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Separability of the Planar $1/\rho^2$ Potential in Multiple Coordinate Systems

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Abstract: With a number of special Hamiltonians, solutions of the Schrödinger equation may be found by separation of variables in more than one coordinate system. The class of potentials involved includes a number of important examples, including the isotropic harmonic oscillator and the Coulomb potential. Multiply separable Hamiltonians exhibit a number of interesting features, including “accidental” degeneracies in their bound state spectra and often classical bound state orbits that always close. We examine another potential, for which the Schrödinger equation is separable in both cylindrical and parabolic coordinates: a z -independent $V \propto 1/\rho^2 = 1/(x^2 + y^2)$ in three dimensions. All the persistent, bound classical orbits in this potential close, because all other orbits with negative energies fall to the center at $\rho = 0$. When separated in parabolic coordinates, the Schrödinger equation splits into three individual equations, two of which are equivalent to the radial equation in a Coulomb potential—one equation with an attractive potential, the other with an equally strong repulsive potential.

Keywords: separation of variable; parabolic coordinates; Schrödinger equation

1. Introduction

There are certain special Hamiltonians for which the Schrödinger equation is separable in more than one coordinate system. The spectra of these Hamiltonians exhibit what are known as “accidental” degeneracies, and a number of the Hamiltonians are extremely important. Well-known examples of systems that are separable in more than one set of coordinates include the free particle (separable in any coordinates for which the Robertson condition is satisfied [1,2]), the three-dimensional isotropic harmonic oscillator (separable in spherical, ellipsoidal, cylindrical, and rectangular coordinates), the Coulomb potential (separable in spherical, prolate ellipsoidal [3], and parabolic coordinates), and the constant magnetic field (separable in rectangular or cylindrical coordinates, depending on the gauge, but in either case with a free choice of the location of the origin). All these examples are also well known for the degeneracies present in their spectra. A slightly less well-known system is a particular anisotropic harmonic oscillator, with potential

$$V(\vec{r}) = \frac{1}{2}M\omega_0^2(x^2 + y^2 + 4z^2) = \frac{1}{2}M\omega_0^2(r^2 + 3z^2). \quad (1)$$

This is a special case of the kinds axially-symmetric harmonic oscillator potentials that are frequently useful in the modeling of molecular vibrations in the presence of external fields [4,5]. (Asymmetric oscillators may also be modeled by an extension of the harmonic oscillator formalism to a non-integral number of effective dimensions [6].)

The fact that the energy spectrum with the specific potential (1) possesses accidental degeneracy is obvious; however, it is not as well known that, just like the Coulomb problem, this potential

problem is separable in parabolic coordinates. Separability in parabolic coordinates is guaranteed if the Hamiltonian involves just a standard nonrelativistic kinetic term and a potential V of the form

$$V(\vec{r}) = \frac{1}{r} [f(\eta) + g(\xi)], \quad (2)$$

for some functions f and g . The quantities η and ξ are two of the parameters of the parabolic coordinate system (η, ξ, ϕ) , where [7]

$$\eta = r + z \quad (3)$$

$$\xi = r - z. \quad (4)$$

(Surfaces of constant η or ξ are orthogonal paraboloids of revolution, each with its focus at the origin.) For the anisotropic harmonic oscillator (1), the two functions are $f(s) = g(s) = \frac{1}{4}M\omega_0^2 s^3$. The use of parabolic coordinates in the Coulomb problem is also especially convenient for dealing with the Stark effect. While the Hamiltonian remains separable in spherical coordinates when an external magnetic field is applied, it remains separable in the parabolic coordinates with a external electric field present.

