Almost singular potentials*

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Explicit solutions are constructed for the lowest bound states of the Schrödinger equation with an attractive potential that behaves typically as $r^{-2+\epsilon}$ at the origin. The energy levels and wavefunctions, which depend on the small parameter ϵ in a nonanalytic way, show some interesting properties; and some relations between this model and aspects of elementary particle physics are noted.

REVIEW OF SINGULAR POTENTIALS

In the usual study of the Schrödinger equation, in a state of orbital angular momentum l (in units with $\hbar^2/2m=1$),

$$\left(-\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr}+\frac{l(l+1)}{r^2}+V(r)-E\right)R_l(r)=0, \quad (1)$$

we have the boundary condition at the origin

$$R_l(r) \underset{r\to 0}{\to} \text{const} \times r^l. \quad (2)$$

In order to make this selection, and to discard the solution which behaves as r^{-l-1}, it is necessary to assume that

$$r^2V(r) \underset{r\to 0}{\to} 0; \quad (3)$$

that is, that the kinetic energy term dominates the potential energy term as r goes to zero. If the potential should be more singular than $1/r^2$ at the origin, then we must investigate the equation more carefully: If this singular potential is repulsive, then we conclude that the correct solution to Eq. (1) does go to zero at the origin, but in some fashion different from (2), and we can proceed to do the usual sort of bound state and scattering calculations; however, if this singular potential is attractive at the origin, we are unable to make any sensible solution to the equation. This latter situation may be described by saying that the potential has an infinite number of bound states going down to $E=-\infty$.

The borderline case, which we will study in detail, involves the potential

$$V(r) \underset{r\to 0}{\to} -g/r^2. \quad (4)$$

If we put this into Eq. (1) and postulate the behavior

$$R_l(r) \underset{r\to 0}{\to} r^s, \quad (5)$$

we get the indicial equation

$$-s(s+1)+l(l+1)-g=0 \quad (6)$$

with the solutions

$$s^{\pm}=-\tfrac{1}{2}\pm[(l+1/2)^2-g]^{1/2}. \quad (7)$$

We see that there is a critical value of the coupling strength,

$$g^*=+(l+\tfrac{1}{2})^2, \quad (8)$$

such that if $g<g^*$, the root s^+ describes the allowed solution and the root s^- describes the improper solution—and everything is normal. However, if $g>g^*$, then then the two roots s are a pair of complex conjugate numbers

$$s^{\pm}=-\tfrac{1}{2}\pm i\sigma \quad (9)$$

and there is no apparent way to select the "good" from the "bad" solutions. This situation is frequently described by saying that we now have a continuous spectrum (instead of a discrete spectrum for bound states), due to the loss of our boundary condition at the origin. Some insight into what has happened can be gained by looking at the wavefunction;

$$R_l(r)\sim a_+r^{-1/2+i\sigma}+a_-r^{-1/2-i\sigma}$$
$$\sim Ar^{-1/2}\sin(\sigma\ln r+\phi). \quad (10)$$

As we trace this function down to $r=0$, starting from any finite value of r, we see that it has an infinite number of nodes; and its value at $r=0$ is not defined, although this wavefunction is still normalizeable in the usual sense. The number of nodes in the solution to Schrödinger's equation at any given energy E is the number of bound states that exist at energies below E; thus we see here that there must be an infinity of bound states below any value of E (the energy level spectrum is bottomless, as well as topless).

In an attempt to make some sense out of this situation, Case[1] applied the condition that two solutions of the Schrödinger equation, belonging to different energy eigenvalues, must be orthogonal. This is equivalent to requiring that the Hamiltonian must be a Hermitian operator, acting upon the proper wavefunctions. He thus derived the condition, for any two solutions R and R',

$$\lim_{r\to 0} r^2\left(R\frac{d}{dr}R'-R'\frac{d}{dr}R\right)=0. \quad (11)$$

With solutions of the form given by Eq. (10) this condition reads

$$AA'\sigma\sin(\phi-\phi')=0, \quad (12)$$

and this is satisfied by requiring the phase angle ϕ to be the same for all states. This gives a discrete bound state spectrum, but the number of bound states is still infinite; furthermore, there is no way to determine the phase angle ϕ.

