

QUANTUM BOUND STATES WITH ZERO BINDING ENERGY

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ABSTRACT

After reviewing the general properties of zero-energy quantum states, we give the explicit solutions of the Schrödinger equation with $E = 0$ for the class of potentials $V = -|\gamma|/r^\nu$, where $-\infty < \nu < \infty$. For $\nu > 2$, these solutions are normalizable and correspond to bound states, if the angular momentum quantum number $l > 0$. [These states are normalizable, even for $l = 0$, if we increase the space dimension, D , beyond 4; i.e. for $D > 4$.] For $\nu < -2$ the above solutions, although unbound, are normalizable. This is true even though the corresponding potentials are repulsive for all r . We discuss the physics of these unusual effects.

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1 Introduction

In studying quantum, nonconfining, potential systems, care is given to describing both the discrete, normalizable, bound states, which exist for energy $E < 0$, and also the non-normalizable, free (including resonant) states, with energy $E > 0$. However, usually little is said about the zero energy states. From systems such as the Coulomb problem, where the $E = 0$ state is in the continuum, it can easily be assumed that all $E = 0$ states are in the continuum and not normalizable. However, there are at least two known examples where, for discrete values of the coupling constant, the $E = 0$ state is bound.

It is the purpose of this note to explore this phenomenon. We will demonstrate an exactly solvable system of power-law potentials where the $E = 0$ states are bound for *continuous* values of the coupling constant. We will elucidate the physics of this situation and also demonstrate that there also exist normalizable states which cannot be interpreted as bound states. Finally, we will show that by increasing the dimensionality of the problem, an effective centrifugal barrier is created which causes states to be bound, even if the expectation value of the angular momentum operator, L^2 , vanishes.

2 Background

Consider the radial Schrödinger equation with angular-momentum quantum number l :

$$ER_l = \left[-\frac{\hbar^2}{2m} \left(\frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} - \frac{l(l+1)}{r^2} \right) + V(r) \right] R_l . \quad (1)$$

For the Coulomb problem, the effective potential

$$U(r) = \frac{\hbar^2}{2m} \frac{l(l+1)}{r^2} - \frac{e^2}{r} \quad (2)$$

has the form shown in Figure 1. The effective potential asymptotes to zero from below as $r \rightarrow \infty$, so that a particle with zero binding energy, $E = 0$, has a positive kinetic energy and is free to travel out to infinity. [Note that in this case the zero-energy solution, in addition to being continuously connected to the continuum, is also a limit point of the bound states, whose energies, E_n , go as $-1/n^2$.]

The physical situation is very different, however, if the potential approaches zero from the top as $r \rightarrow \infty$. This is the case, for example, in the “standard” discussion of alpha decay. Consider a phenomenological description of alpha-decay with a Morse potential. Then, the effective potential, with the angular-momentum barrier included, is

$$U = \mathcal{E}_0 \left[\frac{l(l+1)}{\rho^2} + D \left(-2e^{[-2b(\rho-\rho_0)]} + e^{[-b(\rho-\rho_0)]} \right) \right] , \quad (3)$$

where here, and later, we use the notation,

$$\rho \equiv \frac{r}{a} , \quad \mathcal{E}_0 \equiv \frac{\hbar^2}{2ma^2} , \quad (4)$$

a being a distance scale and \mathcal{E}_0 being an energy scale. In Figure 2 we plot an example of the Morse potential.

Early quantum-mechanical text books [1] discussed the energy ranges $E > 0$ and $E < 0$ for this type of potential, but often did not include the $E = 0$ case in the discussion. Even in the famous lecture notes of Fermi [2] the WKB tunnel time to the outside was discussed only for $E > 0$, even though one can see that it goes to infinity as $E \rightarrow 0$. [This last argument provides an intuitive understanding of the bound-state result we are discussing.]

Now we make this point analytic by considering a solvable system whose effective potential has the features of the alpha-decay potential. This potential is

$$U(r) = \begin{cases} \frac{\hbar^2}{2m} \frac{l(l+1)}{r^2} - V_0 = \mathcal{E}_0 \left[\frac{l(l+1)}{\rho^2} - g^2 \right], & r < a, \\ \frac{\hbar^2}{2m} \frac{l(l+1)}{r^2} = \mathcal{E}_0 \frac{l(l+1)}{\rho^2}, & r > a. \end{cases} \quad (5)$$

where g is a dimensionless ‘‘coupling constant.’’ In this case, the effective potential, shown in Figure 3, is infinite at $r = 0$, falls below zero, rises above zero at some $r = a$, and then goes to zero from above as $r \rightarrow \infty$. This is the spherical box, discussed in many places.

