

# Quantum mechanics of the $1/x^2$ potential

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In quantum mechanics a localized attractive potential typically supports a (possibly infinite) set of bound states, characterized by a discrete spectrum of allowed energies, together with a continuum of scattering states, characterized (in one dimension) by an energy-dependent phase shift. The  $1/x^2$  potential on  $0 < x < \infty$  confounds all of our intuitions and expectations. Resolving its paradoxes requires sophisticated theoretical machinery: regularization, renormalization, anomalous symmetry-breaking, and self-adjoint extensions. Our goal is to introduce the essential ideas at a level accessible to advanced undergraduates. © 2006 American Association of Physics Teachers.

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## I. INTRODUCTION

Ordinarily, an attractive potential admits discrete bound states, together (perhaps) with a continuum of scattering states. In a first course on quantum mechanics, students encounter the infinite square well, the harmonic oscillator, the Dirac delta function, the finite square well, and (in three dimensions) the spherical well and the Coulomb potential, all of which fit this paradigm (though the first two lack scattering states). We do *not* study the  $1/x^2$  potential, and for good reason: It violates every rule in the book, and discredits all the intuition we are trying to instill in our students. In spite of this (or rather, precisely because of it) the  $1/x^2$  potential is a fascinating system, and analyzing its paradoxes provides an illuminating introduction to some of the more subtle techniques in contemporary theoretical physics: regularization and renormalization, anomalous symmetry-breaking, and self-adjoint extensions. In this paper we tell the story from a pedagogical perspective, starting out innocent and naive, and letting the unfolding saga force us to become wiser and more sophisticated.

In Sec. II we introduce the problem in its simplest (one-dimensional) form, and approach it as we would any other quantum system. We quickly encounter a series of puzzles and surprises. In Sec. III we identify the source of the difficulties and modify the potential so as to avoid the trouble. This leads naturally to renormalization and anomalies. In Sec. IV we notice that the Hamiltonian is not Hermitian, and modify the space of permissible functions to make it so; this introduces the method of self-adjoint extensions. In Sec. V we draw lessons from our experience and point to some real-world applications.

## II. PECULIARITIES OF THE $1/x^2$ POTENTIAL

Consider a particle of mass  $m$  in the one-dimensional potential<sup>1</sup>

$$V(x) = \begin{cases} \infty & (x \leq 0) \\ -a/x^2 & (x > 0) \end{cases} \quad (1)$$

shown in Fig. 1. Here  $a$  is a constant with the (MKS) units  $\text{J m}^2$ . In truth, the alarm should already be sounding, for there is no way to construct a quantity with the dimensions of energy from the parameters at hand ( $\hbar$ ,  $m$ , and  $a$ ), and hence no possible formula for the eigenvalues of the

Hamiltonian.<sup>2</sup> But let's pretend for a moment that we did not notice this problem. We look for bound states—normalizable negative-energy solutions of the Schrödinger equation:

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} - \frac{a}{x^2} \psi = E\psi \quad (x > 0), \quad (2)$$

or, multiplying through by  $-2m/\hbar^2$ ,

$$\frac{d^2\psi}{dx^2} + \frac{\alpha}{x^2} \psi = \kappa^2 \psi, \quad (3)$$

where  $\alpha \equiv 2ma/\hbar^2$  and  $\kappa \equiv \sqrt{-2mE}/\hbar$ , subject to the boundary conditions

$$\psi \rightarrow 0 \text{ as } x \rightarrow 0 \text{ and } x \rightarrow \infty. \quad (4)$$

The first boundary condition is necessary to make  $\psi$  continuous at the origin ( $\psi=0$ , of course, for  $x < 0$ ); the second is required for normalization:

$$\int_0^\infty |\psi(x)|^2 dx = 1. \quad (5)$$

Suppose we could find just *one* bound state  $\psi(x)$ , with energy  $E$ . Scaling  $x$  by a factor  $\beta$ , we can immediately construct a new solution,  $\psi_\beta(x) \equiv \psi(\beta x)$ , with energy  $\beta^2 E$ :

$$\begin{aligned} \frac{d^2\psi_\beta}{dx^2} + \frac{\alpha}{x^2} \psi_\beta &= \frac{d^2}{dx^2} \psi(\beta x) + \frac{\alpha}{x^2} \psi(\beta x) = \beta^2 \frac{d^2}{du^2} \psi(u) \\ &+ \beta^2 \frac{\alpha}{u^2} \psi(u) = \beta^2 \kappa^2 \psi(u) = (\beta\kappa)^2 \psi_\beta(x), \end{aligned} \quad (6)$$

where  $u \equiv \beta x$ . But  $\beta$  can be any real number.<sup>3</sup> So if there exist *any* bound states, then there is a bound state for every negative energy! In particular, the  $1/x^2$  potential has *no ground state*. This is disturbing, for a system without a lower limit on its allowed energies would be wildly unstable, cascading down with the release of an unlimited amount of energy. A reasonable inference would be that there are *no* negative energy states, which is indeed the case for  $\alpha < 1/4$  (trivially so, for  $\alpha < 0$ , because the potential is then repulsive).



Fig. 1. The  $1/x^2$  potential.

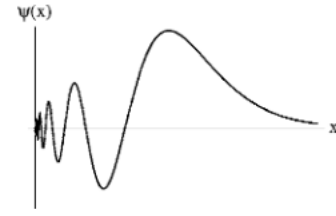


Fig. 2. The bound state wave function,  $\psi_\kappa(x)$ .

One particularly nice way to show that there are no bound states for  $0 < \alpha < 1/4$  is to factor the Hamiltonian.<sup>4</sup> Let  $\alpha = \nu(1 - \nu)$  define the new constant  $\nu$ ,

$$H = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} - \frac{a}{x^2} = -\frac{\hbar^2}{2m} \left( \frac{d}{dx} + \frac{\nu}{x} \right) \left( \frac{d}{dx} - \frac{\nu}{x} \right). \quad (7)$$

For an arbitrary test function  $f(x)$  we have

$$\left( \frac{d}{dx} + \frac{\nu}{x} \right) \left( \frac{d}{dx} - \frac{\nu}{x} \right) f(x) = \left( \frac{d}{dx} + \frac{\nu}{x} \right) \left( \frac{df}{dx} - \frac{\nu}{x} f \right) \quad (8a)$$

$$= \frac{d^2 f}{dx^2} + \frac{\nu}{x^2} f - \frac{\nu}{x} \frac{df}{dx} + \frac{\nu}{x} \frac{df}{dx} - \frac{\nu^2}{x^2} f \quad (8b)$$

$$= \frac{d^2 f}{dx^2} + \frac{\nu(1 - \nu)}{x^2} f = \left( \frac{d^2}{dx^2} + \frac{\alpha}{x^2} \right) f. \quad (8c)$$

Now, the Hermitian conjugate of  $(d/dx + \nu/x)$  is  $(-d/dx + \nu^*/x)$ :

$$\left\langle f \left| \left( \frac{d}{dx} + \frac{\nu}{x} \right) g \right\rangle = \int_0^\infty f^* \left( \frac{dg}{dx} + \frac{\nu}{x} g \right) dx \quad (9a)$$

$$= f^* g \Big|_0^\infty - \int_0^\infty \left( \frac{df}{dx} \right)^* g dx + \int_0^\infty \left( \frac{\nu^*}{x} f \right)^* g dx \quad (9b)$$

$$= \left\langle \left( -\frac{d}{dx} + \frac{\nu^*}{x} \right) f \right| g \right\rangle, \quad (9c)$$

provided that  $f(x)$  and  $g(x)$  go to zero at 0 and  $\infty$ . Thus

$$E = \langle H \rangle = \langle \psi | H | \psi \rangle = -\frac{\hbar^2}{2m} \left\langle \psi \left| \left( \frac{d}{dx} + \frac{\nu}{x} \right) \left( \frac{d}{dx} - \frac{\nu}{x} \right) \psi \right\rangle \quad (10a)$$

$$= \frac{\hbar^2}{2m} \left\langle \left( \frac{d}{dx} - \frac{\nu^*}{x} \right) \psi \left| \left( \frac{d}{dx} - \frac{\nu}{x} \right) \psi \right\rangle. \quad (10b)$$

If  $\nu$  is real, then,

$$E = \frac{\hbar^2}{2m} \int_0^\infty \left| \left( \frac{d\psi}{dx} - \frac{\nu}{x} \psi \right) \right|^2 dx > 0, \quad (11)$$

so negative energy states cannot occur if  $\nu$  is real. But  $\nu(1 - \nu) = \alpha$ , so

$$\nu = \frac{1}{2} \pm \sqrt{\frac{1}{4} - \alpha}, \quad (12)$$

and hence if  $\alpha < 1/4$ , then  $\nu$  is real, and there can be no bound states.

