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Strange bound states in the Schrödinger wave equation: When usual tunneling does not occur

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In most textbooks on quantum mechanics, it is asserted that the bound states of a localized potential have negative energies. To stress that this view should be taken with caution, we give several examples of scalar potentials that tend to zero at infinite distance and yet possess one or several discrete *positive* bound states for the Schrödinger single-particle wave equation. The consequence that usual tunneling may not occur, though it should according to a superficial view, is of interesting pedagogical value.

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I. INTRODUCTION

In standard textbooks on quantum mechanics, the solutions of the time-independent Schrödinger equation for a single particle are often discussed by considering piecewise constant potentials.[1] The simplest such example for a local scalar potential is the square potential well. In this case, as for every potential function of bounded support, the solution in the external region is not square integrable if the particle energy is positive (if not zero, the value of the potential at infinity is identified with the zero level of the energy). From this, it is deduced[2] that these potentials possess only (discrete) negative bound states. On the other hand, there is a continuum of positive energy states that are not square integrable. This conclusion is implicitely extended to local potentials in general,[3] or merely admitted.[4] However, it has been known for a long time[5] (though not widely known by physicists) that some potentials exist that tend to zero at infinity and yet possess square-integrable eigenfunctions with positive energy. Though these potentials have not obvious physical significance, their formal existence is by itself interesting for the student, as a warning against too rapid generalizations. They may also serve as a challenge on usual feelings about tunneling phenomena, since they are examples where usual tunneling does not occur[6] though it should according to conventional view. Furthermore, such potentials may be found by simple methods and involve only elementary functions.

In Sec. II, we recall the method used by von Neumann and Wigner,[5,6] to construct localized potentials with a positive bound state. In Sec. III, we generalize the method to several discrete bound states by using some results for the inverse scattering problem.[7,8] An example is given (involving only functions accessible to the beginning student) of a localized potential that possesses two bound states, one of which with an energy higher than the maximum value of the potential; thus a particle is trapped even when it should be free in classical mechanics.

II. VON NEUMANN–WIGNER EXAMPLE

The corrected[6] von Neumann–Wigner[5] procedure works as follows:

We start with the single-particle wave equation, which reads in reduced units, as

$$[-\nabla^2 + V(\mathbf{r}) - E]\psi(\mathbf{r}) = 0, \tag{1}$$

where $V(\mathbf{r})$ is taken to be a centrally symmetric potential.

Considering only the s wave ($1 = 0$) case, we search solutions of the form

$$\psi(\mathbf{r}) = r^{-1}\varphi(r), \tag{2}$$

where the function $\varphi(r)$ (defined for $r > 0$) is a solution of

$$-\varphi''(r) + V(r)\varphi(r) = E\varphi(r). \tag{3}$$

The free-particle s wave $\psi_0(\mathbf{r}) = \sin(kr)/kr$ satisfies Eq. (1) with $E = k^2 > 0$. Integrable states can be constructed as

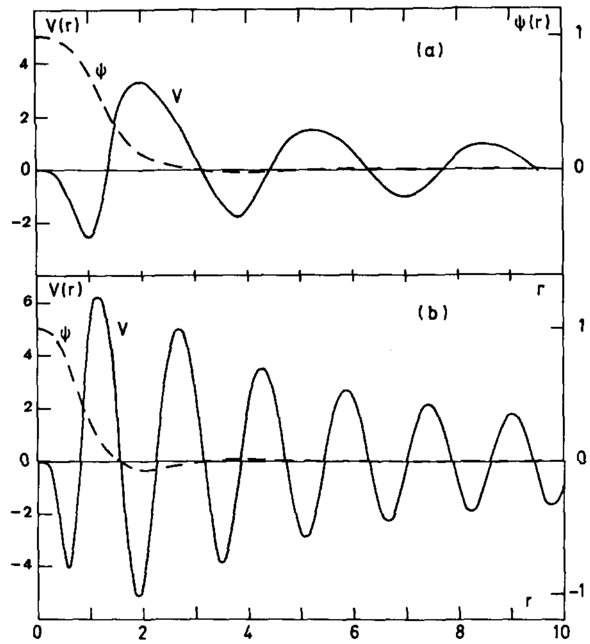

Fig. 1. Two examples of potential $V(r)$ that possess a bound state $\psi(r)$ with positive energy E; (a) $E = 1$; (b) $E = 4$.