The $E = 0$ solution is even simpler than the general case. To our knowledge, this was the first example of a bound state with zero binding energy being explicitly demonstrated for a wide audience [3, 4, 5].

First consider the interior, $r < a$. The solution is a spherical Bessel function, which insures that the wave function is finite at the origin:

$$R_l(r < a) \sim j_l(\kappa r) = j_l(g\rho), \quad \kappa = \sqrt{2mV_0/\hbar^2} = g/a, \quad (6)$$

which is $\sim r^{-1/2} J_{l+1/2}$. From the Schrödinger equation, the exterior solutions ($r > a$, where $V = 0$), go as a power law. The choice is the negative power law since we are interested in normalizable solutions:

$$R_l(r > a) \sim 1/r^{l+1}. \quad (7)$$

The matching condition at $r = a$ is that

$$\frac{d \ln(R_l)}{dr} = \frac{1}{R_l} \frac{dR_l}{dr} \quad (8)$$

be continuous at $r = a$. This means that

$$0 = (l+1)j_l(\kappa a) + (\kappa a)j_l'(\kappa a) = (\kappa a)j_{l-1}(\kappa a). \quad (9)$$

The first equality is the physical condition. The second equality is a standard mathematical result of spherical Bessel functions.

Therefore, the spherical well is a different situation than the Coulomb case, where $E = 0$ is a limit point of the bound-state spectrum. The spherical well has a finite bound-state spectrum. In general the $E = 0$ solutions of the spherical well are not normalizable. However, for a given l , an $E = 0$ solution is normalizable if V_0 is such that κa is equal to a zero of the spherical Bessel function j_{l-1} . That is,

$$j_{l-1}(\kappa a) = 0. \quad (10)$$

τ $\left(\begin{array}{c} \tau \\ \end{array} \right)$

These zeros can easily be calculated and are in tables [6].

Indeed, in Fig. 3 we plot the effective potential $U(r)$ in (5) in units of \mathcal{E}_0 for $l = 1$ and $V_0 = \pi^2 \mathcal{E}_0$ or $g = \pi$. Then, an $E = 0$ bound state exists and corresponds to the first zero, $\kappa a = \pi$, of $j_0(\kappa a) = \sin(\kappa a)/(\kappa a)$.

Another example of this type is the focusing potential of Demkov and Ostrovskii [7, 8], here written in the form

$$V = -\frac{w\mathcal{E}_0}{\rho^2[\rho^\kappa + \rho^{-\kappa}]^2}, \quad \kappa > 0, \quad (11)$$

where w is a dimensionless coupling constant. This system has normalizable, $E = 0$ solutions only for the following discrete values of w [7, 8]:

$$w_N = 4\kappa^2 \left(N + \frac{1}{2\kappa} - 1 \right) \left(N + \frac{1}{2\kappa} \right), \quad (12)$$

$$N = n + \left(\frac{1}{\kappa} - 1 \right) l, \quad n = n_r + l + 1, \quad n_r = 0, 1, 2, \dots \quad (13)$$

3 Zero-Energy Bound States and Singular Discrete States for Power-Law Potentials

Now we present an infinite class of potentials which is exactly solvable for $E = 0$, and has the property that many of the $E = 0$ states are bound. Elsewhere we will go into more detail on this system for both the classical case [9] and the quantum case [10].

For convenience we parametrize these potentials as

$$V(r) = -\frac{\gamma}{r^\nu} = -\frac{g^2 \mathcal{E}_0}{\rho^\nu}, \quad -\infty < \nu < \infty, \quad (14)$$

where g is a dimensionless coupling constant. It will be useful to interchange the variables ν and μ , which are related by

$$\frac{\nu - 2}{2} = \mu, \quad \nu = 2(\mu + 1). \quad (15)$$

In Figure 4 we show an example of such a potential where the $E = 0$ solution will be a bound state ($\nu > 2$).

