


Asymptotically tunable quantum states and threshold scattering anomaliesOfer Neufeld ^{*}*Max Planck Institute for the Structure and Dynamics of Matter and Center for Free-Electron Laser Science, Hamburg 22761, Germany* (Received 3 June 2022; accepted 6 July 2022; published 18 July 2022)

Quantum systems can support irregular eigenstates at their threshold, which can be bound, loosely bound, or half bound. Such states are physically significant, and for instance half-bound states are known to lead to anomalous quantum scattering, where the reflection coefficient vanishes at the threshold rather than approach unity. Here, we present irregular threshold states which are generalizations of the above cases. The asymptotic behavior of these states can be tuned arbitrarily by precise control of the potential; hence, they are denoted “asymptotically tunable.” We provide exact analytical prescriptions on how to generate and control these systems. We explore several examples in 1D, including states that exhibit a power-law-like asymptotic scaling, and hybrid states that exhibit asymmetric boundary conditions (e.g., are fully bounded for $x \rightarrow \infty$ but unbounded for $x \rightarrow -\infty$, etc.). We numerically explore the scattering properties of these systems and find a close connection between the asymptotic behavior of the threshold states, and the appearance of anomalous scattering. We show that the threshold reflection coefficient can exhibit both discontinuities and derivative discontinuities as the system transitions from regular to irregular, which persist even under perturbations, and thus seem to not be quantum critical. These states could be useful for quantum system engineering, and for potential applications in optical systems for manipulating light.

DOI: [10.1103/PhysRevA.106.012210](https://doi.org/10.1103/PhysRevA.106.012210)**I. INTRODUCTION**

The physical properties of a quantum systems are usually determined either by bound states lying below the threshold energy (with $E < 0$), or by scattering states lying above the threshold energy (with $E > 0$). However, there are also cases where other types of quantum states are significant. For instance, resonances with complex eigen-energies describe open systems and metastable phenomena [1,2]. Similarly, bound states in the continuum (with $E > 0$) [3–6] have found several applications in recent years, particularly in optics [7]. In this paper, we discuss physical effects associated with quantum states located exactly at the threshold energy, $E = 0$. A variety of abnormal threshold eigenstates have already been discussed in the literature over the years. These include bound states (square integrable), loosely bound states (asymptotically vanishing, but not square integrable) [8–13], and half-bound states (which uphold Neumann boundary conditions with vanishing derivatives at the asymptotes) [14–19]. Previous works have shown that when the potential supports either low-lying bound states [20–25] or half-bound states [15–18,26,27], the scattering reflection coefficient at $E = 0$ exhibits an anomalous behavior and is smaller than unity.

Here, we present and explore a different family of threshold states in localized potentials, which asymptotically diverge or converge with an arbitrarily tunable functional form. We analytically show how to engineer the system in order to control this asymptotic behavior all the way from bound, to diverging, and provide several examples in 1D. We numerically investigate quantum scattering from these potentials and find a close connection between the asymptotic behavior of the supported threshold state, and the presence of anomalous reflection. We further show that the system can continuously transition from abnormal to normal threshold reflection by tuning a single parameter in the Hamiltonian. However, in some cases this transition exhibits a discontinuity or derivative discontinuity in the scattering coefficients. We demonstrate that these effects persist even under perturbations and are relatively robust.

The paper is ordered as follows: In Sec. II we introduce the analytical approach used to engineer desired threshold states and the logic of our proposal. In Secs. III and IV we explore several interesting cases in 1D systems and demonstrate control of the asymptotic behavior of threshold states. Section V numerically explores the threshold reflection properties of the potentials that support asymptotically tunable states as they transition from abnormal to normal scattering. Section VI summarizes our results.

^{*}oneufeld@schmidtsciencefellows.org

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II. ANALYTICAL APPROACH

The purpose of this paper is to explore quantum systems that support anomalous threshold behavior. We begin by outlining our approach to identify such systems. To this end, we consider the following 1D time-independent Schrödinger

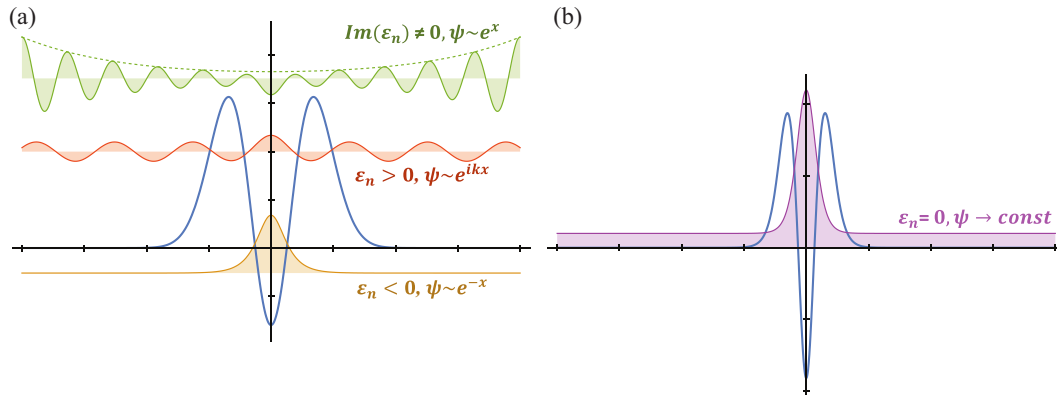


FIG. 1. Illustration of different types of eigenstates in 1D quantum systems, and their asymptotic behavior classified by their eigenenergy. (a) Bound (orange), scattering (red), and resonance (green) states. The dashed green line denotes the exponential divergence of the resonance state. (b) A half-bound threshold state that converges to a constant value asymptotically (vanishing derivative), and is non-square-integrable. Blue line represents the potential function that supports these eigenstates.