By taking the complete potential to be $-g/r^2$, the Schrödinger equation can be exactly solved in terms of Bessel functions, and Case showed that the resulting energy level formula was

$$E = E_0 \exp(-2n\pi/\sigma), \qquad (13)$$

where E_0 is a negative constant—depending on the angle ϕ and thus arbitrary—and the quantum number n is any positive or negative integer or zero. $\{E_0 = -2\exp[2(\phi - \theta)/\sigma]$, where θ is the phase of the gamma function of argument $1 - i\sigma\}$.

In addition to the infinity of bound states at energies approaching minus infinity ($n \to -\infty$), the $1/r$ potential also has an infinity of bound states as the energy approaches zero, from below ($n \to +\infty$). These are really two distinct phenomena: The first arises from the singular nature of the potential at short distances; the second arises from the very long tail of the potential at large distances (reminiscent of the Coulomb potential). Only the first situation—the short distance singularity—is of interest to us here; we shall imagine that the potentials we are interested in fall off faster at large distances so that there is a discrete cutoff to the bound states as the binding energy lessens.

Other attempts have been made to handle the difficulty at $r = 0$ [2] but all these methods are artificial, and we generally conclude that the potentials, singular as $1/r^2$, cannot be sensible if the strength exceeds the critical value g^*.

The situation of a marginally singular equation, such as the $1/r^2$ potential in the Schrödinger equation, will occur in any differential equation when the number of inverse powers of coordinate in the differential operator is equalled by the number of inverse powers of the coordinate in the potential. Thus this situation can be found in the Dirac equation with a Coulomb potential, in the Klein–Gordon equation with a Coulomb potential,[1] and in several models of the Bethe–Salpeter equation.[3,4]

It is sometimes said that there is a correspondence between marginally singular equations and renormalizable field theories. It is not clear precisely what is meant by this statement, but the analogy is probably that, as was shown by Case's work, the divergence difficulties in this marginally singular case can be summarized in a single parameter.

ALMOST SINGULAR POTENTIALS

In this paper we will study a Schrödinger equation model in which the potential is mathematically rigged so as to be not singular, but with a small parameter which will allow us to approach as a limit the marginally singular situation. Two explicit forms for this are

$$\text{Model I:}\quad V = \frac{-g}{r^2}\left(\frac{r}{r_0}\right)^{\epsilon}, \qquad (14)$$

$$\text{Model II:}\quad V = \frac{-g}{r^2}\left[1 + \epsilon \ln\left(\frac{r}{r_0}\right)\right], \qquad (15)$$

$$\epsilon \to 0+ .$$

No standard perturbation theory (expansion in power series in ϵ) will work here because of the singular nature of the perturbing operators. Expressed another way, the resulting formulas will not be analytic functions about $\epsilon = 0$, and it is just from this nonanalytic behavior that some of the most interesting features of this model flow.

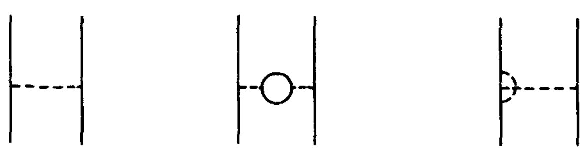
The motivation for studying these models actually is based on more than just a mathematical game. According to quantum field theory, potentials arise from the exchange of virtual quanta. Thus, the exchange of a spin zero quantum of mass μ is described by the propagator

$$1/(q^2 - \mu^2 + i\epsilon), \qquad (16)$$

where q is the 4-vector momentum transfer. Making the Fourier transform to coordinate space, we get a potential which behaves like $\exp(-\mu R)$ for large R (R is the space–time distance between the two interacting particles), and behaves like $1/R^2$ for small distances.

If one performs a time average on this relativistic potential, the result is the familiar Yukawa potential $\exp(-\mu r)/r$. Letting μ become zero, one has the familiar Coulomb potential. Since we are chiefly interested in behavior at small distances in coordinate space, we want to concentrate on the large q behavior in momentum space.