We now demonstrate that the Schrödinger equation is exactly solvable for all $E = 0$ and all $-\infty < \nu < \infty$. To do this, set $E = 0$ in Eq. (1), change variables to ρ , and then multiply by $-\rho^2$. One finds

$$0 = \left[\rho^2 \frac{d^2}{d\rho^2} + 2\rho \frac{d}{d\rho} - l(l+1) + \frac{g^2}{\rho^{2\mu}} \right] R_l(r). \quad (16)$$

τ $\left(\begin{matrix} \tau & \tau \\ & \tau \end{matrix} \right)$

The above is a well-known differential equation of mathematical physics [11]. For $\nu \neq 2$ or $\mu \neq 0$, the solution can be directly given as

$$R_l(r) = \frac{1}{\rho^{1/2}} \mathbf{J}_{\left(\frac{2l+1}{|\nu-2|}\right)} \left(\frac{2g}{|\nu-2|\rho^{(\frac{\nu-2}{2})}} \right) = \frac{1}{\rho^{1/2}} \mathbf{J}_{\left(\frac{l+1/2}{|\mu|}\right)} \left(\frac{g}{|\mu|\rho^\mu} \right), \quad \mu \neq 0. \quad (17)$$

The other possible solution of Eq. (16), involving the functions Y , is ruled out on physical grounds. (See the Appendix of Ref. [10].) Also, note that the power in the argument of the solution is *not* an absolute value of μ . (The singular, free, $\nu = 2$ or $\mu = 0$ case will be discussed in Ref. [10].)

We now find out under what circumstances these states are normalizable. The normalization constants for the wave functions would have to be of the form

$$N_l^{-2} = \int_0^\infty \frac{r^2 dr}{\rho} \mathbf{J}_{\left(\frac{l+1/2}{|\mu|}\right)}^2 \left(\frac{g}{|\mu|\rho^\mu} \right). \quad (18)$$

Changing variables first from r to ρ , and then from ρ to $z = g/(|\mu|\rho^\mu)$, and being careful about the limits of integration for all μ , one obtains

$$N_l^{-2} = \frac{a^3}{|\mu|} \left(\frac{g}{|\mu|} \right)^{2/\mu} I_l, \quad (19)$$

where

$$I_l = \int_0^\infty \frac{dz}{z^{(1+2/\mu)}} \mathbf{J}_{\left(\frac{l+1/2}{|\mu|}\right)}^2(z). \quad (20)$$

Integrals of products of Bessel functions are well studied and are complicated when the orders and arguments approach each other [12]. However, this integral is convergent and given by [13]

$$I_l = \frac{1}{2\pi^{1/2}} \frac{\Gamma\left(\frac{1}{2} + \frac{1}{\mu}\right)}{\Gamma\left(1 + \frac{1}{\mu}\right)} \frac{\Gamma\left(\frac{l+1/2}{|\mu|} - \frac{1}{\mu}\right)}{\Gamma\left(1 + \frac{l+1/2}{|\mu|} + \frac{1}{\mu}\right)}, \quad (21)$$

if the following two conditions are satisfied:

$$\frac{2l+1}{|\mu|} + 1 > \frac{2}{\mu} + 1 > 0. \quad (22)$$

(In obtaining the final result in Eq. (21) the doubling formula for $\Gamma(2z)$ was used.)

Eqs. (21) and (22) lead to two sets of normalizable states. The first is when

$$\mu > 0 \quad \text{or} \quad \nu > 2, \quad l > 1/2. \quad (23)$$

These are ordinary bound states and result because the effective potential asymptotes to zero from above, as in Figure 4. In this case, for $E = 0$, the wave function can reach infinity only by tunneling through an infinite forbidden region. That takes forever, and so the state is bound. Note that the condition on l in Eq. (23) is the minimum nonzero angular momentum allowed in quantum mechanics, $l_{min} = 1$. This agrees with the classical orbit solution which is bound for any nonzero angular momentum [9].

Notice that the above $E = 0$ solutions exist for all $g^2 > 0$, and not just for discrete values of the coupling constant. The reason for this surprising result is the scaling property of power-law potentials. A change of the coupling constant, g^2 , by a positive factor, to $\sigma^2 g^2$, can be accounted for by changing the argument of the wave function from $g/|\mu|\rho^\mu$ to $\sigma g/|\mu|\rho^\mu$. This is essentially a change of the length scale.