But when  $\alpha > 1/4$  there certainly do exist negative energy solutions. The Schrödinger equation can be solved by the method of Frobenius: We write  $\psi(x)$  as a power series,

$$\psi(x) = x^s \sum_{j=0}^\infty a_j x^j \quad (a_0 \neq 0), \quad (13)$$

and substitute this into Eq. (3):

$$\sum_{j=0}^\infty a_j [(j+s)(j+s-1) + \alpha] x^{j-2} = \kappa^2 \sum_{j=0}^\infty a_j x^j. \quad (14)$$

We equate like powers and find that the  $x^{-2}$  term yields  $s(s-1) + \alpha = 0$ , so

$$s = \nu = (1/2) \pm \sqrt{(1/4) - \alpha}; \quad (15)$$

the  $x^{-1}$  term forces  $a_1 = 0$ , and the remaining coefficients are determined by the recursion relation

$$a_j = \frac{\kappa^2}{j(j+2s-1)} a_{j-2} \quad (j = 2, 3, 4, \dots). \quad (16)$$

There are two solutions—one for each sign in Eq. (15). Near the origin they go like  $a_0 x^s$ ; for  $\alpha > 1/4$  this means

$$\sqrt{x} e^{\pm ig \ln x}, \quad (17)$$

where  $g \equiv \sqrt{\alpha - 1/4}$ .

The general solution is a linear combination, but it turns out that only one combination is normalizable:

$$\psi_\kappa(x) = A \sqrt{x} K_{ig}(\kappa x), \quad (18)$$

where  $K_{ig}$  is the modified Bessel function of order  $ig$ ;<sup>5</sup>  $\psi_\kappa$  is real, as long as  $g$  is real (which is to say, for  $\alpha > 1/4$ ), and finite at the origin (so  $\psi_\kappa \rightarrow 0$  as  $x \rightarrow 0$ );  $\psi_\kappa$  itself is square-integrable:<sup>6</sup>

$$\int_0^\infty |\sqrt{x} K_{ig}(\kappa x)|^2 dx = \frac{\pi g}{2\kappa^2 \sinh(\pi g)}, \quad (19)$$

so the normalization constant is

$$A = \kappa \sqrt{\frac{2 \sinh(\pi g)}{\pi g}}. \quad (20)$$

A plot of the wave function is shown in Fig. 2. Notice the oscillations as  $x \rightarrow 0$ , which result from the sinusoidal dependence on  $g \ln x$  in Eq. (17). We are accustomed to the idea that the ground state has no zero crossings, the first excited state has one, the second two, and so on. But the  $1/x^2$  potential has *no* ground state, and *every* (negative energy) solution has an infinite number of zero crossings. If the number of nodes counts the number of lower energy states, then no matter what the energy, there are always infinitely many states even lower.<sup>7</sup>

What about positive energy (scattering) states? For  $E > 0$  the general solution to Schrödinger's equation [Eq. (2)] is

$$\psi_k(x) = \sqrt{x} [AH_{ig}^{(2)}(kx) + BH_{ig}^{(1)}(kx)], \quad (21)$$

where  $k \equiv \sqrt{2mE/\hbar}$ , and  $H^{(1)}$  and  $H^{(2)}$  are Hankel functions. For large  $x$ ,

$$H_{ig}^{(1)}(kx) \sim \sqrt{\frac{2}{\pi kx}} e^{i(kx - \pi/4)} e^{\pi g/2}, \quad (22a)$$

$$H_{ig}^{(2)}(kx) \sim \sqrt{\frac{2}{\pi kx}} e^{-i(kx - \pi/4)} e^{-\pi g/2}, \quad (22b)$$

so

$$\psi_k(x) \sim A \sqrt{\frac{2}{\pi k}} e^{-\pi g/2} e^{i\pi/4} \left[ e^{-ikx} - i \frac{B}{A} e^{\pi g} e^{ikx} \right]. \quad (23)$$

The first term ( $e^{-ikx}$ ) represents a wave incident from the right; the second ( $e^{ikx}$ ) is the reflected wave. Ordinarily, setting  $\psi_k(0)=0$  in Eq. (21) would determine  $B/A$ , and the asymptotic expression Eq. (23) would reduce to<sup>9</sup>

$$\psi_k(x) \sim [e^{-ikx} - e^{i(2\delta + kx)}], \quad (24)$$

indicating that the reflected wave is equal in amplitude to the incident wave (as required by conservation of probability) and shifted in phase by an amount  $\delta(k)$ . But in this case  $\psi_k(0)$  is *automatically* zero (according to Eq. (17),  $|\psi| \sim \sqrt{x}$ ). There is *no* constraint on  $B$ , *no* formula for  $\delta(k)$ , and (most alarming) no enforcement of conservation of probability; the outgoing wave can have *any* amplitude!

**Conclusion:** The  $1/x^2$  potential has no ground state, and the allowed energies are not quantized. As long as  $\alpha > 1/4$ , the Schrödinger equation can be solved (and the boundary conditions satisfied) for every negative energy; the solutions are real and normalizable, and each of them has an infinite number of zero crossings. Scattering states occur for every positive energy, but the boundary condition at  $x=0$  imposes no constraint on the reflection coefficient, and does not determine the phase shift. It would be difficult to imagine a situation more at odds with our expectations.

### III. REGULARIZATION, RENORMALIZATION, AND ANOMALIES

Physically, the  $1/x^2$  potential is just too strong at the origin— $1/x$  is acceptable,<sup>10</sup> but  $1/x^2$  is not. One way to avoid the problem is to move the “wall” over to the right a distance  $\epsilon$ :

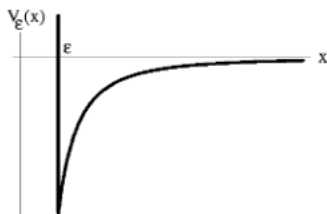


Fig. 3. The regularized potential.

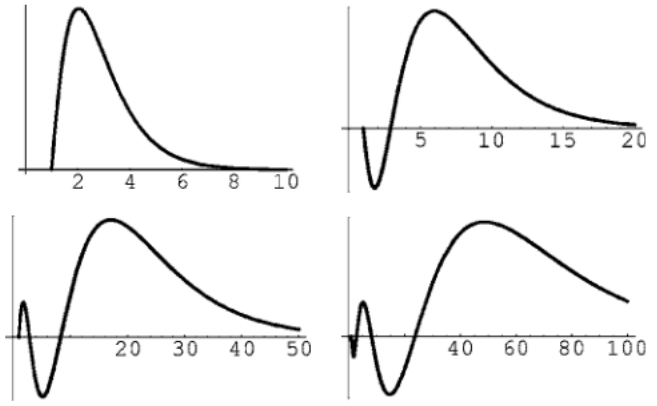


Fig. 4. Ground state and first three excited states, as functions of  $\kappa x$ , for  $V_\epsilon$ , with  $\epsilon=1$  and  $g=3$  (not normalized).

$$V_\epsilon(x) = \begin{cases} \infty & (x \leq \epsilon) \\ -a/x^2 & (x > \epsilon), \end{cases} \quad (25)$$

as shown in Fig. 3. This “regularized” potential suffers none of the ills that afflict  $V(x)$ ; we propose to work with  $V_\epsilon(x)$ , and take the limit  $\epsilon \rightarrow 0$  only at the very end. Of course, the pathologies can be expected to reappear in this limit, but as we shall see, *some* predictions survive, and these we take to be the “true” physical content of the  $1/x^2$  system. This is the strategy of “renormalization.”