Classically, all the potentials we have mentioned with accidental degeneracy are well known for another feature: all their bound orbits close. In this paper, we shall look at another potential that, in a sense, shares this classical feature. Bertrand's theorem is normally taken to hold that the only two central potentials for which all the bound orbits close are the attractive Coulomb potential and the isotropic harmonic oscillator potential. However, this is not quite accurate; there are other examples of potentials with the stated property, but they are typically discounted because they do not have a full spectrum of bound states. For example, all the bound orbits in a constant potential, which exerts no force, close—precisely because there are no bound states. A system with a charged particle in a constant magnetic field also evades the strong restriction imposed by Bertrand's Theorem [8], as the force in this instance is not derived from a central potential. The orbits in the magnetic field are right circular helices. The velocity parallel to the magnetic field is a constant of the motion; only when the velocity in that direction vanishes are the orbits truly bound—in which case they are closed circles. The potential considered in this paper is in a similar category to the two examples just mentioned. We shall see that the attractive $V \propto 1/\rho^2$ potential possesses few bound orbits (for an appropriate interpretation of the meaning of “bound”), but those that it does possess are circular, with exactly zero energy (as expected from the virial theorem).

Separability of the Schrödinger equation in a given set of coordinates means that the energy of a given state may be expressed as a function of three quantum numbers, one corresponding to each coordinate. If separations in multiple coordinate systems are possible, there must be multiple formulas for the energy, based on different sets on quantum numbers. The eigenstates with fixed quantum numbers are generally different in different coordinates; an eigenfunction in one coordinate must be a linear combination of eigenfunctions in the other coordinates. The only way this is possible for an energy eigenstate is if there are multiple eigenstates with exactly the same energy. This shows why separability in multiple coordinate systems requires the presence of accidental degeneracy. Moreover, it is worth noting that the same argument can be applied even to the degeneracy of system with a generic central potential $V(r)$, which is separable in spherical coordinates only. A system with angular momentum ℓ possesses a $(2\ell + 1)$ -fold degeneracy, which is actually related to the fact that the spherical coordinates may be chosen with their polar axis pointing in any direction. The Schrödinger equation is thus separable in an infinite number of different spherical coordinate systems.

However, the existence of accidental degeneracy does not absolutely require that a system be separable in multiple coordinate systems. Any anisotropic three-dimensional harmonic oscillator for which the frequencies of the motions along the three coordinate directions are rational multiples will have classical orbits that eventually close and degeneracies in its quantum mechanical spectrum.

Therefore, there are systems for which the degeneracy is seemingly too “sporadic” to be indicative of any deeper underlying symmetry principle at work.

The existence of alternative bases of quantum numbers is also related, of course, to the existence of additional observables that commute with the Hamiltonian. For the spherical harmonic oscillator and the Coulomb potential, these extra conserved quantities are well known. The harmonic oscillator has separate, commuting Hamiltonians governing the motion along the three orthogonal axes. For the Coulomb problem, there is the Runge–Lenz vector, which points out the direction of the major axis of a bound state elliptical orbit. For the free particle, with its extensive degeneracy, the additional conserved quantity is the momentum itself. Using the algebras generated with the inclusion of any of these conserved quantities, it is possible to determine the bound state spectra of these problems using operator algebra alone.

In the Coulomb problem, part of the accidental degeneracy associated with the additional operators that commute with the Hamiltonian persists even in the relativistic Dirac theory, although the separability in parabolic coordinates actually does not carry over. Another potential, albeit a potential in only one dimension, that is also amenable to similar operator methods is the $V = V_0 \operatorname{sech}^2 ax$ potential; the eigenstates for potentials of different depths V_0 are related by operators [9], and as with the other potentials solvable by operator methods, the operators involved may be interpreted as elements of a $(0 + 1)$ -dimensional supersymmetry algebra [10–13]. (An excellent introductory treatment of quantum-mechanical supersymmetry, especially as applied to the Coulomb problem, may be found in the lecture notes [14].) The harmonic oscillator, Coulomb, and $\operatorname{sech}^2 ax$ potentials just mentioned are all among the shape-invariant potentials, and the main object of study in this paper will be yet another such one. There are a wide variety of mathematical tools that may be useful for solving and addressing questions about these shape-invariant potentials [15,16].