The single-quantum exchange is only the lowest order field theory approximation to the complete interaction of particles. The following are two familiar diagrams from quantum electrodynamics, carried to a higher order of approximation:



The first diagram, single photon exchange, gives the momentum space potential $\sim 1/q^2$. The second diagram is a vacuum polarization correction and the third is a vertex correction. These contributions to the interaction have been calculated, and, if one looks at the high q behavior of the well known results,[5] they give correction factors to the single photon exchange of

$$\left[1 + \frac{\alpha}{3\pi}\ln\left(\frac{-q^2}{m^2}\right)\right] \quad \text{and} \quad \left[1 - \frac{\alpha}{\pi}\ln\frac{m}{\lambda}\ln\left(\frac{-q^2}{m^2}\right)\right] \text{ resp.} \qquad (17)$$

Looking at the Fourier transforms of these functions, we see that the improved field theory potential behaves at small distances as

$$V \sim \frac{\text{const}}{R^2} + \text{const}' \times \frac{\ln R}{R^2}, \qquad (18)$$

which is like our Model II, Eq. (15). Another convenient field theory model is fixed source meson theory. Here one calculates the time independent potential between two sources by usual Schrödinger perturbation theory methods. In second order one gets the usual Yukawa potential, behaving like $1/r$ at small r. In fourth order one finds terms which behave like $(\ln r)/r$; and in sixth order we have found terms that behave like $(\ln r)^2/r$. (If one has purely scalar coupling in this fixed source model, then all these more exotic potential terms cancel out and the pure Yukawa formula is exact. However, with inclusion of spin and/or isotropic spin couplings, then, these new potential terms do survive.)

It is an interesting question to ask what the exact small distance behavior of the complete (i.e., all orders of perturbation theory) field theoretic potential looks like, and we have no idea what the correct answer is. Our Model I potential (14) may be looked upon as a guess, taken as alternative to the perturbation theory guess of Model II, (15).

SOLUTION OF MODEL I

We will solve for the lowest bound states of Eq. (1) with the potential (14). With the change of variables,

$$r = y^{2/\epsilon}/2\sqrt{-E}, \quad R_l = y^{-(1/\epsilon+1/2)}u, \tag{19}$$

the differential equation becomes

$$\left(-\frac{d^2}{dy^2} + \frac{\{[(2l+1)/\epsilon]^2 - \frac{1}{4}\}}{y^2} + \frac{1}{\epsilon^2}\, y^{4/\epsilon-2}\right)u = \Lambda u, \tag{20}$$

where

$$\Lambda = (4g/\epsilon^2)(2r_0\sqrt{-E})^{-\epsilon}. \tag{21}$$

[For $\epsilon = 1$ this is the transformation that reduces the hydrogen atom to a harmonic oscillator.] This looks like a normal Schrödinger equation, having a very large angular momentum; the effective potential $(1/\epsilon^2)y^{4/\epsilon-2}$ has the following behavior in the limit $\epsilon \to 0$: For $y < 1$ this term vanishes, and for $y > 1$ this term becomes positive infinite. Thus we interpret this like an infinite potential barrier and replace it with the familiar boundary condition

$$u(y=1) = 0. \tag{22}$$

The remainder of the equation is solved in terms of Bessel functions; the boundary condition at $y = 0$ is that u must vanish; and so we get the resulting eigenvalue condition:

$$J_\nu(Z_n) = 0, \tag{23}$$

where

$$\nu = (2l+1)/\epsilon \quad \text{and} \quad Z_n = \Lambda^{1/2}. \tag{24}$$

From Jahnke and Emde[6] we have the following formula for the zeroes of Bessel functions of very large order:

$$Z_n = \nu + C_n\nu^{1/3} + D_n\nu^{-1/3} + O(\nu^{-1}) \tag{25}$$

n	C_n	D_n
1	1.8558	1.0332
2	3.2447	3.1584
3	4.3817	5.7598

Putting these results together, we have the energy eigenvalue formula (for $\epsilon \to 0$)

$$E_n = -\frac{1}{4r_0^2}\exp\left(\frac{2}{\epsilon}\ln\frac{g}{(l+1/2)^2}\right)\exp\left(-\frac{4C_n}{\epsilon^{1/3}(2l+1)^{2/3}}\right). \tag{26}$$