Having introduced a parameter ( $\epsilon$ ) with the units of length, we are now able to construct an expression with the dimensions of energy:

$$\frac{a}{\epsilon^2} f(\alpha), \quad (26)$$

where  $f$  is a function of the dimensionless quantity  $\alpha = 2ma/\hbar^2$ . The system is no longer scale invariant; it possesses both a ground state<sup>11</sup> and a discrete spectrum of bound states. These have the same functional form as in Eq. (18), but the boundary condition is now  $\psi_\kappa(\epsilon)=0$ , which implies that

$$K_{ig}(\kappa\epsilon) = 0, \quad (27)$$

which is *not* automatically satisfied, and serves to quantize the energy. Figure 4 shows the ground state and the first three excited states for the case  $\alpha=9.25$  ( $g=3$ ).<sup>12</sup> Figure 5 shows the ground state energy (or rather,  $\kappa_1\epsilon$ ) for  $g$  ranging up to 7.

If  $\kappa\epsilon \ll 1$ ,<sup>13</sup> we can provide a relatively simple formula for the allowed energies:<sup>14</sup>

$$K_{ig}(z) \approx -\sqrt{\frac{\pi}{g \sinh(\pi g)}} \times \sin \left[ g \ln \left( \frac{z}{2} \right) - \arg \Gamma(1 + ig) \right] \quad (z \ll 1), \quad (28)$$

so  $K_{ig}(\kappa\epsilon)=0$  implies

$$g \ln \left( \frac{\kappa\epsilon}{2} \right) - \arg \Gamma(1 + ig) + n\pi = 0, \quad (29)$$

where  $n$  is an integer. The ground state is  $n=1$ ,<sup>15</sup> and the excited states are  $n=2, 3, \dots$ , with



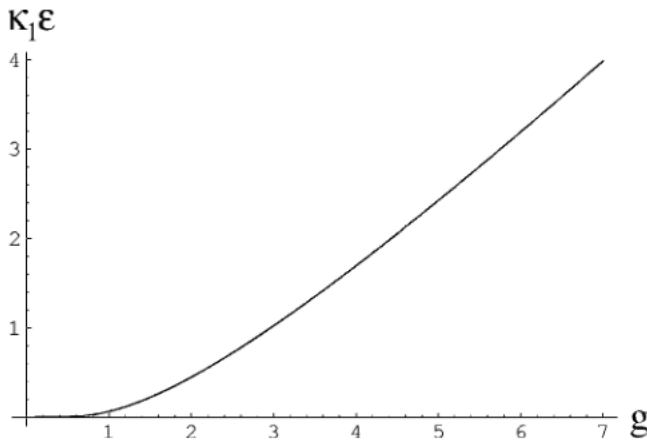


Fig. 5. The ground state  $\kappa_1\epsilon$  as a function of  $g$ .

$$\kappa_n = \frac{2}{\epsilon} e^{[\arg \Gamma(1+ig) - n\pi]/g}, \quad (30)$$

or

$$E_n = -\frac{2\hbar^2}{m\epsilon^2} e^{2[\arg \Gamma(1+ig) - n\pi]/g}. \quad (31)$$

There are infinitely many discrete bound states, as one might expect.<sup>16</sup>

For positive energies (scattering) the wave function is still given by Eq. (21), but now

$$\psi_k(\epsilon) = 0, \quad (32)$$

and hence  $AH_{ig}^{(2)}(k\epsilon) + BH_{ig}^{(1)}(k\epsilon) = 0$ , so

$$\frac{B}{A} = -\frac{H_{ig}^{(2)}(k\epsilon)}{H_{ig}^{(1)}(k\epsilon)}. \quad (33)$$

Referring to Eqs. (23) and (24), we find that the phase shift satisfies<sup>17</sup>

$$e^{2i\delta} = i\frac{B}{A}e^{\pi g} = -i\frac{H_{ig}^{(2)}(k\epsilon)}{H_{ig}^{(1)}(k\epsilon)}e^{\pi g} = -i\frac{[H_{ig}^{(1)}(k\epsilon)]^*}{H_{ig}^{(1)}(k\epsilon)}. \quad (34)$$

Notice that conservation of probability has been enforced by Eq. (32). Thus

$$\delta = -\arg[H_{ig}^{(1)}(k\epsilon)] - \frac{\pi}{4}. \quad (35)$$

This function is plotted in Fig. 6.

As the graphs suggest,  $\arg[H_{ig}^{(1)}(x)]$  is extremely steep near the origin. Indeed, for  $|z| \ll 1$ ,

$$H_{ig}^{(1)}(z) \approx e^{ig \ln(z/2)} \frac{1 + \coth \pi g}{\Gamma(1+ig)} - e^{-ig \ln(z/2)} \frac{\Gamma(1+ig)}{\pi g}, \quad (36)$$

so<sup>19</sup>

$$\tan[\arg H_{ig}^{(1)}(z)] \approx \coth\left(\frac{\pi g}{2}\right) \times \tan[g \ln(z/2) - \arg \Gamma(1+ig)], \quad (37)$$

and hence

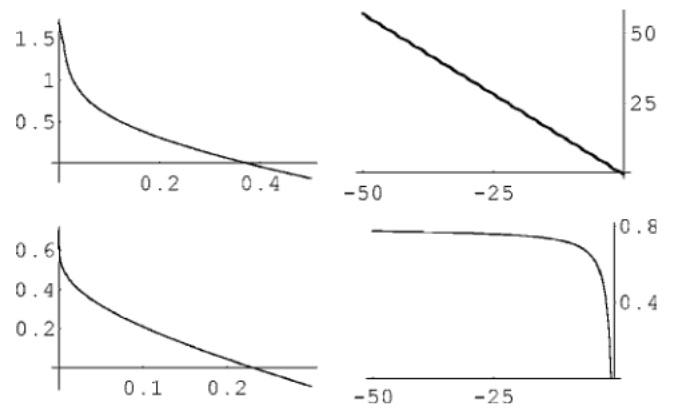


Fig. 6. Graphs of  $\delta$  as a function of  $k\epsilon$ , for  $g=0.5$  (top) and  $g=0$  (bottom). The graphs on the right show the behavior near the origin (the horizontal scale is in powers of 10); they suggest that there is no limit when  $g=0.5$ , whereas  $\delta \rightarrow \pi/4$  when  $g=0$  (though that limit is only approached when  $k\epsilon \ll 10^{-10}$ ).

$$\tan \delta \approx \frac{\tan \xi + \tanh(\pi g/2)}{\tan \xi - \tanh(\pi g/2)}, \quad (38)$$

where

$$\xi \equiv g \ln(k\epsilon/2) - \arg \Gamma(1+ig). \quad (39)$$

As  $k\epsilon \rightarrow 0$ ,  $\xi \rightarrow -\infty$ , and  $\tan \xi$  fluctuates wildly: Whenever  $\xi$  hits an integer multiple of  $\pi$ ,  $\tan \xi = 0$ , so (unless  $g=0$ )  $\tan \delta = -1$ ; whenever  $\xi$  is a half-integer multiple of  $\pi$ ,  $\tan \xi \rightarrow \pm\infty$ , so  $\tan \delta = 1$ . Clearly,  $\delta$  does not approach a limit. The case  $g=0$  is special, and it is best to treat it separately: For  $|z| \ll 1$ ,

$$H_0^{(1)}(z) \approx 1 + \frac{2i}{\pi} [\ln(z/2) + C] = 1 + \frac{2i}{\pi} \ln(\gamma z/2), \quad (40)$$

where  $C=0.577\,215$  is Euler's constant and  $\gamma \equiv e^C = 1.78\,1072$ .<sup>20</sup> Thus  $\tan[\arg H_0^{(1)}(z)] \approx 2 \ln(\gamma z/2)/\pi$ , and hence

$$\tan \delta \approx \frac{\ln(\gamma k\epsilon/2) + \pi/2}{\ln(\gamma k\epsilon/2) - \pi/2}. \quad (41)$$

At this point we would like to send  $\epsilon \rightarrow 0$ , to recover the pure  $1/x^2$  potential. Naively, Eq. (31) suggests that  $E_1$  will go to  $-\infty$ —precisely the trap we were hoping to avoid. But closer inspection reveals that the boundary condition, Eq. (27), only determines the *product*  $\kappa_1\epsilon$ . Suppose we stipulate that  $E_1$  (and hence  $\kappa_1$ ) remain *constant* as  $\epsilon \rightarrow 0$ . From Fig. 5 we see that this assumption forces  $g \rightarrow 0$ , leaving<sup>16</sup>

$$\kappa_1 = \frac{2}{\gamma\epsilon} e^{-\pi/g} \quad (\epsilon \rightarrow 0, g \rightarrow 0). \quad (42)$$

The excited states, Eq. (30), are squeezed out

$$\kappa_n = \frac{2}{\gamma\epsilon} e^{-n\pi/g} = \kappa_1 e^{-(n-1)\pi/g} \rightarrow 0 \quad (n=2,3,4,\dots), \quad (43)$$

but there remains a single bound state at finite (though indeterminate) energy.