equation, given in atomic units by

$$\left(-\frac{1}{2}\frac{\partial^2}{\partial x^2} + V(x)\right)\psi_n(x) = \varepsilon_n\psi_n(x), \quad (1)$$

where $V(x)$ is a general potential-energy function, and ψ_n describes the n th eigenstate of the Hamiltonian with the associated eigenenergy ε_n . This eigenvalue problem is standardly solved with outgoing boundary conditions, giving rise to a variety of physical states. It is instructive to overview the various allowed solutions in the case of a localized potential, i.e., when the potential function vanishes at infinity ($V(x \rightarrow \pm\infty) \rightarrow 0$, we assume without loss of generality that the threshold lies at zero energy). In this case, one may formally solve Eq. (1) at the asymptotes using plane waves, $\psi_n(x \rightarrow \pm\infty) \propto e^{\pm ikx}$, where $k = (2\varepsilon_n)^{1/2}$. Consequently, it is convenient to categorize physical states according to their eigenenergies as illustrated in Fig. 1. For $\varepsilon_n < 0$, one obtains bound states that asymptotically vanish at infinity [$\psi_n(x \rightarrow \pm\infty) \rightarrow 0$] and are square integrable [$\int |\psi_n(x)|^2 dx = 1$]. Bound states standardly vanish exponentially at the asymptotes (in 3D systems bound states can also exist in the continuum with subexponential decay [3–6], but in 1D this is not possible for localized potentials [28]). For $\varepsilon_n > 0$, one obtains scattering (or continuum) states which do not converge asymptotically, and are non-square-integrable. Besides bound and scattering states, resonances are also possible solutions of Eq. (1). These arise when the eigenvalues ε_n are allowed to be complex, and lead to metastable phenomena [1,2]. Resonances exponentially diverge at the asymptotes and are non-square-integrable [1,2]. Finally, there is one more family of solutions that is often disregarded, which is obtained exactly at the threshold, $\varepsilon_n = 0$. These are so-called threshold states. Notably, there are no particular boundary conditions that threshold states must uphold, providing some freedom in their asymptotic behavior. For instance, previous works have found threshold states to be bound and square integrable, loosely bound (asymptotically vanishing but non-square-integrable), or half bound, upholding Neumann boundary conditions [$\psi_n(x \rightarrow \pm\infty) \rightarrow \text{const} \neq 0$, $\partial_x \psi_n(x \rightarrow \pm\infty) \rightarrow 0$], as illustrated in Fig. 1(b).

To analytically explore these states, we invert Eq. (1) to the following form:

$$V(x) = \frac{1}{2} \frac{\psi_n''(x)}{\psi_n(x)}, \quad (2)$$

where we used $\varepsilon_n = 0$, and $\psi_n''(x)$ represents the second derivative of ψ_n . This approach has been found useful for a variety of applications (see, e.g., Refs. [27,29,30]), and we will show here that it is well suited to explore threshold phenomena. Equation (2) highlights the one-to-one mapping between the eigenstates of the Hamiltonian and $V(x)$ —the knowledge of a single eigenstate is sufficient to fully recover the functional form of $V(x)$ up to a constant. This mapping is particularly useful for engineering threshold states: By plugging in any trial wave function, one immediately obtains the potential function that supports it as an eigenstate. If this trial wave function behaves asymptotically different than the standard bound, continuum, or resonance states (i.e., it cannot be expressed as a single plane wave), then the resulting potential either supports a threshold state, or is nonlocalized (which is irrelevant to our discussion). For instance, plugging into Eq. (2) a Gaussian wave function (that vanishes faster than an exponential rate) leads, as expected, to a harmonic potential that is nonlocalized. Alternatively, if one plugs into Eq. (2) a half-bound state that converges to a constant value at infinity, one retrieves a localized potential that supports such a state at the threshold, as illustrated in Fig. 1(b).

The above considerations can be combined with Sturm's theorem in 1D (also known as “the node theorem,” stating that the n th wave function has exactly $n - 1$ nodes [31]) to yield further spectral control. That is, by “guessing” wave functions with a particular number of nodes and desired parity in Eq. (2), one may also fix the number of bound states supported by the resulting potential. In particular, if the trial wave function is nodeless, then it is necessarily also the lowest real-energy eigenstate and the potential does not support bound states.

In the following we use Eq. (2) to generate potential functions that support threshold states, obtaining the analytical expressions for the wave functions. For simplicity, we limit our analysis to nodeless states, such that the potentials do not support any lower-lying bound states (though the analysis is

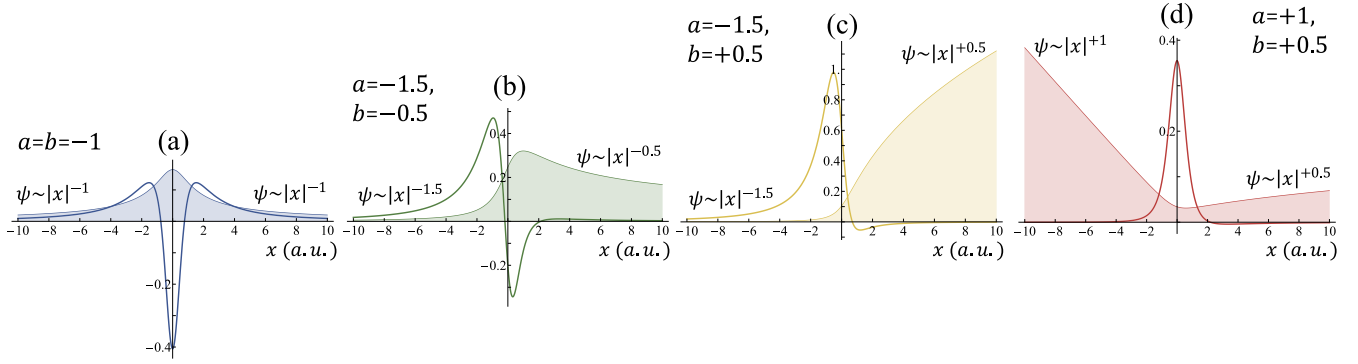


FIG. 2. Asymptotically tunable threshold states and the associated potentials that support them according to Eqs. (3) and (4) for different values of the parameters a and b . The asymptotic behavior of the threshold state is indicated in each subplot with the values of the parameters; a.u. stands for atomic units.