For $-2 \leq \nu \leq 2$ or $-2 \leq \mu \leq 0$ (as well as the solutions with $l = 0$ and $\mu > 0$ or $\nu > 2$) the solutions are free, continuum solutions.

However, there is one remaining class of normalizable solutions which is quite surprising. For any l and all $\nu < -2$ or $\mu < -2$, the reader can verify that the conditions of Eq. (22) are also satisfied. Thus, even though one here has a repulsive potential that falls off faster than the inverse-harmonic oscillator and the states are *not* bound, the solutions are normalizable!

The corresponding classical solutions yield infinite orbits, for which the particle needs only a finite time to reach infinity [9]. But it is known that a classical potential which yields trajectories with a finite travel time to infinity also yields a discrete spectrum in the quantum case [14]. This conclusion is in agreement with the situation here. Although normalizable quantum solutions exist not just for $E = 0$ but also for a continuous range of E , by imposing special boundary conditions a discrete subset can be chosen which defines a self-adjoint extension of the Hamiltonian [15, 16, 17].

This system has many other interesting features, both classically and quantum mechanically. We refer the reader elsewhere to discussions of these properties [9, 10].

4 Bound States in Arbitrary Dimensions

One can easily generalize the problem of the last section to arbitrary D space dimensions. Doing so yields another surprising physical result.

To obtain the D -dimensional analogue of Eq. (16), one simply has to replace 2ρ by $(D-1)\rho$ and $l(l+1)$ by $l(l+D-2)$ [18]:

$$0 = \left[\rho^2 \frac{d^2}{d\rho^2} + (D-1)\rho \frac{d}{d\rho} - l(l+D-2) + \frac{g^2}{\rho^{2\mu}} \right] R_{l,D} . \quad (24)$$

The solutions also follow similarly as

$$\begin{aligned} R_{l,D} &= \frac{1}{\rho^{D/2-1}} \mathbf{J}_{\left(\frac{2+D-2}{|\nu-2|}\right)} \left(\frac{2g}{|\nu-2|\rho^{\frac{\nu-2}{2}}} \right) \\ &= \frac{1}{\rho^{D/2-1}} \mathbf{J}_{\left(\frac{l+D/2-1}{|\mu|}\right)} \left(\frac{g}{|\mu|\rho^\mu} \right) . \end{aligned} \quad (25)$$

To find out which states are normalizable one first has to change the integration measure from $r^2 dr$ to $r^{D-1} dr$ and again proceed as before. The end result is that if the wave functions are

τ $\left(\begin{array}{c} \tau \\ \tau \end{array} \right)$

normalizable, the normalization constant is given by

$$N_{l,D}^{-2} = \frac{a^D}{|\mu|} \left(\frac{g}{|\mu|} \right)^{2/\mu} I_{l,D} \quad , \quad (26)$$

where

$$I_{l,D} = \int_0^\infty \frac{dz}{z^{(1+2/\mu)}} \mathbf{J}^2_{\left(\frac{l+D/2-1}{|\mu|}\right)}(z) \quad . \quad (27)$$

We see that the above integral is equal exactly to that in (20), except that l is replaced by the effective quantum number

$$l_{eff} = l + \frac{D-3}{2} \quad . \quad (28)$$

Therefore,

$$I_{l,D} = \frac{1}{2\pi^{1/2}} \frac{\Gamma\left(\frac{1}{2} + \frac{1}{\mu}\right)}{\Gamma\left(1 + \frac{1}{\mu}\right)} \frac{\Gamma\left(\frac{l+D/2-1}{|\mu|} - \frac{1}{\mu}\right)}{\Gamma\left(1 + \frac{l+D/2-1}{|\mu|} + \frac{1}{\mu}\right)} \quad , \quad (29)$$

which is defined and convergent for

$$\frac{2l + D - 2}{|\mu|} + 1 > \frac{2}{\mu} + 1 > 0 \quad . \quad (30)$$

This yields the surprising result that there are bound states for all $\nu > 2$ or $\mu > 0$ when $l > 2 - D/2$. Explicitly this means that the minimum allowed l for there to be zero-energy bound states are:

$$\begin{aligned} D = 2 \quad , \quad l_{min} &= 2 \quad , \\ D = 3 \quad , \quad l_{min} &= 1 \quad , \\ D = 4 \quad , \quad l_{min} &= 1 \quad , \\ D > 4 \quad , \quad l_{min} &= 0 \quad . \end{aligned} \quad (31)$$

This effect of dimensions is purely quantum mechanical and can be understood as follows: Classically, the number of dimensions involved in a central potential problem has no intrinsic effect on the dynamics. The orbit remains in two dimensions, and the problem is decided by the form of the effective potential, U , which contains only the angular momentum barrier and the dynamical potential.

