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Bound quantum states with no classical turning points

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For a two-parameter class of local potentials which support a bound state with energy E_1 embedded in the continuous spectrum, we determine the conditions that the potential has m wells with barriers of height greater than E_1. Although $E_1 > V(\infty)=0$, such wells act as traps for a classical particle, with classical turning points wherever a barrier height reaches the energy of the particle. However, the parameters of the potential may easily be chosen so that there are no classical turning points, even though the potential supports a bound quantum state.

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Bound quantum states with energies embedded in the continuous part of the energy spectrum were first proposed by von Neumann and Wigner [1], and recently have once more become a subject of study [2,3]. We refer to Ref. [2] for details and a fuller bibliography. A local potential in a nonrelativistic Schrödinger equation which possesses such continuum bound states will always have a long range oscillating tail. We denote the height of the mth peak of the potential (counting from the origin) by V_m, where $V_{m+1} < V_m$ because the amplitude of the oscillations is slowly decreasing. In the corresponding classical problem with $E_1 < V_m$, the particle can be trapped in any of m wells with classical turning points, even though the particle energy is greater than is required for a free particle at a great distance from the force center. However, a quantum bound state with $E_1 > V_1$ has no classical analog in particle dynamics. Nevertheless, such a state with no classical turning points has been observed in an experiment by Capasso *et al.* [4]. Weber [5] has developed a simple solvable model inspired by the Capasso experiment, but this model is not of the von Neumann–Wigner type. It is interesting, therefore, to determine when classical turning points exist for von Neumann–Wigner continuum bound states. We answer this question here for a subclass of von Neumann–Wigner potentials.

As in Ref. [2], we choose units such that $2m=1$ and $\hbar=1$, and we work with the radial Schrödinger equation for a particle with zero angular momentum in the form

$$\left[-\frac{d^2}{dr^2}+V(r)-E\right]\psi(r,E)=0. \tag{1}$$

We choose the energy of the continuum bound state to be $E_1=k_1^2$, and its wave function to be

$$\psi(r,E_1)=2\sqrt{k_1}f(s)\sin k_1 r, \tag{2}$$

where $s(r)$ is the nondecreasing function of r defined by

$$s(r)=4k_1\int_0^r d\xi\ \sin^2 k_1\xi=2k_1 r-\sin 2k_1 r, \tag{3}$$

and $f(s)$ is a square integrable function of s with no zeros in the range $0\leqslant s<\infty$. The von Neumann–Wigner potential associated with the continuum bound state wave function of Eq. (2) is

$$V(r)=\frac{16k_1}{f(s)}\left[\sin k_1 r\ \cos k_1 r\ \frac{df(s)}{ds}+\sin^4 k_1 r\ \frac{d^2 f(s)}{ds^2}\right]. \tag{4}$$

We further restrict attention to von Neumann–Wigner potentials with

$$f(s)=(\lambda+s)^{-n}, \tag{5}$$

where λ and n are parameters subject only to the constraints $\lambda>0$ and $n>1/2$. For convenience, we write

$$x\equiv 2k_1 r \tag{6}$$

and

$$z\equiv\lambda+s=\lambda+x-\sin x. \tag{7}$$

With this abbreviated notation and with Eqs. (3) and (5), the potential (in units of E_1) becomes

$$U(r)\equiv V(r)/E_1=4n\left[(n+1)\left(\frac{1-\cos x}{z}\right)^2-2\frac{\sin x}{z}\right]. \tag{8}$$

The potential of Eq. (8) oscillates with an amplitude which decreases as r (or, equivalently, z) increases. For a classical particle with energy E_1, several of the peaks of $V(r)$ may be greater than E_1, thus producing a number of wells in which a classical particle could be trapped. We shall refer to such wells as "classical traps." Since the amplitude of the potential's oscillations decreases with increasing r, there can be only a finite number of such traps, the exact number being determined by the values of n and λ. From Eq. (8), it is clear that increasing λ causes a decrease in the amplitude of the potential's oscillations, and therefore a decrease in the number of classical traps. For a fixed value of n, there will be a maximum possible number $m_{\max}(n)$ of classical traps, whatever the value of λ. For any n, if λ is sufficiently large there may be no classical traps at all, even though the potential supports a bound quantum state with energy E_1. In what follows, we shall determine critical values $\lambda_c(n,m)$ of λ such that for $\lambda<\lambda_c(n,m)$ the potential has at least m wells with classical turning points for a particle of energy E_1, while for $\lambda>\lambda_c(n,m)$ the potential has at most $m-1$ such wells. In particular, if $\lambda>\lambda_c(n,1)$ then the potential supports a bound quantum state with no classical turning points whatsoever. We shall also show how to determine $m_{\max}(n)$, the maximum number of possible classical traps.