general). We note that our approach is complementary to the supersymmetric quantum mechanics approach [32] that was previously used to investigate threshold phenomena [6,12,18].

III. THRESHOLD-STATE ENGINEERING

We now explore types of threshold quantum states where the asymptotic behavior can be directly manipulated. For this, we utilize the approach described above, and consider the

following trial wave function:

$$\psi(x) = \left(\arctan(x) + \frac{\pi}{2} \right)^{-a} \left(\frac{\pi}{2} - \arctan(x) \right)^{-b}, \quad (3)$$

where a and b are real tunable parameters, and we note that $\psi(x)$ in Eq. (1) is not normalized. Plugging Eq. (3) into Eq. (2), one obtains the following potential:

$$V(x) = \frac{f_0(x) + f_1(x)\arctan(x) + f_2(x)\arctan^2(x) + f_3(x)\arctan^3(x)}{(x^2 + 1)^2(4\arctan^2(x) - \pi^2)^2}, \quad (4)$$

where $f_0(x)$, $f_1(x)$, $f_2(x)$, and $f_3(x)$ are the following linear functions:

$$\begin{aligned} f_0(x) &= 2\pi^2((a+b) + (a-b)^2 + \pi(a-b)x) \\ f_1(x) &= -4\pi(2(a-b)(a+b+1) + \pi(a+b)x) \\ f_2(x) &= 8((a+b)(a+b+1) + \pi(b-a)x) \\ f_3(x) &= 16(a+b)x \end{aligned} \quad (5)$$

$V(x)$ and $\psi(x)$ are plotted in Figs. 2(a)–2(d) for some exemplary values of a and b . It is worthwhile examining the asymptotic behavior of these functions. $V(x)$ in Eq. (4) has a numerator that converges to a constant value of $8\pi^2b(b-1)$ as x tends to infinity, and a constant value of $8\pi^2a(a-1)$ as x tends to minus infinity, regardless of the values of a and b (because the terms that are linear in x cancel out for $|x| \gg 1$). The denominator on the other hand diverges at the asymptotes with a parabolic scaling $\sim 16\pi^2x^2$. Thus, this potential is localized in space for any values of the parameters a and b , and exhibits a composite barrier-well type structure (see Fig. 2). Interestingly, the threshold state supported by this potential exhibits an asymptotic behavior that strongly depends on the values of a and b . One can show that its series expansion at infinity, to leading order, is

$$\psi(x) \rightarrow \pi^a x^b, \quad (6)$$

while at minus infinity it is

$$\psi(x) \rightarrow \pi^b (-x)^a. \quad (7)$$

Therefore, $\psi(x)$ exhibits a power-law behavior at the asymptotes that can be arbitrarily controlled by tuning a and b . In particular, when $a, b > 0$, the state diverges and is non-square-integrable, while it can be bound or loosely bound for $a, b < 0$. For an asymmetric choice of $a \neq b$, one may design a threshold state that is “bound” at infinity (i.e., decays faster than $x^{-0.5}$), but is loosely bound or diverges at minus infinity. Remarkably, this control is irrespective of the fact that $V(x)$ is always localized and analytic. Lastly, we point out that the particular choice of $\psi(x)$ was quite arbitrary in our analysis, and there are many other choices that lead to similar types of control.

At this point, we can extend our analysis to a plethora of other “weird” states. This possibility stems from the generality and simplicity of the above approach—once a particular $\psi(x)$ and $V(x)$ pair is obtained, the result is analytic and guaranteed. For instance, we suggest the following simple form for a nodeless half-bound state:

$$\psi(x) = \alpha + (1 - \alpha)\text{sech}^2(x), \quad (8)$$

where α is a real parameter that is bound from 0 to 1, and the potential that supports such states is straightforwardly derived by substituting Eq. (8) in Eq. (2) (for analytic expressions see the Appendix). This state is complementary to those suggested in Ref. [18] using supersymmetric quantum mechanics [32]. Such a model system can be quite useful, since for $\alpha = 0$ this state is fully bound with an eigenenergy below the threshold (exponentially decaying at infinity), while for $\alpha > 0$