$\psi(\mathbf{r}) = \psi_0(\mathbf{r})f(r)$, if $f(r)$ drops to zero as $r^{-p}(p > \frac{1}{2})$ for $r \to \infty$.

Substituting in Eq. (3) and using Eq. (2) yields

$$V(\mathbf{r}) = E - k^2 + f''(r)/f(r) + 2k\cot(kr)f'(r)/f(r). \quad (4)$$

From Eq. (4), one sees that, in order that $V(r)$ remain bounded, f'/f must vanish at the zeros of $\sin(kr)$. For example, one can choose $f(r)$ to be a differentiable function of the variable:

$$s(r) = 4k\int_0^r \sin^2(kr')dr' = 2kr - \sin(2kr). \quad (5)$$

The choice made originally[5,6] corresponds to

$$f(r) = [A^2 + s^2(r)]^{-1}, \quad (6)$$

where A is an arbitrary nonzero real constant.

This ensures that $\psi(\mathbf{r})$ is square integrable; substituting in Eq. (4) and taking $E = k^2$ yields the potential

$$V(r) = 16k^2\{-8A^2\sin^4 kr f^2(r) + [6\sin^4 kr - (2kr - \sin 2kr)\sin 2kr]f(r)\}. \quad (7)$$

One verifies easily that $V(r) \sim -16k^2(\sin 2kr)/2kr$ for $r \to \infty$.

Thus one has constructed a localized potential $V(r)$ with a bound eigenstate with energy $E = k^2 > 0$. Figure 1 shows two examples of $V(r)$ and the corresponding $\psi(r)$ (times A^2) for the specific choice $A^2 = 8k^2$ and the respective energies $E = 1$, $E = 4$. The above method can supply other potentials with similar properties.[6] However, it gives only one bound state.

III. SEVERAL BOUND STATES

The above approach can in fact be generalized in a simple way. To do this, we shall use some results of the Gelfand–Levitan formulation of the inverse scattering problem,[7] in the simple form recently[8] presented in this Journal. Those results concern, as usual, bound states with negative energies, and we shall merely use them by continuating for positive energies. Since this general subject is largely studied by (and in fact confined in) mathematicians, we shall not study in detail the method, but merely verify that it yields results suitable for our purpose.

We start with a set of discrete energies

$\{E_i = k_i^2\}(i = 1, n)$ and normalization constants $\{c_i\}$

for the unknown wave functions. Transposing the simple method outlined in Ref. 8 yields the n eigenfunctions of Eq. (3) with eigenvalues E_i as

$$\varphi_i(r) = c_i^{-1/2}\sum_{j=1}^{n} U^{-1}(x)_{ij}\,\varphi_0(r, k_j), \quad (8)$$

where φ_0 is the function used in Sec. II, i.e., $\varphi_0(r,k) = \sin kr/k$

and $U(r)$ is the $n\times n$ matrix defined by

$$U(r)_{ij} = c_i^{-1}\delta_{ij} + \int_0^r dt\,\varphi_0(t,k_i)\varphi_0(t,k_j). \quad (9)$$

Thus

$$U(r)_{ii} = c_i^{-1} + (4k_i^3)^{-1}(2k_ir - \sin 2k_ir),$$
$$U(r)_{ij} = (2k_ik_j)^{-1}[-(k_i + k_j)^{-1}\sin(k_i + k_j)r + (k_i - k_j)^{-1}\sin(k_i - k_j)r] \quad (i\neq j) \quad (10)$$

and the potential is given by[8]

$$V(r) = -2\frac{d^2}{dr^2}[\ln\det U(r)] = -2\frac{(\det U)''}{\det U} + 2\left(\frac{(\det U)'}{\det U}\right)^2. \quad (11)$$

It is readily verified that in the case $n = 1$, the result so obtained is akin to the results given in Sec. II.

We illustrate below the case $n = 2$, where the calculations are still reasonably simple.