The critical value $\lambda_c(n,m)$ will be such that the height of the mth maximum of $V(r)$ is exactly equal to E_1. Thus we need to find simultaneous solutions of the two equations

$$4n\left[(n+1)\left(\frac{1-\cos x}{z}\right)^2-2\frac{\sin x}{z}\right]=1 \tag{9}$$

and

$$\frac{dU}{dr}\equiv 2k_1\frac{dU}{dx}=0. \tag{10}$$

Equation (9) is equivalent to

$$4n(n+1)(1-\cos x)^2-8nz\sin x-z^2=0, \tag{11}$$

while Eq. (10) is equivalent to

$$(n+1)(1-\cos x)^3-(n+2)z(1-\cos x)\sin x+z^2\cos x=0. \tag{12}$$

We eliminate z^2 between these two equations and then solve for z to obtain

$$z=\frac{(n+1)(1-\cos x)^2[1+(4n-1)\cos x]}{[(7n-2)\cos x+(n+2)]\sin x}. \tag{13}$$

We next substitute this into Eq. (11) and simplify the result. After some work, this yields

$$(3n-1)(2n-1)^2\cos^2 x+2(16n^3-4n^2-3n+1)\cos x \\ +(4n^3+8n^2-n-1)=0. \tag{14}$$

The only solution of this quadratic equation for $\cos x$ consistent with $|\cos x|\leqslant 1$ is

$$\cos x=\gamma(n), \tag{15}$$

where

$$\gamma(n)=[-(16n^3-4n^2-3n+1) \\ +4n^2\sqrt{13n^2-10n+2}]/(3n-1)(2n-1)^2 \tag{16}$$

is an increasing function of n for $1/2<n<\infty$, with $\lim_{n\to 1/2}\gamma(n)=-1$ and $\lim_{n\to\infty}\gamma(n)=(\sqrt{13}-4)/3=-0.1315$. From Eq. (15), the desired maximum of $V(r)$ occurs at $r=r_c=x_c/2k_1$, where $x_c=\pm\arccos\gamma(n)+2m\pi$, with $0\leqslant\arccos\gamma(n)\leqslant\pi$ and with m a non-negative integer which must be at least 1 if the lower sign is chosen.

We now return to Eq. (13). With $\cos x_c$ given by Eq. (16), we find that $z_c\sin x_c<0$. However, $z_c>0$, so that $\sin x_c<0$ and therefore

$$x_c(n)=-\arccos\gamma(n)+2m\pi \quad (m\geqslant 1). \tag{17}$$

The function $x_c(n)$ increases monotonically from $n=1/2$ to $n=\infty$, with bounds

$$(2m-1)\pi<x_c<2m\pi-\arccos(-\tfrac{4}{3}+\tfrac{1}{3}\sqrt{13}) \tag{18a}$$

$$=(2m-0.5420)\pi. \tag{18b}$$

From Eqs. (13) and (16), the critical value $\lambda_c(n,m)$ of λ is

$$\lambda_c(n,m)=z_c-x_c+\sin x_c, \tag{19a}$$

$$=z_c-\sqrt{1-[\gamma(n)]^2}+\arccos\gamma(n)-2m\pi, \tag{19b}$$

where

$$z_c=-\frac{(n+1)[1-\gamma(n)]^2[1+(4n-1)\gamma(n)]}{[(7n-2)\gamma(n)+(n+2)]\sqrt{1-[\gamma(n)]^2}} \tag{20}$$

is obtained by substituting x_c from Eq. (17) into Eq. (13). The value of m is related to the number of wells in $V(r)$ which could trap a classical particle by the existence of classical turning points. Thus for $\lambda_c(n,m+1)<\lambda<\lambda_c(n,m)$ the potential possesses m classical traps for a particle with energy E_1. Since λ_c must be positive, there will be an upper limit $m_{\max}(n)$ to the possible values of m, given by

$$m_{\max}(n)=\mathrm{Int}\left(\frac{1}{2\pi}\{z_c(n)-\sqrt{1-[\gamma(n)]^2}+\arccos\gamma(n)\}\right), \tag{21}$$

where Int( ) indicates the integer part of the argument. If $\lambda>\lambda_c(n,1)$ then the potential has no classical turning points for a classical particle with energy equal to the energy E_1 of the quantum bound state supported by the potential.

