+1} \exp(-2z)}{2(1+\mathrm{i})\sqrt{pz}} . \tag{4.14}$$

This is the small exponential for the linear potential. The simple procedure employed here works because the phases $(-\mathrm{i})^k$ of the terms in (4.8) depend on k. It would fail if all the terms in the asymptotic series had the same sign; that situation corresponds to the 'Stokes phenomenon'[13, 14], and requires more sophisticated resummation [15, 16]

The red dots in figure 6 illustrates how effectively this resummation improves the least-term termination approximation, for energies of the lowest four levels of the untruncated linear potential. Table 1 shows the numerical errors in the sum for the lowest five levels. The relatively large errors in the final column reflect the fact that (4.14) is just the lowest-order approximation to the remainder R, sufficient to capture the small exponential.

E	N_{opt}	$\left\|S_{¥} - S_0\right\|$	$\left\|S_{¥} - S_{N_{\text{opt}}}\right\|$	$\left\|S_{¥} - S_{N_{\text{opt}}} - R_{\text{summed}}\right\|$	$\left\|R_{\text{summed}} / R - 1\right\|$
1.019	1	0.0775	0.0469	0.0144	0.31
2.338	5	0.0277	0.0010	1.010×10^{-4}	0.10
3.248	8	0.0174	3.87×10^{-4}	2.507×10^{-6}	0.06
4.088	11	0.0124	1.33×10^{-6}	6.396×10^{-8}	0.05
4.820	14	0.0098	5.39×10^{-8}	2.044×10^{-9}	0.04

Table 1. Errors in the sum $S_{¥}\left(z\left(E\right)\right)$ for the lowest five levels of the untruncated linear potential (1.2), corresponding to approximating by the leading term S_0 of the series (4.3), optimal termination N_{opt}, and including the resummed tail R_{summed}.

The corresponding well contribution to the quantization condition, including optimal termination and the approximated resummaton, is

$$Q_{w,\text{linear},\text{summed}}\left(E\right) = \tan\left(z\left(E\right) + \tfrac{1}{4}p + \operatorname{Im}\log\left(S_{[2z]}\left(z\left(E\right)\right) + R_{\text{summed}}\left(z\left(E\right)\right)\right)\right). \quad (4.15)$$

This is for the odd states. For the even states, the only change is the replacement of tan by cot. In particular, the small exponential (4.14) is the same. Thus, the even and odd energies of the untruncated linear potential, i.e. the zeros of Ai and Ai′, are, in this improved semiclassical approximation, determined by the solutions of

$$\zeta\left(E\right) + \operatorname{Im}\log\left(S_{[2\zeta]}\left(\zeta\left(E\right)\right) + R_{\text{summed}}\left(\zeta\right)\right) = \left(n - \tfrac{1}{2}\right)\pi, \quad \left(n = 1,2,\cdots\right). \quad (4.16)$$

For a general untruncated potential V_{well}, the theory for the small exponential corresponding to (4.14) is essentially the same. The divergence of semiclassical approximations is a general phenomenon, whose origin lies in the fact that successive approximations involve successive derivatives (essentially of $\sqrt{E - V_{\text{well}}\left(x\right)}$), and high derivatives diverge; this is a consequence of Darboux's theorem [8, 9]. For second-order differential equations of the

Schrödinger type (2.1), the tail to be resummed is exactly (4.9), and the small exponential is (4.14), after the replacement

$$2z\left(E\right) \rightarrow 2\int_{0}^{x_c(E)} \mathrm{d}x\sqrt{E - V_{\text{well}}\left(x\right)}\ . \tag{4.17}$$

This quantity is the difference of the exponents in the growing and decaying solutions; in more general situations, such as the approximation of integrals with several saddle-points, this difference of relevant exponents is called the 'singulant'[8].