In quantum mechanics there are actually two places where an effect of dimension appears. The first is in the factor $l(l+D-2)$ of the angular-momentum barrier. The second is more fundamental. It is due to the operator

$$U_{qm} = -\frac{(D-1)}{\rho} \frac{d}{d\rho} \quad . \quad (32)$$

The contribution of U_{qm} to the “effective potential” can be calculated by using the ansatz

$$R_{l,D}(\rho) \equiv \frac{1}{\rho^{(D-1)/2}} \chi_{l,D}(\rho) . \quad (33)$$

This transforms the D -dimensional radial Schrödinger equation into a 1-dimensional Schrödinger equation:

$$0 = \left[-\frac{d^2}{d\rho^2} + U_{l,D}(\rho) \right] \chi_{l,D} . \quad (34)$$

In Eq. (34), the effective potential $U_{l,D}(\rho)$ is given by

$$\begin{aligned} U_{l,D}(\rho) &= \frac{(D-1)(D-3)}{4\rho^2} + \frac{l(l+D-2)}{\rho^2} + V(\rho) \\ &= \frac{l_{eff}(l_{eff}+1)}{\rho^2} + V(\rho) , \end{aligned} \quad (35)$$

with l_{eff} given in Eq. (28). Since the Schrödinger equation (34) depends only on the combination l_{eff} , the solution $\chi_{l,D}(\rho)$ does not depend on l and D separately. This explains, in particular, the values of l_{min} given in Eq. (31).

Although the above ansatz is well known, the dimensional effect has apparently not been adequately appreciated. One reason may be attributed to the fact that in going from $D = 3$ to $D = 1$, l_{eff} remains equal to l . However, in our problem this effect leads to such a counter-intuitive result, that it cannot be overlooked.

The dimensional effect essentially produces an additional centrifugal barrier which can bind the wave function at the threshold, even though the expectation value of the angular momentum vanishes. Note that this is in distinction to the classical problem, where there would be no “effective” centrifugal barrier to prevent the particle from approaching $r \rightarrow \infty$.

5 Summary

After obtaining exact, $E = 0$ solutions of the Schrödinger equation for power-law potentials, we demonstrated three interesting effects:

- (1) There exist bound states at the threshold, *for all $l > 0$ and all $\gamma > 0$* . These states persist if one changes the coupling constant γ by a positive factor. [In contrast, $E = 0$ bound states exist for the spherical well and the focusing potentials only for very special values of the coupling constants, and never for all $l > 0$ simultaneously.]
- (2) There exist normalizable solutions for $\nu < -2$, i.e., for highly repulsive potentials, singular at $\rho \rightarrow \infty$.
- (3) For higher-space dimensions, each additional dimension adds a half unit to the effective angular-momentum quantum number, l_{eff} , of Eq. (28). An effective centripetal barrier, solely due to this

dimensional effect, i.e., for $L^2 = 0$, is capable of producing a bound state. This result is a remarkable manifestation of quantum mechanics and has no classical counterpart.

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Figure Captions

Figure 1: A dimensionless representation of the Coulomb effective potential. We show the effective potential $U = 1/\rho^2 - 4/\rho$.

Figure 2: The Morse effective potential of Eq. (3) in units of $\mathcal{E}_0 = \hbar^2/(2ma^2)$, We take $l = 2$, $D = 11$, $b = 2.5$, and $\rho_0 = 1$.

Figure 3. The effective potential $U(\rho)$ of Eq. (5), in units of \mathcal{E}_0 , for a spherical-well, with $l = 1$ and $V_0 = \pi^2\mathcal{E}_0$ or $g = \pi$. With these parameters, there is exactly one bound state, at $E = 0$.

Figure 4: The effective potential obtained from Eq. (14) for $\nu = 4$ in units of $\mathcal{E}_0/2$, as a function of $\rho = r/a$. The form is $U(\rho) = 4/\rho^2 - 1/\rho^4$.