We can use Eq. (42) to eliminate the cutoff  $\epsilon$  in favor of  $\kappa_1$ , in the scattering problem:

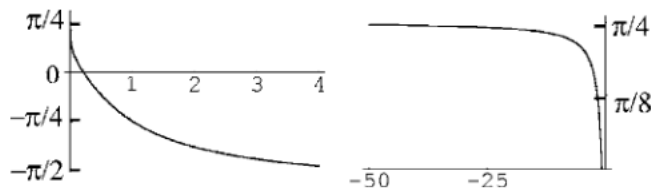


Fig. 7. The scattering phase shift  $\delta(k/\kappa_1)$ , Eq. (47), for  $g \ll 1$ . The graph on the right shows the behavior near the origin (the horizontal scale is in powers of 10).

$$k\epsilon = \frac{k}{\kappa_1} \frac{2}{\gamma} e^{-\pi/g}. \quad (44)$$

So for low energy scattering, Eq. (39) becomes

$$\xi \approx g \ln(k/\kappa_1) - \pi, \quad (45)$$

$$\tan \xi \approx \tan[g \ln(k/\kappa_1)] \approx g \ln(k/\kappa_1), \quad (46)$$

and Eq. (38) reads

$$\tan \delta \approx \frac{\ln(k/\kappa_1) + \pi/2}{\ln(k/\kappa_1) - \pi/2}. \quad (47)$$

Curiously, the phase shift is independent of  $g$  (although we have stipulated that  $g \ll 1$ ).<sup>21</sup> For extremely low-energy scattering,  $k \ll \kappa_1$ , the phase shift is evidently  $\pi/4$  (see Fig. 7).

**Conclusion:** The regularized potential, Eq. (25), has a non-problematic spectrum of discrete bound states, and a continuum of scattering states with well-defined phase shifts. Naively, the limit  $\epsilon \rightarrow 0$  (which restores the pure  $1/x^2$  potential) reintroduces all of the pathological features of the original. But closer examination reveals a loophole: If as we send  $\epsilon \rightarrow 0$  we simultaneously let  $g \rightarrow 0$ , in such a way as to hold  $\kappa_1$  constant (Fig. 8), then a single bound state with energy

$$E_1 = -\frac{\hbar^2 \kappa_1^2}{2m} \quad (48)$$

survives, and the scattering phase shift is given by

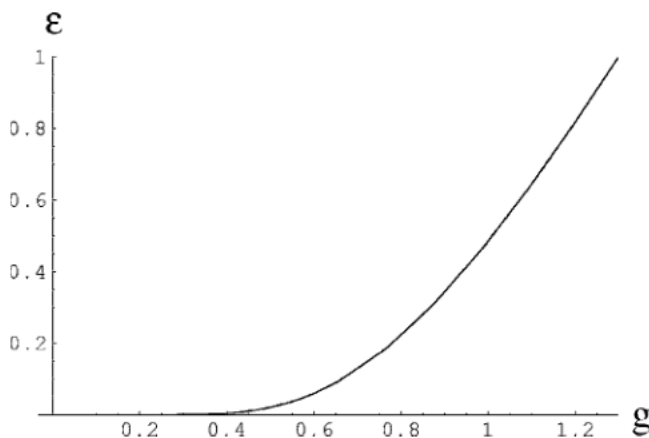


Fig. 8. Graph of  $\epsilon$  as a function of  $g$ , Eq. (42), with  $\kappa_1=0.1$ .

$$\delta(k) = \tan^{-1} \left[ \frac{\ln(k/\kappa_1) + \pi/2}{\ln(k/\kappa_1) - \pi/2} \right]. \quad (49)$$

This scheme does not determine  $\kappa_1$ , and it forces  $\alpha \rightarrow 1/4$ , but the physical implications of the theory are perfectly sensible.

The renormalization procedure we have just described may sound artificial, but it is not altogether unreasonable.<sup>22</sup> After all, in practice we would have no way of knowing whether the potential is really  $1/x^2$  all the way down to  $x=0$ ; what we actually *measure* is the ground state energy and the scattering phase shift. The former provides us with a *relation* between  $\epsilon$  and  $g$ , Eq. (42), but it does not determine either one separately, and the latter, Eq. (49), stands as a testable prediction irrespective of the actual (but unmeasurable) value of the cutoff.<sup>23</sup>

What about the symmetry argument based on scale invariance (or, if you prefer, dimensional analysis) that seemed to prove conclusively that the  $1/x^2$  potential can have no ground state (if it has one negative allowed energy, then every negative energy is an eigenvalue)? Well, we broke that symmetry when we introduced the cutoff, and the break persists even as we eliminate  $\epsilon$  from the theory in favor of  $\kappa_1$ , and (implicitly) send  $\epsilon \rightarrow 0$ . This is an example of “anomalous” symmetry breaking. There are three standard mechanisms for breaking a symmetry in physics:

1. *External* (or *dynamical*): An imposed force spoils the symmetry (for example, at the surface of the earth gravity breaks the three-dimensional isotropy of space).
2. *Spontaneous*: The ground state of a system is degenerate, and historical accident selects a particular one (for example, the magnetization of a small piece of iron, which *could* have pointed in any direction, but in *fact* has to point in some specific direction).
3. *Anomalies*: The process of renormalization breaks the symmetry.<sup>24</sup>

#### IV. SELF-ADJOINT EXTENSIONS

In Sec. II we examined the patient and diagnosed the illness. In Sec. III we provided a partial cure. Now it is time to identify the root cause of the disease and propose a more comprehensive treatment. The fundamental problem with the  $1/x^2$  potential is that the Hamiltonian

$$H = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} - \frac{a}{x^2} = -\frac{\hbar^2}{2m} \left( \frac{d^2}{dx^2} + \frac{\alpha}{x^2} \right) \quad (50)$$

is not Hermitian (more precisely, it is not *self-adjoint*). In quantum mechanics self-adjoint operators occupy a privileged position, because they alone represent *observable* quantities. Most of our experience and intuition is predicated on the self-adjointness of the Hamiltonian, and when this fails, the intelligibility of the theory goes with it.

An operator is defined not only by its *action*,  $A$ , but also by its *domain*,  $\mathcal{D}_A$ , the space of functions  $\{\psi\}$  on which it acts. Physicists tend to forget the second part, because in most cases the domain is not problematic. Of course,  $\psi$  and  $A\psi$  must lie in the Hilbert space of square-integrable functions,  $L_2$  (in our case, on the interval  $0 < x < \infty$ ), to ensure that inner products are well-defined. In fact, to guarantee the existence of the Hermitian conjugate (or “adjoint”)  $A^\dagger$ ,

$$\langle \phi | A \psi \rangle = \langle A^\dagger \phi | \psi \rangle, \quad (51)$$

the allowed functions must be *dense* in  $L_2$ .<sup>25</sup> Typically there will be other conditions on  $\mathcal{D}_A$  as well.