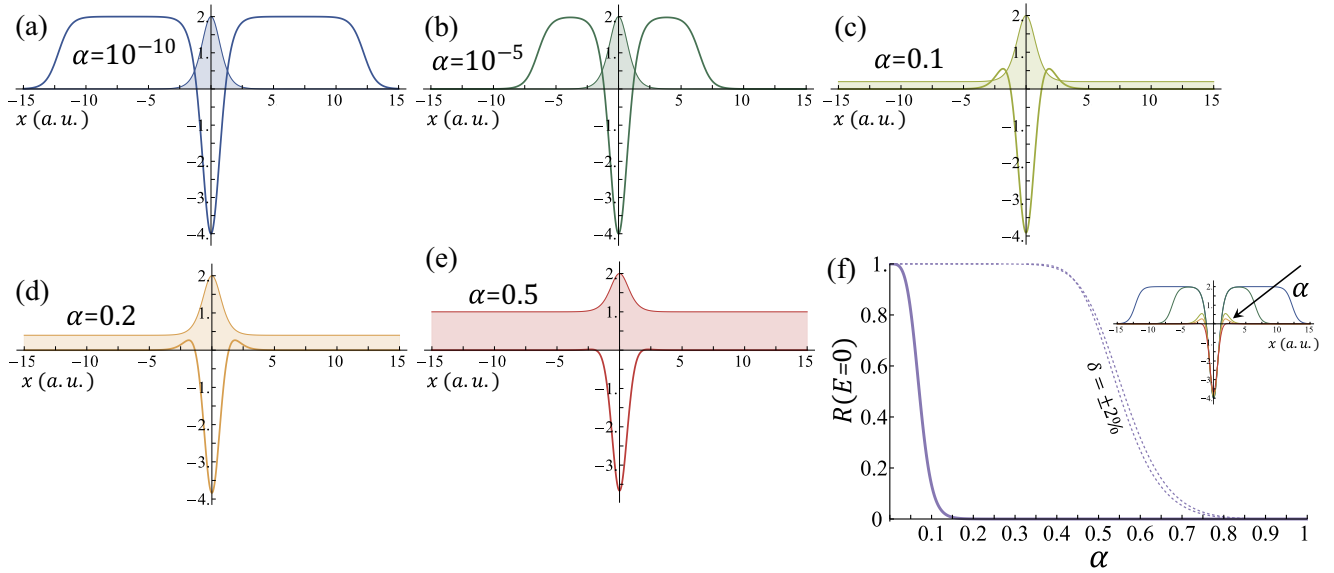


FIG. 3. Half-bound threshold states and the associated potentials that support them according to Eq. (8) for exemplary parameters. (a)–(e) Eigenstates for different values of α . The states converge to the constant value α at the asymptotes. (f) Numerically calculated quantum threshold reflection coefficient vs the parameter α from the unperturbed potential (solid line), and using a perturbed potential with an overall $\delta = 2\%$ amplitude variation (dashed). Inset in (f) indicates how the potential function changes as α is tuned, where the arrow marks the direction of increase in α .

it is half bound. By tuning α , one can study the system as it transitions between the two regimes (see plots for several values of α in Fig. 3).

As a final example, we consider loosely bound and diverging threshold states that scale logarithmically at the asymptotes. For loosely bound states we employ

$$\psi(x) = \frac{1}{\ln(1 + \beta + x^2)}, \quad (9)$$

while for diverging states we employ

$$\psi(x) = \ln(1 + \gamma + x^2), \quad (10)$$

where β and γ are real positive parameters. In both cases the potentials are straightforwardly derived (see the Appendix), and are localized. Some illustrative cases are plotted in Fig. 4.

We emphasize that the exemplary cases shown here for types of threshold states are only a select few. The approach to design and control their properties is fully general, and one may tailor a potential function to suit any desired functional form. For instance, one may similarly tailor states to scale logarithmically at infinity, but exhibit a power-law-like scaling at minus infinity, and so on and so forth. In a similar manner, this approach can be directly extended to higher-dimensional systems. For instance, in 3D one may use spherically symmetric trial wave functions that diverge (converge) with a desired scaling in r for the radial part of the Schrödinger equation.

IV. DEGENERATE THRESHOLD SOLUTIONS

At this point, and before moving on to calculate physical observables in systems supporting asymptotically tunable threshold states, we acknowledge an important mathematical point: For a second-order linear ordinary differential equation, two independent solutions always exist. Thus, the presented

wave functions, $\psi(x)$, constitute only half of the potential solution space. Standardly in quantum mechanics, other families of solutions are discarded if they exhibit ill-behaved boundary conditions (e.g., exponentially divergent at the asymptotes for the harmonic oscillator potential). Since we have not used a strong boundary constraint here (but rather demanded a particular parity and scaling at the asymptotes), we are not guaranteed a unique solution, and we must contemplate the role of the other independent solution, termed $\psi_2(x)$ from this point on. Given $\psi(x)$ solves Eq. (1) for $\varepsilon = 0$, we can directly obtain $\psi_2(x)$ as [33]

$$\psi_2(x) = \psi(x) \int \frac{dx}{[\psi(x)]^2}, \quad (11)$$

which can be plugged back into Eq. (1) to show that it is also a solution. Figure 5 presents this “other” solution for several of the exemplary cases explored in the section above. Several observations should be noted. First, while $\psi(x)$ was chosen to have an even parity (i.e., it is a nodeless positive definite state), $\psi_2(x)$ exhibits a node and odd parity. Notably, one should be able to make any threshold-state transition into a bound state by slightly (and continuously) changing the Hamiltonian. For $\psi(x)$ this poses no issue, since it is nodeless and can easily turn into the first bound state without violating Sturm’s theorem [31]. $\psi_2(x)$ on the other hand could not make this transition since, having a node, it would violate Sturm’s theorem [31]. This provides some physical intuition that $\psi_2(x)$ likely does not physically contribute to connected observables. Second, $\psi_2(x)$ can generally diverge faster than $\psi(x)$ at the asymptotes. For instance, in the case shown in Fig. 5(b) where $\psi(x)$ is determined by Eq. (3) for the parameters $a = -1.5$, $b = 0.5$, $\psi(x)$ converges at $x \rightarrow -\infty$ with a scaling of $\psi \propto (-x)^{-1.5}$, while from Eq. (11) $\psi_2(x)$ diverges as $\psi_2 \propto (-x)^{2.5}$. This by itself is not a fundamental