For large n,

$$\lambda_c(n,m)=\tfrac{1}{9}[6n(\sqrt{13}+5)-(\sqrt{13}-1)](2\sqrt{13}-5)^{1/2} \\ +\arccos[\tfrac{1}{3}(\sqrt{13}-4)]-2m\pi+O(n^{-1}), \tag{22a}$$

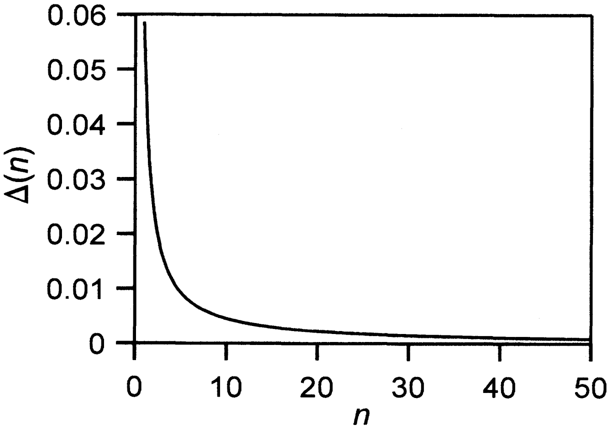

FIG. 1. The discrepancy between the exact $\lambda_c(n,m)/2\pi$ and the linear approximation $\bar{\lambda}_c(n,m)/2\pi$, namely, $\Delta(n)\equiv[\lambda_c(n,m)-\bar{\lambda}_c(n,m)]/2\pi$, shown as a function of n for $1\leq n\leq 50$.

$$=8.530\,84n+1.272\,17-2m\pi+O(n^{-1}). \quad (22b)$$

Even for $n=1$, the critical value $\lambda_c(n,m)$ is reasonably well approximated by

$$\lambda_c(n,m)\approx\bar{\lambda}_c(n,m)=2\pi(0.202\,47+1.3577n-m). \quad (23)$$

It follows that

$$m_{\max}(n)\approx \mathrm{Int}(0.202\,47+1.3577n). \quad (24)$$

Figure 1 shows $\Delta(n)\equiv[\lambda_c(n,m)-\bar{\lambda}_c(n,m)]/2\pi$ as a function of n for $1\leq n\leq 50$. It is clear that Eq. (24) will yield an erroneous result only rarely, namely, when 0.202 47 $+1.3577n$ is very close to an integer. As n approaches its lower limit 0.5, the approximation of Eq. (23) is less satisfactory. Thus

$$\lim_{n\to 1/2}\lambda_c(n,1)=2\sqrt{3}-\pi=0.3225>0 \quad (25)$$

so that $m_{\max}(n)\geq 1$ for all $n>0.5$, whereas Eq. (24) would predict $m_{\max}(n)=0$ for $n<0.5874$. In Table I we present the critical values $\lambda_c(n,m)$ for $n=1.0$, 1.5, 2.0, 2.5, and 3.0, computed from Eq. (19b), and we illustrate the potentials with several values of λ for $n=1$ in Fig. 2 and with $\lambda=\lambda_c(n,m)$ for $n=2.5$ and $m=1$, 2, and 3 in Fig. 3.

We can understand the results of this investigation as follows. From Eq. (24) we see that the maximum number of classical traps for a particle of energy E_1 increases with increasing n. This is due to the increasing strength of the potential defined by Eq. (8). Clearly the magnitude of n is the the most important factor controlling the