5. Concluding remarks

There are two main results from this study of truncated potentials. First, the exact quantization condition can be written in the form (2.5), in which the contributions associated with the untruncated well and the truncation are separated. Second, the semiclassical asymptotics of the quantization condition involves two comparable small exponentials: associated with the truncation, and with the untruncated well. These are

$$\begin{aligned} &\text{truncation: } e_t\left(E\right) = \exp\left(-\frac{2}{\hbar}\int_{x_c(E)}^{L} \mathrm{d}x'\sqrt{V_{\text{well}}\left(x'\right) - E}\right) \\ &\text{well: } e_w\left(E\right) = \exp\left(-\frac{2}{\hbar}\int_{0}^{x_c(E)} \mathrm{d}x'\sqrt{E - V_{\text{well}}\left(x'\right)}\right). \end{aligned} \tag{5.1}$$

For the linear potential (1.2), the exponentials are

$$\text{truncation: } e_t\left(E\right) = \exp\left(-\frac{4}{3}\left(L - E\right)^{3/2}\right), \quad \text{well: } e_w\left(E\right) = \exp\left(-\frac{4}{3}E^{3/2}\right). \tag{5.2}$$

Thus the truncation exponential dominates for $L/2<E<L$, i.e. nearer the top of the well, and the well exponential dominates for $0<E<L/2$, i.e. near the bottom of the well.

Our intention has been to explore a 'minimal model'[17] of the influence of nonanalyticity on quantization. Several extensions can be envisaged, such as

• Exactly solvable model potentials different from (1.2). for example a harmonic well, where the exact quantization condition (2.5) would involve parabolic cylinder functions, or the Pöschl-Teller potential, involving Legendre functions.

• Different forms of nonanalyticity, in which the truncation is more gentle than the discontinuity of slope in (1.1). We conjecture that if the lowest discontinuous derivative of the potential is the nth, the same small exponentials will appear, but with prefactors proportional to $\hbar^n$ (cf. (3.2)). For a related study, for reflections above nonanalytic potential barriers, see [18].

• More sophisticated resummations of the tails of series such as (4.8), where approximations such as (4.5) are corrected by incorporating the fact that the coefficients of high-order terms of divergent series are related to the coefficients of the low-order terms; this is the phenomenon of 'resurgence' [8, 12], leading to 'hyperasymptotic' approximation schemes [19-21], involving successive exponential improvements: for the first zero of Ai, the relative error is of order 10^{-7}. A less general but comparably accurate alternative [22] is based on extending approximations such as (4.12) to higher orders in $1/\left[2z\right]$.

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References

1. Messiah,A.,1962, *QuantumMechanics* (North-Holland,Amsterdam)
2. Bohm, D.,1951, *Quantum theory* (Prentice-Hall, Inc, Englew ood Cliffs, N.J.)
3. DLMF,2010, *NIST Handbook of Mathematical Functions* (University Press,Cambridge) http://dlmf.nist.gov.
4. Vallée,O.&Soares,M.,2010, *Airyfunctionsandapplicationstophysics (2ndEd.)* (ImperialCollegePress,London)
5. Kocher, C. A.,1977, Criteria for bound -state solutons in quantum mechanics *Am.J.Phys.* **45**,71 -74
6. Jacoby,J.A.,Curran,M.,Wolf,D.R.&Freericks,J.K.,2019,Provingthe existence of bound states for attractive potentials in one -dimension and two-dimensionswithoutcalculus *Eur.J.Phys.* **40**,045404(32pp)
7. Berry,M.V.&Mount,K.E.,1972,Semiclassicalapproximationsinwave mechanics *Reps.Prog.Phys.* **35**,315 -97
8. Dingle, R. B.,1973, *Asymptotic Expansions: their Derivation and Interpretation* (AcademicPress,NewYorkandLondon)
9. Olver, F. W. J.,1997, *Asymptotics and special functions* (A.K. Peters, Wellesley,Mass)
10. Dunham,J.L.,1932,TheWentzel -Brillouin-KramersMethodofSolving theWaveEquation *Phys.Rev.* **41**,713 -720
11. Bayes,T.,1763,AletterfromthelateReverendMr.ThomasBayes,F.R.S. toJohnCanton,M.A.andF.R.S. *Phil.Trans.Roy.Soc.* **53**,269 -271
12. Berry,M.V.&Howls,C.J.,2015, *Divergentseries:tamingthetailsinThe Princeton Companion to Applied M athematics* eds. Higham, N. (UniversityPress,Princeton).
13. Stokes, G. G.,1864, On the discontinuity of arbitrary constants which appearindivergentdevelopments *Trans.Camb.Phil.Soc.* **10**,106 -128