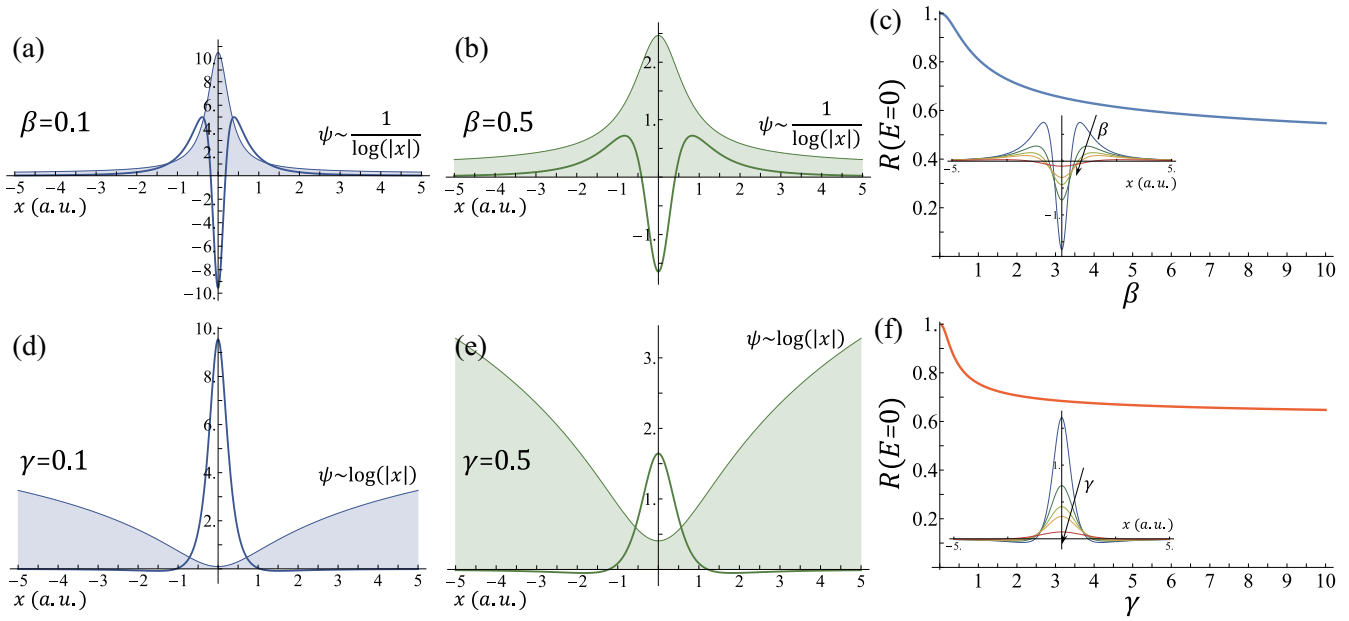


FIG. 4. Logarithmically diverging and converging threshold states and the associated potential functions that support them according to Eqs. (9) and (10), for exemplary parameters. (a), (b) Eigenstates for different values of β . The states are loosely bound and non-square-integrable. (c) Numerically calculated quantum threshold reflection coefficient, $R(E = 0)$, vs the parameter β . Inset in (c) indicates how the potential function changes as β is tuned, where the arrow marks the direction of increase in β . (d), (e) Eigenstates for different values of γ . The states are logarithmically diverging and non-square-integrable. (f) Numerically calculated quantum threshold reflection coefficient vs the parameter γ . Inset in (f) indicates how the potential function changes as γ is tuned, where the arrow marks the direction of increase in γ ; the logarithm is base 10.

issue, since it simply establishes that $\psi_2(x)$, just like $\psi(x)$, is an irregular threshold state with nonstandard asymptotic scaling (in that regard both families of independent solutions represent asymptotically tunable threshold states). On the other hand, from Eq. (4) we have that the potential converges with $V \propto (-x)^{-2}$, such that $\psi_2(x)$ diverges faster than $V(x)$ converges. Thus, $\psi_2(x)$ is a zero-energy (threshold) solution only by an exact cancellation of various contributions in a type of detailed balance that seems unphysical, since small perturbations would lead to infinite energies. Lastly, from the perspective of the main physical observable that will be explored below (the reflection–transmission coefficients at the threshold), the physical state itself does not play a direct role

because it is initially unoccupied. In that respect, the potential function $V(x)$, which is nonambiguous, determines all scattering properties. Indeed, the threshold states are only indirectly involved because they determine $V(x)$ via the conceptual inversion process, but once that has been assigned, the role of $\psi(x)$ [or $\psi_2(x)$] has ended.

To summarize this discussion, all of these considerations indicate the following: (i) The presented potentials always support irregular asymptotically tunable threshold states, since those are constructed by any superposition of the full solution space. (ii) The conclusions that will be presented below for the anomalous scattering are not affected by a possible second degenerate threshold solution. (iii) $\psi_2(x)$ likely