We see that this formula becomes very singular in the limit of $\epsilon = 0$. The first exponential factor, which is the same for all states, establishes the very large numerical *scale* of the eigenvalues. (Note that if g were less than $g^* = (l+\frac{1}{2})^2$, then the sign in this exponent would change and the limit would be $E = 0$ instead of $E = -\infty$.) The second exponential factor gives us the *structure* of the eigenvalue spectrum. This factor also is singular in the limit of $\epsilon = 0$ but not as strongly as the leading factor. The rather bizarre dependence—$\exp(1/\epsilon^{1/3})$—could hardly have been anticipated. Thus we find that not only the depth of the lowest eigenvalues, but their ratios as well are governed by very large pure numbers produced by the mathematics of this problem. Thus, for $l = 0$,

$$E_2/E_1 = \exp(-5.6/\epsilon^{1/3}). \tag{27}$$

SOLUTION OF MODEL II

Now we shall solve for the lowest bound states of Eq. (1) with the potential (15). Here we start with the transformations

$$R_l = r^{-1/2}u, \quad r = xr_1, \quad E = -\lambda/r_1^2, \tag{28}$$

where

$$r_1 = r_0\exp\{-(1/g\epsilon)][g-(l+1/2)^2]\} \tag{29}$$

to get the equation

$$\left(\frac{d^2}{dx} + \frac{1}{x}\frac{d}{dx} + g\epsilon\frac{\ln x}{x^2} - \lambda\right)u = 0. \tag{30}$$

Next we write

$$x = \exp[\eta/(g\epsilon)^{1/3}], \quad \lambda = \exp[-2\mu/(g\epsilon)^{1/3}] \tag{31}$$

to get

$$\left(\frac{d^2}{d\eta^2} + \eta - (g\epsilon)^{-2/3}\exp[2(\eta-\mu)/(g\epsilon)^{1/3}]\right)u = 0. \tag{32}$$

This is looked upon similarly to Eq. (20) in that the last term behaves, in the limit of $\epsilon \to 0$, like an infinite potential barrier at $\eta = \mu$. Therefore, we need only solve the equation

$$\left(\frac{d^2}{d\eta^2} + \eta\right)v(\eta) = 0 \tag{33}$$

with the boundary conditions

$$v(-\infty) = 0, \quad v(\eta = \mu_n) = 0, \tag{34}$$

to get our eigenvalues

$$E_n = -\frac{1}{r_0^2}\exp\left(\frac{2}{g\epsilon}[g-(l+\tfrac{1}{2})^2] - \frac{2\mu_n}{(g\epsilon)^{1/3}}\right) \tag{35}$$

Equation (33) may be solved in terms of Bessel functions; with the required boundary condition at $\eta \to -\infty$ ($r = 0$), we find

$$v = A\eta^{1/2}[J_{1/3}(\tfrac{2}{3}\eta^{3/2}) + J_{-1/3}(\tfrac{2}{3}\eta^{3/2})]. \tag{36}$$

Thus the values μ_n are just the zeroes of this tabulated function. Actually, if one looks at the derivation of the earlier quoted formula (25) for the zeroes of Bessel functions of large order,[7] it is found that the exponential transformation (31) is involved, leading to the same Eq. (33) that we are now studying. The resulting identification is

$$\mu_n = 2^{1/3}C_n \tag{37}$$

in terms of the coefficients given earlier. The energy formulas for the two models are quite similar in structure.

SOLUTION OF A GENERALIZED MODEL

The similarity in results of these two models suggest that we try to solve the generalized almost singular potential,

$$V = -(g/r^2)f(r), \tag{38}$$

where the modifying factor f is very close to unity, except at very small distances. With the transformation $R = r^{-1/2}u$ we write

$$\left(-\frac{1}{r}\frac{d}{dr}r\frac{d}{dr} + U - E\right)u = 0, \tag{39}$$

where

$$U = [(l+1/2)^2 - gf(r)]/r^2. \tag{40}$$

We assume that $g > g^*$ and also that f is such as to make the potential less attractive at very small distances. Thus U is positive at small r and negative at large r. We identify the point where U passes through zero as r_1, and then we write

$$U(r_1) = 0, \quad r = r_1 e^{\theta}, \quad E = -\frac{1}{r_1^2}\exp(-2\lambda), \tag{41}$$

$$\left(\frac{d^2}{d\theta^2} + W(\theta) - \exp[2(\theta - \lambda)]\right)u = 0, \tag{42}$$