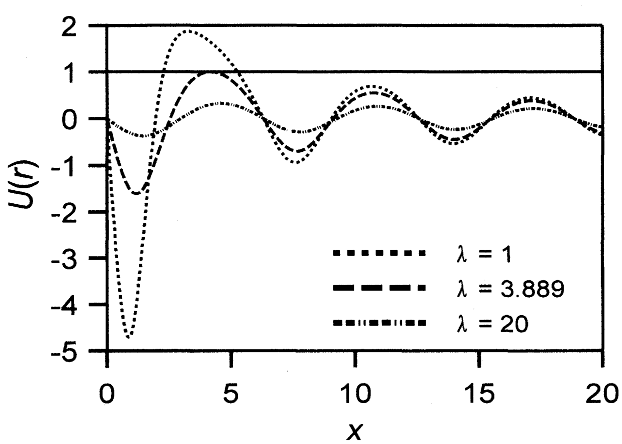

FIG. 2. Potentials $U(r)=V(r)/E_1$ plotted against $x=2k_1r$ for $n=1$ and three values of λ including the critical value $\lambda_c(1,1)$. For $n=1$, Table I shows that $m_{\max}(1)=1$, so that a potential with $n=1$ can support at most one classical trap. All three of the illustrated potentials, including that for $\lambda=20$, support a continuum bound state with energy E_1.

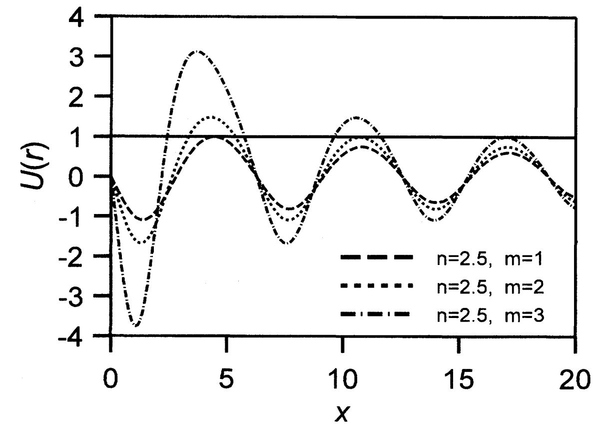

FIG. 3. Potentials $U(r)=V(r)/E_1$ plotted against $x=2k_1r$ for $n=2.5$, with $\lambda=\lambda_c(n,m)$ and with $1\leq m\leq m_{\max}(n)$. The height of the mth peak of the potential is exactly equal to the energy E_1 of the continuum bound state. Increasing λ beyond $\lambda_c(n,m)$ decreases the magnitude of the potential, so that there are fewer classical traps. In particular, if $\lambda>\lambda_c(n,1)$ then the potential has no wells capable of trapping a classical particle with the energy of the bound quantum state.

TABLE I. Critical values $\lambda_c(n,m)$ of the potential parameter λ for several values of n, with $1\leq m\leq m_{\max}(n)$. If $\lambda<\lambda_c(n,m)$ then the potential has at least m classical turning points for a particle with energy E_1, while if $\lambda>\lambda_c(n,m)$ then the potential has fewer than m classical turning points. If $\lambda>\lambda_c(n,1)$ then the potential has no classical turning points at all for a particle having the energy E_1 of the continuum bound state.

n	$m=1$	$m=2$	$m=3$	$m=4$
1.0	3.889			
1.5	8.008	1.724		
2.0	12.210	5.927		
2.5	16.440	10.157	3.874	
3.0	20.663	14.400	8.117	1.833

strength of the potential, although this is also partially controlled by λ. The height V_1 of the first maximum may be increased by decreasing λ, but there is an n-dependent upper bound given by the limit as $\lambda \rightarrow 0$. For example, if $n=1$ and $\lambda=0$ then the first maximum of $V(r)$ occurs when $2k_1 r \equiv x = 2.836$ and has height $V_1 = 7.775E_1$. The maximum number $m_{\max}(n)$ of classical traps for a fixed value of n will be the number of traps in the potential in the limit as $\lambda \rightarrow 0$. Since the strength of the potential increases as n increases, it is no surprise that $m_{\max}(n)$ also increases with increasing n. Increasing λ reduces the strength of the potential, so that the number of traps is decreased by 1 each time a maximum of $V(r)$ drops below E_1. The critical value $\lambda_c(n,m)$ is the value of λ at which the mth maximum of $V(r)$ just reaches E_1, so that one more classical trap is about to disappear. Since λ has no upper bound, the strength of the potential can be made arbitrarily small by increasing this parameter. Hence the critical value $\lambda_c(n,1)$, at which the last classical trap in $V(r)$ is about to vanish, must be finite. For $\lambda > \lambda_c(n,1)$ the potential has no classical traps at all for a particle of energy E_1; nevertheless the potential, even with $\lambda > \lambda_c(n,1)$, has been constructed in such a way that it supports a bound quantum state with this energy.

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