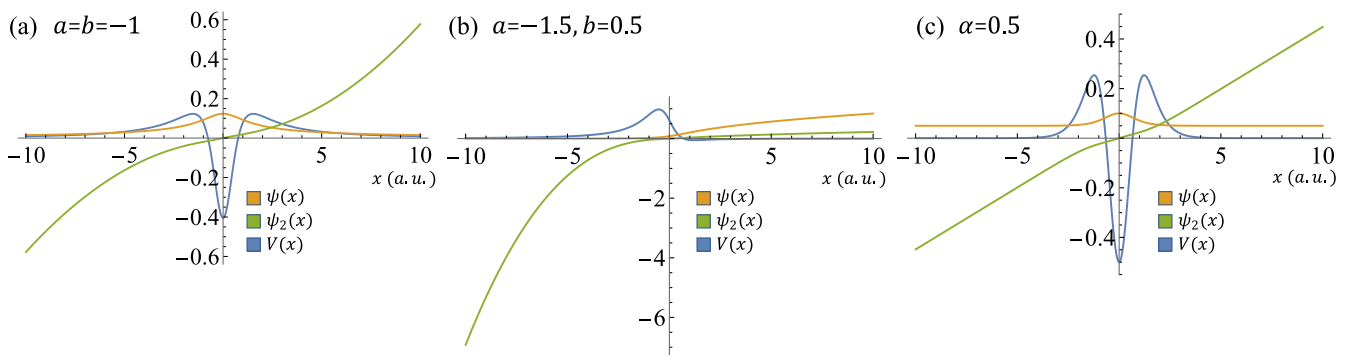


FIG. 5. Independent energy-degenerate threshold solutions to the Schrödinger equation in some exemplary cases, where ψ denotes the analytical nodeless solutions, and ψ_2 denotes the other independent solution that can be obtained from ψ with Eq. (11). (a), (b) Independent solutions where ψ is obtained from Eq. (3) for the parameters $a = b = -1$, and $a = -1.5, b = 0.5$, respectively. (c) Similar to (a) and (b), but where ψ is obtained from Eq. (8) for $\alpha = 0.5$.

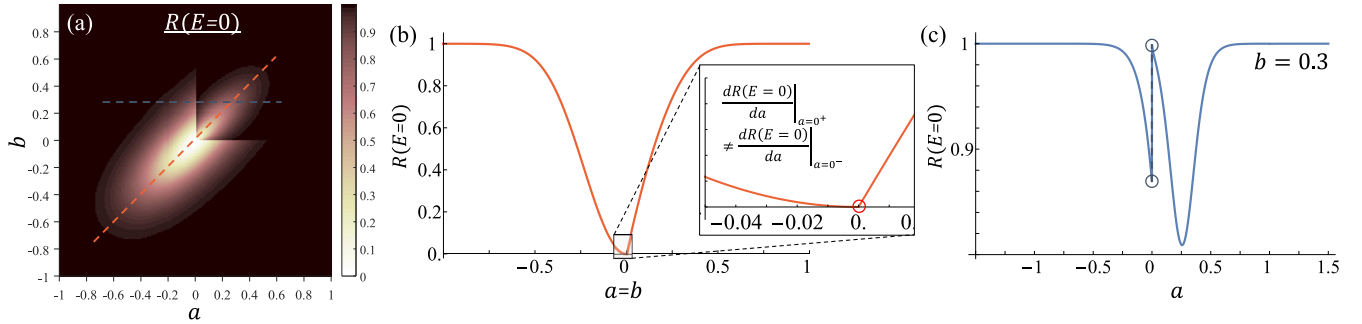


FIG. 6. Quantum threshold reflection coefficient from the potential in Eq. (4) for different values of the parameters a and b . (a) Reflection coefficient calculated for all values of a and b . (b) Cut along the diagonal of (a) for the case of $a = b$, showing derivative discontinuity [red dashed line in (a) shows the diagonal cut]. Inset shows zoom-in around the derivative discontinuity at $a = b = 0$. (c) Same as (b) but along a cut of $b = 0.3$ [dashed blue line in (a)], showing a discontinuity in the reflection coefficient at $a = 0$.

does not have a main physical contribution to any observed effects. At the same time, we note that some care is needed, because the main role of the threshold states in the anomalous reflection process remains vague, and we cannot definitively rule out that both states might play some role (e.g., they might play a role in the scattering discontinuities that will be explored below).

V. SCATTERING ANOMALIES

Having presented a variety of systems that support asymptotically tunable threshold states, we move on to explore their physical properties, focusing on the threshold quantum scattering behavior. To this end, we numerically calculate the reflection coefficient at the threshold for the potential functions described above, $R(E = 0)$, and explore its dependence with respect to the asymptotic behavior of the supported states. Technical details on the methodology are found in the Appendix.

We begin with the potential function in Eq. (4) that supports threshold states that diverge (converge) with a power law-like scaling at the asymptotes. Figure 6 presents $R(E = 0)$ from this potential for various values of the parameters a and b . Some immediate observations can be made: (i) As expected, R is fully symmetric under $a \rightarrow b$. (ii) The system exhibits anomalous reflection [$R(E = 0) \neq 1$] for a variety of potential parameters, including when the supported threshold states are bound, loosely bound, half bound, outright diverge, and all combinations thereof. (iii) As the absolute values of a and b increase, the reflection reaches unity, which is the standardly expected value for regular systems [34]. This occurs despite the fact that for any value of a and b the potential supports irregular threshold states (in the sense that these states asymptotically do not decay exponentially for $a, b < 0$, and that they diverge for $a, b > 0$). (iv) The transition from anomalous to regular reflection can be fully continuous and smooth along some parameter contours (e.g., $a = -0.5, -1 < b < 1$), but also exhibits discontinuities and derivative discontinuities along others. For instance, Fig. 6(b) clearly shows a derivative discontinuity in the threshold reflection coefficient for $a = b$ as a transitions through zero. More noticeably, there is a discontinuity in $R(E = 0)$ for $a = 0$ and

$b = 0$ in a wide parameter regime [see sharp lines in Fig. 6(a) and exemplary cut in Fig. 6(c)].

At this point, we recall that several works have investigated the connection between the presence of half-bound states or shallow-bound states at the threshold to anomalous quantum scattering [25,26]. Here we have demonstrated that a wide range of different states can also lead to such anomalous behavior, and that the strength of the anomaly seems to be correlated with the asymptotic behavior of the supported irregular states (since beyond certain values of a and b regular reflection is restored).