If there exists a domain such that for all  $\psi$  and  $\phi$  in  $\mathcal{D}_A$

$$\langle \phi | A \psi \rangle = \langle A \phi | \psi \rangle \quad (52)$$

(that is, the actions of  $A$  and  $A^\dagger$  are identical), then the operator is Hermitian (mathematicians would say “symmetric”) over that domain. However, it may happen that as long as  $\psi$  is in  $\mathcal{D}_A$  (the domain of the *operator*),  $\phi$  can be in a *larger* domain,  $\mathcal{D}_{A^\dagger}$  (the domain of the *adjoint*),<sup>26</sup> and yet Eq. (52) still holds. In that case ( $\mathcal{D}_{A^\dagger} \supset \mathcal{D}_A$ ) we may be able to *extend* the domain of the operator (which will automatically *restrict* the domain of the adjoint) until the two domains coincide. In this circumstance, with  $A=A^\dagger$  and  $\mathcal{D}_{A^\dagger}=\mathcal{D}_A$ , the operator is said to be *self-adjoint*. For self-adjoint operators, in other words, both the action *and* the *domain* of the adjoint are the same as for the operator itself.

The process we have sketched is called “self-adjoint extension.” You start with a Hermitian operator on a specified domain, and extend  $\mathcal{D}_A$  (thereby contracting  $\mathcal{D}_{A^\dagger}$ ) until the domains are identical. This process raises several questions, which were first addressed by Weyl and later generalized by von Neumann and Stone.<sup>27</sup> How can you tell whether a given operator admits a self-adjoint extension? Is the extension (if it exists) unique? How do you construct the self-adjoint domain? The answers are buried in abstruse mathematical literature that is largely inaccessible to physicists,<sup>28</sup> but two recent articles provide a relatively straightforward guide for the uninitiated.<sup>29,30</sup>

We begin by asking whether  $H$  in Eq. (50) is Hermitian. Suppose  $\phi(x)$  and  $\psi(x)$  are two functions in  $L_2(0, \infty)$  such that  $H\phi$  and  $H\psi$  are also in  $L_2(0, \infty)$ . Using integration by parts (twice), we have

$$\langle \phi | H \psi \rangle = \frac{-\hbar^2}{2m} \int_0^\infty \phi^* \left( \frac{d^2 \psi}{dx^2} + \frac{\alpha}{x^2} \psi \right) dx \quad (53a)$$

$$= -\frac{\hbar^2}{2m} \left[ \phi^* \frac{d\psi}{dx} \Big|_0^\infty - \psi \frac{d\phi^*}{dx} \Big|_0^\infty + \int_0^\infty \left( \frac{d^2 \phi^*}{dx^2} + \frac{\alpha}{x^2} \phi^* \right) \psi dx \right] \quad (53b)$$

$$= \langle H \phi | \psi \rangle - \frac{\hbar^2}{2m} \left( \phi^* \frac{d\psi}{dx} - \psi \frac{d\phi^*}{dx} \right) \Big|_0^\infty. \quad (53c)$$

Evidently  $H$  is Hermitian,

$$\langle \phi | H \psi \rangle = \langle H \phi | \psi \rangle, \quad (54)$$

if the boundary term in Eq. (53c) is zero (for all  $\psi$  and  $\phi$ ). There is no problem at infinity, where the functions and their derivatives can safely be taken to vanish;<sup>31</sup> the trouble arises at the lower limit. If we want  $H$  to be Hermitian, we shall have to restrict its domain. Earlier, we stipulated (for reasons of continuity) that wave functions go to zero at the origin, but in spite of appearances this condition does *not* suffice to kill the boundary term, because the *derivatives* can (and in the critical cases *do*) diverge. For example, we found in Eq. (15) that solutions to the Schrödinger equation behave near the origin like

$$u_\pm(x) = x^{s_\pm}, \quad (55a)$$

with

$$s_\pm = \frac{1}{2} \pm \sqrt{\frac{1}{4} - \alpha}. \quad (55b)$$

So, using  $\psi = u_+$  and  $\phi = u_-$ , we have<sup>32</sup>

$$\begin{aligned} \left( u_-^* \frac{du_+}{dx} - u_+ \frac{du_-^*}{dx} \right) \Big|_0 &= x^{(s_-)^*} s_+ x^{(s_+-1)} - x^{s_+} s_-^* x^{(s_-^*-1)} \\ &= (s_+ - s_-^*) x^{(s_++s_-^*-1)} = \sqrt{1-4\alpha}. \end{aligned} \quad (56)$$

Unless  $\alpha=1/4$  (a special case that keeps recurring and to which we shall return) some *other* condition must be imposed.

What if we insist that allowed functions vanish in a finite (but arbitrarily small) *neighborhood*<sup>33</sup> of the origin? Then the boundary term vanishes trivially, and  $H$  is Hermitian (on this domain). But if  $\psi$  is in this very restricted domain,  $\phi$  could be *any* square-integrable function, and the boundary term will still vanish. So the domain of the adjoint is very much larger than the domain of the operator, and hence  $H$  is not self-adjoint. *Question:* Does  $H$  admit a self-adjoint extension, and if so, what is the self-adjoint domain?<sup>34</sup> In von Neumann’s procedure the first step is to look for eigenfunctions of  $H$  with imaginary eigenvalues:<sup>35</sup>

$$H \phi_\pm = \pm i \eta \phi_\pm, \quad (57)$$

where  $\eta$  is real and positive.<sup>36</sup> Thus

$$\left( \frac{d^2}{dx^2} + \frac{\alpha}{x^2} \right) \phi_\pm = \kappa_\pm^2 \phi_\pm, \quad (58)$$

where

$$\kappa_\pm \equiv \frac{\sqrt{\mp i 2m \eta}}{\hbar} = e^{\mp i \pi/4} \beta, \quad (59)$$

with  $\beta \equiv \sqrt{2m \eta}/\hbar$ . The general solution is

$$\phi_\pm(x) = \sqrt{x} [A_\pm H_{ig}^{(1)}(i\kappa_\pm x) + B_\pm H_{ig}^{(2)}(i\kappa_\pm x)], \quad (60)$$

where (as always)  $g = \sqrt{\alpha - 1/4}$ , and  $A_\pm$  and  $B_\pm$  are arbitrary constants. But  $H_{ig}^{(2)}(i\kappa_\pm x)$  is not in  $L_2$  (and hence not in  $\mathcal{D}_H$ ), because at large  $x$  [Eq. (22b)]<sup>37</sup>

$$\begin{aligned} H_{ig}^{(2)}(i\kappa_\pm x) &\approx \sqrt{\frac{2}{\pi i \kappa_\pm x}} e^{-i(i\kappa_\pm x - \pi/4)} e^{-\pi g/2} \\ &= \sqrt{\frac{2}{\pi \kappa_\pm x}} e^{-\pi g/2} e^{\kappa_\pm x}, \end{aligned} \quad (61)$$

and because  $\kappa = \beta(1 \mp i)/\sqrt{2}$ ,  $H_{ig}^{(2)}$  diverges exponentially. Thus

$$\phi_\pm(x) = A_\pm \sqrt{x} H_{ig}^{(1)}(i\kappa_\pm x). \quad (62)$$

Let  $n_+$  be the number of linearly independent solutions for  $\phi_+$ , and  $n_-$  the corresponding number for  $\phi_-$ ;  $n_1$  and  $n_2$  are called “deficiency indices,” and they play a major role in the theory. Weyl and von Neumann showed that if  $n_+ = n_- = n$ , there exists an  $n^2$ -parameter family of self-adjoint extensions. (If  $n=0$ , the operator is already self-adjoint, and if  $n_+ \neq n_-$ , there is no self-adjoint extension.) In our case,  $n_+$



$=n_-=1$ , and it remains only to characterize the one-parameter family of self-adjoint domains. The prescription is as follows:  $\psi$  is in the self-adjoint domain if

$$\langle \Phi | H \psi \rangle = \langle H \Phi | \psi \rangle, \quad (63)$$

where  $\Phi \equiv \phi_+ + \lambda \phi_-$  for some  $\lambda$ , which is to say [Eq. (53c)] if

$$\lim_{x \rightarrow 0} \left[ \Phi^* \frac{d\psi}{dx} - \psi \frac{d\Phi^*}{dx} \right] = 0. \quad (64)$$