Equation (10) yields readily

$$\det U = [c_1^{-1} + (4k_1^3)^{-1}(2k_1r - \sin 2k_1r)] \times [c_2^{-1} + (4k_2^3)^{-1}(2k_2r - \sin 2k_2r)] - (2k_1k_2)^{-2}[(k_1 - k_2)^{-1}\sin(k_1 - k_2)r - (k_1 + k_2)^{-1}\sin(k_1 + k_2)r], \quad (12)$$

$$U^{-1}(r)_{ii} = U(r)_{jj}/\det U,$$
$$U^{-1}(r)_{ij} = -U(r)_{ij}/\det U.$$

The functions $\varphi_i(r)$ ($i = 1, 2$) are thus given by Eq. (8) as

$$\varphi_i(r) = c_i^{-1/2}[k_i^{-1}\sin(k_ir)U(r)_{jj} - k_j^{-1}\sin(k_jr)U(r)_{12}]/\det U \quad (i\neq j = 1, 2). \quad (13)$$

And the corresponding potential is, using Eqs. (10) and (11),

$$V(r) = 2(\det U)^{-2}[U_{11}k_2^{-2}\sin^2(k_2r) + U_{22}k_1^{-2}\sin^2(k_1r) - 2U_{12}(k_1k_2)^{-1}\sin(k_1r)\sin(k_2r)]^2 - 2(\det U)^{-1}[U_{11}k_2^{-1}\sin(2k_2r) + U_{22}k_1^{-1}\sin(2k_1r) - 2U_{12}(k_1^{-1}\sin(k_1r)\cos(k_2r) + k_2^{-1}\sin(k_2r)\cos(k_1r))]. \quad (14)$$

One can easily check that the solutions verify Eq. (3) and that

$$\varphi_i(r) \sim c_i^{1/2}r \quad r \to 0,$$
$$\varphi_i(r) \sim c_i^{-1/2}2k_i\sin(k_ir)/r \quad r \to \infty,$$

so that the wave functions are square integrable.

The potential behaves as

$$V(r) \sim -4[k_1\sin(2k_1r) + k_2\sin(2k_2r)]/r \quad r \to \infty.$$

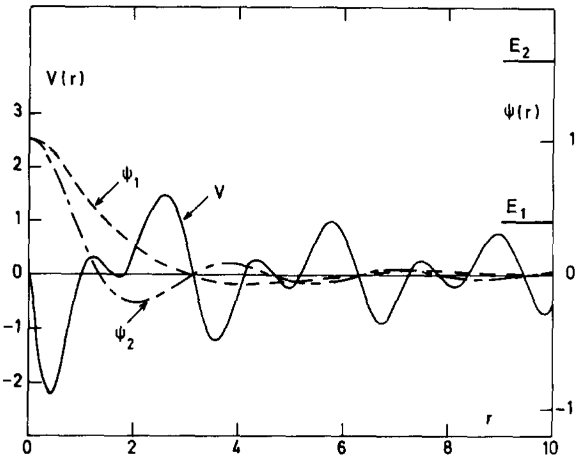

Fig. 2. Example of a potential $V(r)$ that possesses two bound states $\psi_1(r)$, $\psi_2(r)$ with positive energies $E_1 = 1$, $E_2 = 4$. Note that the particle with energy E_2 should not be trapped by classical mechanics.

Thus we have constructed a localized potential that possess two bound states with positive energy.

Figure 2 displays these results for the specific choices $c_1 = c_2 = 1$, $E_1 = 1$, $E_2 = 4$.

Other examples could be constructed by taking higher values for n and/or generalizing the method to different spectral[8] functions.

IV. CONCLUDING REMARKS

Viewing these results is a good warning to students. We have displayed localized potentials that possess one or several bound states with positive energy, so that usual tunneling does not occur. Furthermore, in Fig. 2, one has a particle with energy greater than the maximum value of the potential. It is not bound in classical mechanics, yet quantum mechanics bound it.

These results appear at first sight odd, but the oddity is only a consequence of preconceived ideas involving too rapid generalizations, and in particular of neglecting the potential at large distances and/or applying the WKB approximation in an uncritical way.

Concerning the physical significance of these results, it is worth making two remarks. First, the wave functions decay with a power law, contrary to the exponential decay of usual bound states. Second, in the same way, the potentials constructed by this method behave as a modulated r^{-1} for $r \to \infty$; this involves a slow decrease, and an infinite number of zeros. (and in fact, they do not satisfy the constraints needed[4] to demonstrate that positive energy states are not bound).

Their physical significance as representing real potentials is not obvious. Although they may be considered as mere curiosities, some applications have been studied in the case of multiple-particle systems (see for instance Refs. 6 and 9). Likewise, some applications could possibly be found when studying wave propagation in plasmas, where unexpected trapped waves could occur.

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