Previous works have also shown that the anomalous threshold reflection is a quantum critical phenomenon [16,25,26]. That is, vanishingly small perturbations to the potential function (such as changing its amplitude or some other parameters in the Hamiltonian) cause a collapse of the half-bound states (resulting in either bound or scattering states instead), exponentially restoring the reflection coefficient to unity. We further explore this notion by calculating the threshold reflection from our particular half-bound model [Eq. (8)]. In this case, we find that by tuning a single parameter in the Hamiltonian, α , the reflection can be fully controlled all the way from unity to zero [see Fig. 3(f), solid line]. The transition from anomalous to regular reflection is fully continuous and noncritical along α , even though a half-bound state is present through the transition for any $\alpha \neq 0$. This concept is put to further testing by calculating the threshold reflection from the system when it is perturbed by an overall amplitude variation in the potential, i.e., $V(x) \rightarrow (1 \pm \delta)V(x)$. The perturbations indeed cause considerable changes in the threshold reflection coefficient, such that larger values of α are needed to obtain nonunity reflection [Fig. 3(f), dashed lines compared to solid lines]. Still, even under perturbations as large as $\pm 5\%$ the anomalous behavior persists, and a continuous and smooth transition is always observed from regular to irregular reflection as α is varied. Moreover, for values of $\alpha > 0.85$ the perturbation hardly changes the value of the threshold reflection, which is maintained close to zero. Overall, this suggests that this particular half-bound model shows anomalies that are relatively robust under perturbations.

We next explore the sensitivity of $R(E = 0)$ from the potential function in Eq. (4) that supports asymptotically tunable threshold states to small perturbations (which are not half

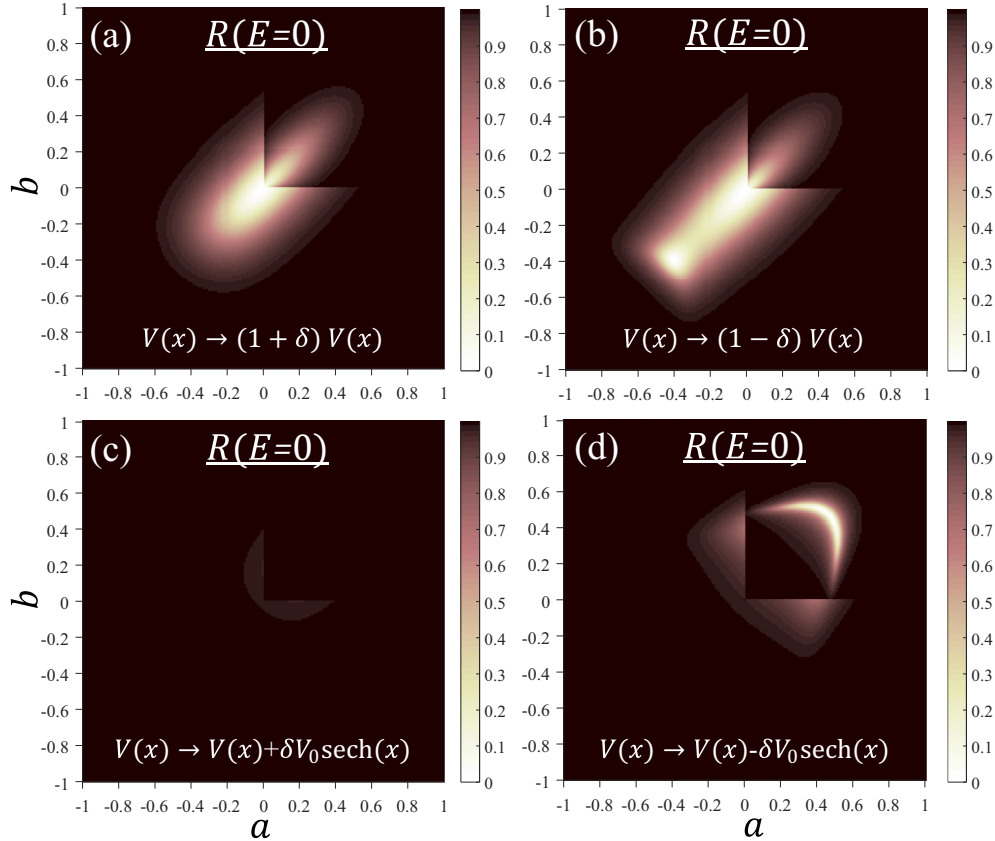


FIG. 7. Sensitivity of quantum threshold reflection coefficient to perturbations, for the potential in Eq. (4). (a), (b) $R(E = 0)$ calculated for different values of the parameters a and b , but where the total amplitude of the potential is perturbed by $\delta = \pm 2\%$. (c), (d) Same as (a) and (b), but where the perturbation is an added $\text{sech}(x)$ function with an amplitude of $\delta = \pm 2\%$ of the original potential amplitude.

bound). It is especially interesting to examine the sensitivity of the sharp discontinuity features in Fig. 6. We consider here two types of perturbations: (i) changing the overall amplitude of the potential by δ , denoted as $V(x) \rightarrow (1 \pm \delta)V(x)$, and (ii) adding a small perturbative function $\pm \delta \text{sech}(x)$ to the potential (which on its own supports a bound state for any well depth), denoted by $V(x) \rightarrow V(x) \pm \delta \text{sech}(x)$. Figure 7 shows the threshold reflection coefficient under these perturbations for $\delta = 2\%$. As seen in Figs. 7(a) and 7(b), the reflection coefficient is not very sensitive to changes in the amplitude of the potential. It maintains its structure and dependence on the parameters a and b . However, it is much more sensitive to the addition of small binding or antibinding functions [see Figs. 7(c) and 7(d)]. Still, even here the anomaly survives, including the presence of both discontinuities and derivative discontinuities in the threshold quantum reflection coefficient. These types of states thus support relatively robust irregular threshold phenomena that seem to not be quantum critical.