14. Stokes,G.G.,1902,Onthediscontinuityofarbitra ryconstantsthatappear asmultipliersofsemi -convergentseries *ActaMath.* **26**,393 -397
15. Berry, M. V.,1989, Uniform asymptotic smoothing of Stokes's discontinuities *Proc.Roy.Soc.Lond.* **A422**,7 -21
16. Berry, M. V.,1989, Stokes' phenomenon; smoothing a Victorian discontinuity *Publ.Math.oftheInstitutdesHautesÉtudesscientifique* **68**, 211-221
17. Batterman, R. W. & Rice, C. C.,2014, Minimal Model Explanations *Philos.Sci.* **81**,349 -376
18. Berry, M. V.,1982, Semiclassical weak reflections above analytic and nonanalyticpotentialbarriers *J.Phys.A* **15**,3693 -3704
19. Berry, M. V. & Howls, C. J.,1990, Hyperasymptotics *Proc. Roy. Soc. Lond.* **A430**,653 -668
20. Berry, M. V. & Howls, C. J.,1991, Hyperasymptotics for integrals with saddles *Proc.Roy.Soc.Lond.* **A434**,657 -675
21. Berry, M. V.,1992, *Asymptotics, superasymptotics, hyperasymptotics in Asymptoticsbeyondallorders* eds.Segur,H.&Tanveer,S.(Plenum, New York),pp.1 -14
22. Airey, J. R.,1937, LII. The "converging factor" in asymptotic series and thecalculationofBessel, Laguerre andotherfunction s *Phil.Mag.(Series7* **24**,521 -552

Figurecaptions

Figure1 .Truncatedpotential,withenergylessthanthetruncation.

Figure2 .Redcurves:evenandoddenergylevelsinthetruncatedpotential (1.2),forincreasingtruncationdistance *L*;dottedlines:levelsoftheuntruncated linearpotential,i.e.zerosofA i′ (evenlevels)andAi(oddlevels).

Figure 3. Test of the small well limiting form (2.11) for the ground-state energy $E_{1,\mathrm{even}}$.

Figure 4. Errors in approximations to the truncation function Q_t. Dashed curve: large X approximation $Q_{t,\,\mathrm{large}}$ (3.3); red curve: approximation $Q_{t,\,\mathrm{combined}}$ (3.5) fitting the large and small X limits.

Figure 5. Lowest levels after their appearance when $L=L_{\mathrm{birth}}$ (..) (magnification of part of figure 2): red curves: exact; dashed curves: using the approximation $Q_{t,\mathrm{combined}}$ (3.5); dotted lines, levels of untruncated linear potential (1.2), i.e. zeros of Ai and Ai′. (a) Lowest even level (ground state); (b) lowest odd state; (c) first excited even state; (d) first excited odd state.

Figure 6. Black dots: errors in the approximations $S_N\left(z\left(E\right)\right)$ (4.3) to the sum $S_{¥}\left(z\left(E\right)\right)$ (4.7) for successive truncations N, showing the divergence of the series; the large dots indicate the smallest term: $N=N_{\mathrm{opt}}(E)$. Red dots: errors when the series optimally terminated at $N_{\mathrm{opt}}(E)$ is corrected by the resummed tail $R_{\mathrm{summed}}(E)$ (4.14), for energies E of the four lowest levels of the untruncated potential (1.2): (a) E=1.019 (N_{opt}=1); (b) E=2.338 (N_{opt}=5); (c) E=3.248 (N_{opt}=9); (d) E=4.008 (N_{opt}=12).

Table 1. Errors in the sum $S_{¥}\left(z\left(E\right)\right)$ for the lowest five levels of the untruncated linear potential (1.2), corresponding to approximating by the leading term S_0 of the series (4.3), optimal termination N_{opt}, and including the resummed tail R_{summed}.