Evidently we need to know the behavior of  $\phi_{\pm}$  for small  $x$ . From Eq. (36),

$$H_{ig}^{(1)}(i\kappa_{\pm}x) \approx e^{ig \ln(i\kappa_{\pm}x/2)} \frac{1 + \coth \pi g}{\Gamma(1 + ig)} - e^{-ig \ln(i\kappa_{\pm}x/2)} \frac{\Gamma(1 + ig)}{\pi g}, \quad (65)$$

provided that  $g \neq 0$ . But  $\kappa_{\pm} = \exp(\mp i\pi/4)\beta$ , so

$$\ln(i\kappa_{\pm}x/2) = \ln(\beta x) - \ln 2 + i\ell_{\pm}\pi/4, \quad (66)$$

where  $\ell_+ \equiv 1$  and  $\ell_- \equiv 3$ . Thus

$$e^{ig \ln(i\kappa_{\pm}x/2)} = e^{ig \ln \beta x} e^{-ig \ln 2} e^{-i\ell_{\pm}g\pi/4} \quad (67)$$

and hence

$$\phi_+ \approx A_+ \sqrt{x} [D e^{ig \ln \beta x} - F e^{-ig \ln \beta x}], \quad (68a)$$

$$\phi_- \approx A_- \sqrt{x} [D e^{-\pi g/2} e^{ig \ln \beta x} - F e^{\pi g/2} e^{-ig \ln \beta x}], \quad (68b)$$

where

$$D \equiv e^{-ig \ln 2} e^{-\pi g/4} \left[ \frac{1 + \coth \pi g}{\Gamma(1 + ig)} \right], \quad (69a)$$

$$F \equiv e^{ig \ln 2} e^{\pi g/4} \left[ \frac{\Gamma(1 + ig)}{\pi g} \right]. \quad (69b)$$

It follows that

$$\Phi \approx \sqrt{x} [G e^{ig \ln \beta x} - J e^{-ig \ln \beta x}] \quad (x \ll 1), \quad (70)$$

where

$$G \equiv D(A_+ + \lambda A_- e^{-\pi g/2}), \quad (71a)$$

$$J \equiv F(A_+ + \lambda A_- e^{\pi g/2}). \quad (71b)$$

Therefore

$$\frac{d\Phi}{dx} \approx \frac{1}{\sqrt{x}} \left[ \left( \frac{1}{2} + ig \right) G e^{ig \ln \beta x} - \left( \frac{1}{2} - ig \right) J e^{-ig \ln \beta x} \right]. \quad (72)$$

Using Eqs. (70) and (72), the boundary condition [Eq. (64), or more simply its complex conjugate] becomes

$$\sqrt{x} [e^{2ig \ln(x/x_0)} - 1] \frac{d\psi^*}{dx} - \frac{1}{\sqrt{x}} \left[ \left( \frac{1}{2} + ig \right) e^{2ig \ln(x/x_0)} - \left( \frac{1}{2} - ig \right) \right] \psi^* \rightarrow 0 \quad (73)$$

(as  $x \rightarrow 0$ ), where

$$x_0 \equiv \frac{1}{\beta} \left( \frac{G}{J} \right)^{i/2g} \quad (74)$$

is a free constant<sup>38</sup>—the anticipated parameter that characterizes the particular self-adjoint extension. For example, if  $\alpha=0$  (so  $g=i/2$ ), Eq. (73) reduces to

$$\frac{1}{\sqrt{x}} \left[ x_0 \frac{d\psi}{dx} + \psi \right] \rightarrow 0, \quad (75)$$

which is the self-adjoint extension for the free particle on  $0 \leq x < \infty$ .<sup>39</sup>

In the critical case  $g=0$  ( $\alpha=1/4$ ) Eq. (65) is replaced by

$$H_0^{(1)}(i\kappa_{\pm}x) \approx 1 - \frac{\ell_{\pm}}{2} + \frac{2i}{\pi} \ln(\gamma\beta x/2) \quad (76)$$

[see Eq. (40)], and

$$\phi_{\pm} \approx A_{\pm} \sqrt{x} \left[ \pm \frac{1}{2} + \frac{2i}{\pi} \ln(\gamma\beta x/2) \right], \quad (77)$$

so

$$\Phi \approx \sqrt{x} [G + J \ln(\gamma\beta x/2)], \quad (78)$$

with

$$G \equiv \frac{1}{2}(A_+ - \lambda A_-), \quad (79a)$$

$$J \equiv \frac{2i}{\pi}(A_+ + \lambda A_-), \quad (79b)$$

and

$$\frac{d\Phi}{dx} \approx \frac{1}{2\sqrt{x}} [G + 2J + J \ln(\gamma\beta x/2)]. \quad (80)$$

According to Eq. (64), then, a function  $\psi$  is in the self-adjoint domain if

$$\sqrt{x} \ln(x/x_0) \frac{d\psi}{dx} - \frac{1}{\sqrt{x}} \left[ 1 + \frac{1}{2} \ln(x/x_0) \right] \psi \rightarrow 0, \quad (81)$$

where in this case  $x_0 \equiv (2/\gamma\beta) e^{-G/J}$  is the free parameter characterizing the particular self-adjoint extension.<sup>40</sup>

Where does all this leave us? If we want the  $1/x^2$  Hamiltonian, Eq. (50), to be self-adjoint, we must tighten up the naive boundary condition  $\psi(0)=0$ , Eq. (4), in favor of a self-adjoint extension [Eq. (73) if  $\alpha \neq 1/4$  and Eq. (81) for the critical case  $\alpha=1/4$ ].<sup>41</sup> The choice of a *particular* extension (which is to say, a particular value of  $x_0$ ) is arbitrary, and in this sense there exists an entire one-parameter family of distinct physical theories described by the  $1/x^2$  potential. *Question*: Do they admit reasonable bound state spectra? We know that the normalized eigenstates of  $H$  are given by Eq. (18):

$$\psi_{\kappa}(x) = A \sqrt{x} K_{ig}(\kappa x) = \frac{i\pi}{2} A \sqrt{x} H_{ig}^{(1)}(i\kappa x), \quad (82)$$

where  $\kappa \equiv \sqrt{-2mE}/\hbar$ . Which (if any) of these reside in the self-adjoint domain of  $H$ ?

In the critical case  $g=0$ , Eq. (40) yields (for small  $x$ )

$$\psi_{\kappa}(x) \approx -A \sqrt{x} \ln(\gamma\kappa x/2), \quad (83)$$

and

$$\frac{d\psi_\kappa}{dx} \approx -A \frac{1}{\sqrt{x}} \left[ 1 + \frac{1}{2} \ln(\gamma\kappa x/2) \right]. \quad (84)$$

Inserting these expressions into Eq. (81) yields the condition  $A \ln(\gamma\kappa x_0/2) \rightarrow 0$ . This holds only if  $\gamma\kappa x_0/2=1$ , which is to say, if  $\kappa=2/\gamma x_0$ . Evidently there is exactly *one* bound state for  $\alpha=1/4$ , just as we found (by a completely different route) in Sec. III [Eq. (48)]. But we cannot *calculate* the allowed energy, because it depends on the arbitrary parameter  $x_0$  (just as, in the renormalization method, it depended on the arbitrary cutoff  $\epsilon$ ).

The case  $g \neq 0$  is a little more complicated. Equation (28) gives (for small  $x$ )

$$\psi_\kappa(x) \approx B\sqrt{x} \sin \theta, \quad (85)$$

where  $B \equiv -A\sqrt{\pi/g \sinh(\pi g)}$  and

$$\theta(x) \equiv g \ln(\kappa x/2) - \arg \Gamma(1 + ig). \quad (86)$$

It follows that

$$\frac{d\psi_\kappa}{dx} \approx B \frac{1}{\sqrt{x}} \left[ \frac{1}{2} \sin \theta + g \cos \theta \right]. \quad (87)$$

According to Eq. (73), then,  $\psi_\kappa$  is in the self-adjoint domain if

$$g \ln\left(\frac{2}{\kappa x_0}\right) + \arg \Gamma(1 + ig) = n\pi \quad (n = 0, \pm 1, \pm 2, \dots) \quad (88)$$

for  $g$  real ( $\alpha > 1/4$ ), or  $2/\kappa x_0 = 1$  for  $g$  imaginary ( $\alpha < 1/4$ ). In the former case we obtain an infinite set of eigenvalues; in the latter case just one.