Lastly, we explore the reflection properties from our exemplary system that supports asymptotically logarithmically scaling threshold states [Eqs. (9) and (10)]. Figures 4(c) and 4(f) present the threshold reflection from this system, showing that similar control is obtained by tuning a single parameter in the Hamiltonian (β or γ). We emphasize that these parameters control only the spatially local properties of the threshold states. As a result, the control over the reflection coefficient is somewhat limited. We also note that contrary to the previous

example in Fig. 6, here as one changes the potential to support more strongly diverging states (increase γ) the reflection coefficient reduces and saturates. We believe that the saturation results from the spatially local nature of the control parameters, as for all values of β and γ the asymptotic scaling of the supported threshold states is the same. This highlights the strong, and complex, connection between quantum reflection at zero energy, and the asymptotic properties of the supported threshold states.

VI. SUMMARY

In this paper we introduced a new type of irregular threshold quantum states, denoted as asymptotically tunable states. These states can be fully controlled to reproduce any type of asymptotic behavior, e.g., power-law-like divergence (convergence), logarithmic-like scaling, and so on. We have analytically demonstrated that a vast variety of such systems exist, gave an exact analytic prescription on how to find them, and provided expressions for both the potential functions and the supported anomalous states for a few unique cases in 1D. We investigated the reflection properties from these systems and showed that they support anomalous reflection, which is fully tunable, and whose strength seems to be correlated to the asymptotic properties of the threshold states. Importantly, we provided models for systems that transition from regular to irregular threshold reflection when a single parameter

in the Hamiltonian is varied. This transition may be fully continuous, or in some cases, abrupt, with discontinuities and derivative discontinuities for the quantum reflection (even though the potential and supported states are fully analytic and smooth at all times). The effect is reminiscent of a quantum phase transition at zero temperature. Lastly, we showed that such phenomenon is not necessarily quantum critical, and that certain systems are relatively robust against perturbations.

We expect our work to find applications in atomic and molecular systems, e.g., for tailoring a desired scattering property, or engineering the system's spectral properties. Alternatively, optical systems under the paraxial approximation (that are mathematically equivalent to the Schrödinger equation) provide readily accessible setups to demonstrate the existence of the states, as for instance has been shown for bound states in the continuum [7], resonances [35,36], and recently for half-bound states [27]. Here we envision that controllable threshold anomalies might open possibilities in tailoring light propagation and guiding. We also hope that this work will inspire further research of such systems, which could lead to the discovery of anomalies in other physical observables, and has potential for quantum control.

ACKNOWLEDGMENTS

O.N. gratefully acknowledges the support of a Schmidt Science Fellowship, and thanks Anael Ben Asher and Nimrod Moiseyev for interesting discussions. O.N. also acknowledges helpful comments from an anonymous referee.

APPENDIX

1. Numerical details

We provide here technical details on the numerical calculations for the reflection coefficients. We numerically calculated the reflection coefficients on nonequidistant Cartesian grids, using the transfer matrix method [37–39] (rather than with direct propagation methods [40]). In this approach, the time-independent Schrödinger equation is solved with outgoing waves at one boundary, and both incoming and outgoing waves at the other boundary. In particular, we used the simplest variant of the method that assumes a plane-wave solution for the scattering problem between every two grid points, where the coefficients of the waves are propagated along the

grid with transfer matrices. The reflection and transmission coefficients were calculated directly from the system's total transfer matrix.

For some of the cases examined, large grids were needed when the potential functions decay slowly with a power-law scaling. For instance, for scattering from the potential in Eq. (4), we used a grid of total size $L = 500$ bohr, with an outer spacing of 0.1 bohr, and an inner mesh around the origin (up to 20 bohr around the center) of 10^{-3} bohr. The nonequidistant grids were used in order to have denser sampling around the origin, where the potential functions change rapidly (while in the asymptotic regions changes are much less abrupt). In all cases grid sizes and spacings were tested for convergence.

The reflection coefficient at the threshold was either calculated directly (when the potential function approached the threshold from below), or by extrapolation (when the potential function approached the threshold from above). For extrapolation, the reflection coefficient was calculated over a large energy range (in steps of 5×10^{-5} hartree from 0 up to 5×10^{-3} hartree), and a piecewise cubic interpolating Hermite polynomial was fitted to the data, and extrapolated to zero energy.

2. Exact expressions for potentials

We give here the exact expressions for the potentials that support some of the irregular threshold states explored in the main text. The potential that supports the half-bound threshold state in Eq. (8) is

$$V(x) = 2 \frac{2 - 3\text{sech}^2(x)}{2 + \alpha[1 + \cosh(2x)]} - 3\text{sech}^2(x). \quad (\text{A1})$$

The potential that supports the threshold state in Eq. (9) that converges logarithmically and is loosely bound is

$$V(x) = \frac{4x^2 + (x^2 - 1 - \beta)\ln(1 + \beta + x^2)}{(1 + \beta + x^2)^2 \ln^2(1 + \beta + x^2)}. \quad (\text{A2})$$

The potential that supports the threshold state in Eq. (10) that diverges logarithmically is

$$V(x) = \frac{1 + \gamma - x^2}{(1 + \gamma + x^2)^2 \ln(1 + \gamma + x^2)}. \quad (\text{A3})$$

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