where

$$W = -r^2 U = -(l+\tfrac{1}{2})^2 + gf(r_1 e^{\theta}). \tag{43}$$

Now we expand about $\theta = 0$, where U, and therefore W, vanishes:

$$W = \alpha\theta + O(\alpha^2\theta^2). \tag{44}$$

The parameter α is assumed to be very small, as in our previous models it is proportional to ϵ. One more variable change

$$\theta = \eta\alpha^{-1/3}, \quad \lambda = \mu\alpha^{-1/3} \tag{45}$$

and we have

$$\left[\frac{d^2}{d\eta^2} + \eta + O(\alpha^{2/3}\eta^2) - \alpha^{-2/3}\exp\left(\frac{2(\eta-\mu)}{\alpha^{1/3}}\right)\right]u = 0, \tag{46}$$

and so in the limit of $\alpha \to 0$ we have the earlier solution (33), (34).

We can actually do a little bit better by watching more closely what happens around the point $\eta = \mu$, that is, at

$$r = r_1\exp(\mu/\alpha^{1/3}) \equiv r_2. \tag{47}$$

By matching solutions of the equation approaching this barrier from both sides we pick up one more correction term to the energy, and our final formula is

$$E_n = -\frac{1}{r_1^2}\exp\left(-\frac{2^{4/3}C_n}{\alpha^{1/3}} + 2(\ln 2 - C)\right), \tag{48}$$

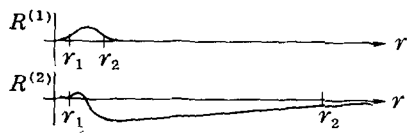
where C is Euler's constant. This formula reproduces the two earlier results as special cases—except for the last factor, which was lacking before.

DESCRIPTION OF THE WAVEFUNCTIONS

The several transformations of variables may obscure the picture of what the eigenfunctions for these deeply bound states look like. The wavefunction goes to zero at the origin and has its first turning point at the very small distance r_1. Then it may oscillate; finally it has its second turning point at r_2 – which is still a very small distance compared to the basic unit of length, r_0, but is a rather large distance compared to r_1 (see (47)). Furthermore the distance r_2 will be very strongly dependent on the quantum number n, for example

$$r_2(\text{for } n=2)/r_2(\text{for } n=1) = \exp(\mu_2 - \mu_1)/\alpha^{1/3}$$

We also note that the tail of the function decays with length r_2. Pictures of the functions will look as follows:



The functions are, of course, orthogonal to one another; but there is a more interesting property contained here. If one should have some reasonably smooth operator (such as a dipole length) and calculate its matrix element between these two states, the result will be a small number—depending on the ratio of the distances r_2—due to the great disparity in the spatial extent of the two wavefunctions.

Thus a transition rate between the nth state and the mth state (m less than n) would be characterized by the small number:

$$G^2 = \left[\frac{r_2^{(m)}}{r_2^{(n)}}\right]^3 \xrightarrow{m=1,n=2} \exp\left(\frac{-5.25}{\alpha^{1/3}}\right),$$

$$\alpha = 10^{-1}, \quad G^2 \approx 10^{-5}$$

$$\alpha = 10^{-2}, \quad G^2 \approx 10^{-11},$$

$$\alpha = 10^{-3}, \quad G^2 \approx 10^{-23}.$$

CONCLUSIONS

This study of almost singular potentials in the Schrödinger equation has led to some interesting results and suggests some interesting ideas for future study. The small parameter built into the model (called ϵ or α) allows us to construct solutions without introducing a cutoff or similar device; the answers can be expanded for small values of this parameter, although it is not a power series expansion. The resulting energy level spectrum is characterized by very large numbers—resulting from an exponentiation of the small parameter originally introduced—and the same is found for the overlap of the wavefunctions that would occur in any calculation of transition probabilities under some external interaction. These general features are characteristic of the basic properties of elementary particles: large ratios of masses (as between baryons and leptons) and severe heirarchy of interactions (strong, weak).

A next step should be to explore the behavior of almost singular potentials in the context of some relativistic equations, rather than the Schrödinger equation. One immediate problem will be the following: in the above study the energy E took on very large negative values;

in relativistic calculations (for example, in the Klein–Gordon equation) the analogous role is played by the quantity $E^2 - m^2$ and one does not know what to say about states with negative values of E^2.

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