**Conclusion:** To make the  $1/x^2$  Hamiltonian self-adjoint we are obliged to impose more stringent boundary conditions [Eq. (73) or (81)] than we naively supposed. This imposition necessarily introduces a free parameter  $x_0$  with the dimensions of length, thereby breaking the scale invariance of the theory. The result is a reasonable spectrum of allowed states, whose energies, however, we are unable to predict, because they depend on the value of the arbitrary parameter.<sup>42</sup>

## V. CONCLUSION

The  $1/x^2$  potential is clearly problematic. We can fix it (sort of) by renormalization or by self-adjoint extension, but a reasonable person would likely conclude that the problem itself is artificial and unphysical—maybe there is no such thing as a  $1/x^2$  potential in nature. Perhaps some potentials are just plain illegal in quantum mechanics. It seems odd, though, that we never encounter such difficulties in *classical* mechanics.

Well, in the first place there *are* classical precursors.<sup>43</sup> Moreover, there *do* exist systems represented (at least, to good approximation) by a  $1/x^2$  potential (at any rate by its three-dimensional analog). The best example is the motion of a charged particle in the field of a stationary electric dipole, for instance, an electron in the vicinity of a polar molecule. Here the potential is  $-ep \cos \theta/r^2$ , and (surprisingly) the radial Schrödinger equation is mathematically identical to Eq. (2).<sup>44</sup> The critical parameter  $\alpha=1/4$  was noted in early studies of this system,<sup>45</sup> which has attracted renewed attention recently.<sup>46</sup> Like it or not, we have to take this problem seriously.

## ACKNOWLEDGMENTS

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<sup>1</sup>Of course,  $V(x)$  is unbounded as  $x \rightarrow 0$ , but this by itself is not problematic—the same is true of the Coulomb potential and the delta function well. Our study of the  $1/x^2$  potential was inspired by (and in the early parts modeled on) S. A. Coon and B. R. Holstein, “Anomalies in quantum mechanics: The  $1/r^2$  potential” *Am. J. Phys.* **70**, 513–519 (2002).

<sup>2</sup>Is there any other potential with this defect? In other words, is there another function of position that contains no dimensional constants and has the same units as  $1/x^2$ ? There is—the two-dimensional delta function,  $\delta^2(\mathbf{r}) = \delta(x)\delta(y)$ . Our story can be told using the two-dimensional delta function, but because the extra dimension makes the details a little more cumbersome and because the  $1/x^2$  potential is arguably more realistic, we prefer to consider it as the model. In fact, for states with circular symmetry the two-dimensional delta function is mathematically equivalent to the  $1/x^2$  potential with  $\alpha=1/4$  [Eq. (3)]—see Exercise 1 in Ref. 30. For discussion of the two-dimensional delta function see L. R. Mead and J. Godines, “An analytical example of renormalization in two-dimensional quantum mechanics,” *Am. J. Phys.* **59**, 935–937 (1991); R. Jackiw, “Delta-function potentials in two- and three-dimensional quantum mechanics,” in *M. A. B. Bég Memorial Volume*, edited by A. Ali and P. Hoodbhoy (World Scientific, Singapore, 1991), pp. 25–42.

<sup>3</sup>Notice that if  $\psi(x)$  is normalizable, so too is  $\psi_\beta(x)$ .

<sup>4</sup>K. S. Gupta and S. G. Rajeev, “Renormalization in quantum mechanics,” *Phys. Rev. D* **48**, 5940–5945 (1993).

<sup>5</sup>G. Arfken and H.-J. Weber, *Mathematical Methods for Physicists* (Academic, Orlando (2000), 5th ed., Chap. 11. The other solution,  $\sqrt{x}I_{ig}(\kappa x)$ , diverges for large  $x$ .

<sup>6</sup>I. S. Gradshteyn and I. M. Ryzhik, *Tables of Integrals, Series, and Products* (Academic, San Diego, (1980), Eqs. (6.576.4) and (8.332.3). Incidentally, states with different  $\kappa$  are not orthogonal.

<sup>7</sup>One might ask what the usual approximation schemes have to say about this potential. Not much. For the general power law  $V(x)=ax^\nu$  on  $0 < x < \infty$ , the WKB approximation yields  $E_n \approx a[(n-1/4)\hbar\sqrt{2\pi m a \Gamma(1/\nu + 3/2)/\Gamma(1/\nu + 1)}]^{2\nu/(\nu+2)}$  [see D. J. Griffiths, *Introduction to Quantum Mechanics* (Prentice Hall, Englewood Cliffs, NJ, 2004), 2nd ed., Problem 8.11], and the exponent is infinite when  $\nu=-2$ . The variational principle only confirms what we already knew—that the ground state is lower than every negative energy.

<sup>8</sup>Reference 6, p. 962, Eqs. (3) and (4).

<sup>9</sup>Some authors use a plus sign in Eq. (24), which adds  $\pi/2$  to the phase shift. We prefer the minus sign, because it reduces to  $\delta=0$  when the potential is zero.

<sup>10</sup>For a list of accessible references see C. V. Siclen, “The one-dimensional hydrogen atom,” *Am. J. Phys.* **56**, 9–10 (1988).

<sup>11</sup>Indeed, because allowed energies must exceed  $V_{\min}$ ,  $E_1 > -a/\epsilon^2$ .

<sup>12</sup>For these parameters  $\kappa_1\epsilon=1.024\,645$ ,  $\kappa_2\epsilon=0.350\,972$ ,  $\kappa_3\epsilon=0.122\,830$ , and  $\kappa_4\epsilon=0.043\,089$ .

<sup>13</sup>For the ground state this inequality would appear to require  $g \ll 3$  (see Fig. 5), but in practice the approximation is good up to  $g=3$ . For the excited states  $\kappa$  is smaller, and the approximation is valid for even higher  $g$ .

<sup>14</sup>Reference 5, Eqs. (11.112) and (11.118), and Ref. 6, Eqs. (8.331) and (8.332).

<sup>15</sup>This holds for  $g < 3$ , as we can easily confirm by comparing the graph of Eq. (30) with Fig. 5. For larger values of  $g$  the approximation itself is invalid for the ground state. Incidentally, Eq. (29) has solutions for negative  $n$ , but these are spurious, because they violate the assumption  $\kappa\epsilon \ll 1$ .

<sup>16</sup>The limiting case  $g=0$  is obviously problematic—indeed,  $K_0(z)$  has no zeros for positive  $z$ . For  $|z| \ll 1$ ,  $\Gamma(1+z) \approx 1-Cz$ , where  $C=0.577\,215$  is Euler’s constant, so for small  $g$   $\arg \Gamma(1+ig) \approx -Cg$ , and Eq. (30) is replaced by  $\kappa_n=(2/\gamma\epsilon)\exp(-n\pi/g)$ , where  $\gamma \equiv \exp(C)=1.781\,072$ . See Ref. 6, Eq. (8.321.1), and p. xxviii.

<sup>17</sup>We used the identity  $H_{ig}^{(2)}(x)=[H_{-ig}^{(1)}(x)]^*=e^{-\pi g}[H_{ig}^{(1)}(x)]^*$  (valid for real  $x$ )



- and real  $g$ ). See Ref. 6, p. 969.
- <sup>18</sup>We used Ref. 6, Eq. (8.405.1), to express  $H_\nu^{(1)}$  in terms of  $J_\nu$  and  $N_\nu$ , Eq. (8.440) to approximate  $J_\nu$ , Eq. (8.443) to approximate  $N_\nu$ , and Eq. (8.332.3) to eliminate  $\Gamma(1-ig)$ .
- <sup>19</sup>Reference 6, Eqs. (8.331) and (8.332.1).
- <sup>20</sup>Reference 6, Eqs. (8.441.1) and (8.444.1), and p. xxviii.
- <sup>21</sup>Note that this is a *correlated* limit in which  $\epsilon$  and  $g$  both go to zero in such a way as to hold  $\kappa_1$  in Eq. (42) fixed. This is *not* the same as going straight to  $g=0$  and then letting  $\epsilon \rightarrow 0$  [Eq. (41)], which only reproduces the limiting value  $\pi/4$ .
- <sup>22</sup>This is not the only way to tame the  $1/x^2$  potential. Other regularizations have been proposed. See, for example, C. Schwartz, "Almost singular potentials," J. Math. Phys. **17**, 863–867 (1976); H. E. Camblong, L. N. Epele, H. Fanchiotti, and C. A. Garca Canal, "Dimensional transmutation and dimensional regularization in quantum mechanics, I. General theory," and "II. Rotational invariance," Ann. Phys. **287**, 14–100 (2001). Our approach follows Ref. 4. It is important in principle to demonstrate that all regularizations lead to the same physical predictions. If they do *not*, the theory is non-renormalizable and there is very little that can be done with it.
- <sup>23</sup>Of course, if we could detect *several* bound states, or measure the phase shifts at sufficiently high energy, then we could map out any departures from the  $1/x^2$  potential; renormalization offers a means for doing so. By the way, something very similar happens in quantum electrodynamics, where the theory, naively construed, yields an infinite mass for the electron. The introduction of a cutoff renders the mass finite but indeterminate. We take the *observed* mass of the electron as *input* and use it to eliminate any explicit reference to the cutoff. The resulting renormalized theory has been spectacularly successful, yielding by far the most precise (and precisely confirmed) predictions in all of physics.
- <sup>24</sup>The classic example of an anomaly is the decay of the neutral pion,  $\pi^0 \rightarrow \gamma + \gamma$ , which could not occur without the breaking of chiral symmetry.
- <sup>25</sup>See, for instance, E. Zeidler, *Applied Functional Analysis: Applications to Mathematical Physics* (Springer, New York, 1997), pp. 116–117.
- <sup>26</sup>Note the logical structure here: We choose  $\mathcal{D}_A$ , but  $\mathcal{D}_A^\dagger$  is then *determined*—it is the space of functions  $\phi$  (in  $L_2$ ) such that if  $\psi$  is in  $\mathcal{D}_A$  then Eq. (52) holds.
- <sup>27</sup>H. Weyl, "Über gewöhnliche Differentialgleichungen mit Singularitäten und die zugehörigen Entwicklungen willkürlicher Funktionen," Math. Ann. **68**, 220–269 (1910); J. von Neumann, "Allgemeine Eigenwerttheorie Hermitescher Funktionaloperatoren," *ibid.* **102**, 49–131 (1929); M. H. Stone, "On one-parameter unitary groups in Hilbert space," Ann. Math. **33**, 643–648 (1932).
- <sup>28</sup>N. I. Akhiezer and I. M. Glazman, *Theory of Linear Operators in Hilbert Space* (Dover, New York, 1993); M. Reed and B. Simon, *Methods of Modern Mathematical Physics* (Academic, London, 1975); G. Hellwig, *Differential Operators of Mathematical Physics* (Addison-Wesley, Reading, MA, 1964).
- <sup>29</sup>G. Bonneau, J. Faraut, and G. Valent, "Self-adjoint extensions of operators and the teaching of quantum mechanics," Am. J. Phys. **69**, 322–331 (2001).
- <sup>30</sup>V. S. Araujo, F. A. B. Coutinho, and J. F. Perez, "Operator domains and self-adjoint operators," Am. J. Phys. **72**, 203–213 (2004).
- <sup>31</sup>There exist pathological functions that are square-integrable and yet do not go to zero at infinity, but there is no penalty for excluding them here. See, for example, D. V. Widder, *Advanced Calculus* (Dover, New York, 1998), 2nd ed., p. 325.
- <sup>32</sup>We assume here that  $\alpha < 1/4$ ; for  $\alpha > 1/4$  we could run the same argument using  $\psi = \phi = u_+$  to obtain the same result.
- <sup>33</sup>More explicitly, functions in  $\mathcal{D}_H$  vanish if  $0 \leq x \leq \epsilon$  or  $x \geq \tau$  for arbitrarily small  $\epsilon$  and arbitrarily large  $\tau$ .
- <sup>34</sup>We follow the treatment in Ref. 30, where the special case  $\alpha = 1/4$  is posed as an exercise.
- <sup>35</sup>Of course, the eigenvalues of a *Hermitian* operator are real, so  $\phi_+$  and  $\phi_-$  cannot be in  $\mathcal{D}_H$ ; rather, the eigenfunctions we seek lie in  $\mathcal{D}_{H^\dagger}$ .
- <sup>36</sup>Mathematicians usually take  $\eta = 1$ , but this choice offends the physicist's concern for dimensional consistency. In any case, it combines with other arbitrary constants at the end.
- <sup>37</sup>This approximation assumes  $\text{Re}(ig) > -1/2$ , which is fine as long as  $\alpha > 0$  (the potential is attractive). It is of some interest to explore self-adjoint extensions of the *repulsive*  $1/x^2$  potential, but we shall not do so here.
- <sup>38</sup>Here  $x_0$  is simply a convenient packaging of the arbitrary constants  $m$ ,  $A_\pm$ ,  $\lambda$ , and  $\eta$ . It is clear from Eq. (73) [if not from Eq. (74)] that  $x_0$  carries the dimensions of length, and hence the choice of a particular self-adjoint extension entails breaking the scale invariance that led to all the difficulties in Sec. II.
- <sup>39</sup>This case violates our assumption in Ref. 37, so it should be taken with a grain of salt. See Ref. 30, Example 1, for a more rigorous analysis.
- <sup>40</sup>This result agrees with Eq. (80) of Ref. 30, with  $r \rightarrow x$  and  $\varphi \rightarrow \psi/x$ .
- <sup>41</sup>The term "self-adjoint extension" is potentially misleading, because at first sight it appears to involve a *contraction*, not an expansion, of the domain. The point is that you must start out with a *Hermitian* operator, and  $H$  is not Hermitian with respect to the set of functions that satisfy the boundary condition  $\psi(0) = 0$ . That is why we first had to *restrict* the domain (see Ref. 33), and the "extension" is with respect to that much more limited domain.
- <sup>42</sup>By changing the boundary conditions it could be argued that we are radically altering the physical system, albeit at a single point. The process is analogous (in some cases identical) to adding a delta function to the potential, and it is hardly surprising that this changes the spectrum of allowed states. But the question was whether there is *anything* we could do to salvage the  $1/x^2$  potential, and if the remedy is necessarily radical, so be it.
- <sup>43</sup>C. Zhu and J. R. Klauder, "Classical symptoms of quantum illnesses," Am. J. Phys. **61**, 605–611 (1993); N. A. Wheeler, "Relativistic classical fields," unpublished notes, Reed College, 1973, pp. 246–251.
- <sup>44</sup>J.-M. Lévy-Leblond, "Electron capture by polar molecules," Phys. Rev. **153**, 1–4 (1967).
- <sup>45</sup>M. H. Mittleman and V. P. Myerscough, "Minimum moment required to bind a charged particle to an extended dipole," Phys. Lett. **23**, 545–546 (1966); W. B. Brown and R. E. Roberts, "On the critical binding of an electron by an electric dipole," J. Chem. Phys. **46**, 2006–2007 (1966).
- <sup>46</sup>C. Desfrancois, H. Abdoul-Carime, N. Khelifa, and J. P. Schermann, "From  $1/r$  to  $1/r^2$  potentials: Electron exchange between Rydberg atoms and polar molecules," Phys. Rev. Lett. **73**, 2436–2439 (1994); Coon and Holstein (Ref. 1); many articles by H. E. Camblong and collaborators, especially "Quantum anomaly in molecular physics," Phys. Rev. Lett. **87**, 220402-1–4 (2001).