The harmonic oscillator and Coulomb systems are also known for the fact that certain classical and semiclassical approximations yield exact results when applied to these systems. The Bohr–Sommerfeld quantization rule derived from the Wentzel–Kramers–Brillouin (WKB) approximation gives the exact energies for a harmonic oscillator system in one dimension—and thus also for an isotropic or anisotropic harmonic oscillator in any number of dimensions. Harmonic oscillators also have coherent states, with the zero-point uncertainties in position and momentum added onto a classically orbiting wave function centroid. For the Coulomb potential, there is the fact that the full nonperturbative scattering cross section is the same as the cross sections derived classically or from the first-order Born approximation. Moreover, for the $V = V_0 \operatorname{sech}^2 ax$ potential also, a certain approximation is exact; the potential is reflectionless, so the classical reflection coefficient is always precisely correct. The exact successes of these various approximations are highly appealing features of these special potential types, although it is not clear whether we should expect anything similar when dealing with more esoteric multiply separable potentials.

This paper will examine the $1/\rho^2 = 1/(x^2 + y^2)$ potential in three spatial dimensions. The attractive version of the potential has been observed physically, in the interaction of a long charged wire with a polarizable atoms and molecules [17–19]. For an atom with polarizability α in a spatially slowly varying external electric field \vec{E}_0 , the interaction energy is $-\frac{1}{2}\alpha\vec{E}_0^2$. When the atom is exposed to the electrostatic field of a charged wire carrying linear charge density λ , the $\vec{E}_0 = \frac{2\lambda}{\rho}\hat{\rho}$ behavior of the field gives rise to an effective potential

$$V = -\frac{2\alpha\lambda^2}{\rho^2}. \quad (5)$$

The organization of this paper is as follows. Section 2 introduces the features that make the $1/\rho^2 = 1/(x^2 + y^2)$ potential special classically. Finding analytical solutions of the equations of motion is easy, and there are relatively few bound, stable orbits, but those that do exist close. The simplicity of the classical problem leads us to suspect that the corresponding quantum mechanical theory may also exhibit special properties.

In Section 3, we demonstrate that the Hamiltonian with a $1/\rho^2$ potential belongs to the elite family that are separable in multiple coordinate systems—cylindrical and parabolic, in this case. The scattering state wave functions of this potential in two space dimensions have already been studied [20], but it is only with the inclusion of the third dimension that the dual separations become possible. Therefore, new symmetry phenomena are expected to be found in the three-dimensional axisymmetric potential, although it is not really clear in advance what special behavior could be expected. If the potential possessed bound states, we would expect them to have additional degeneracies. However, the attractive $1/\rho^2$ potential does not support a stable spectrum of bound negative-energy states; the attractive singularity at $\rho = 0$ is too strong. On the other hand, for the repulsive $1/\rho^2$ potential, we have identified a number of special features, which are discussed in Section 4. Our conclusions are summarized in Section 5.

2. Classical Features of the $1/\rho^2$ Potential

Central potential problems in three (or more) dimensions may be reduced to two-dimensional problems using the conservation of angular momentum. The differential equation for the orbital curve $r(\phi) = [u(\phi)]^{-1}$ then has the simple, well-known form

$$\frac{d^2 u}{d\phi^2} = -u - \frac{M}{L^2 u^2} F\left(\frac{1}{u}\right), \quad (6)$$

where $F(r) = -dV/dr$ is the radial force. The u term on the right-hand side of (6) corresponds to the centrifugal term in the effective potential governing the radial motion. For potentials $V \propto r^n$, the orbital shape can be expressed in terms of elementary trigonometric functions for $n = 2, 0, -1$, or -2 [8]. These are, respectively, the harmonic oscillator, the free particle, the Coulomb potential, and the inverse square potential of interest here. For certain other integral and rational values of the exponent n , the solutions may be expressed in terms of elliptic, hypergeometric, or other progressively more general functions.

Because it is straightforward to reduce the central force problem from three to two dimensions, there is very little practical difference at the classical level between computations with a three-dimensional central potential $V(r)$ and the two-dimensional analog $V(\rho)$. (The same cannot be said in quantum mechanics though; for example, a two-dimensional attractive potential always possesses at least one bound state, but in three dimensions the bound state need not be present.) The classical radial equation of motion in two-dimensional space, with a potential $V(\rho) = \kappa/\rho^2$, using the effective potential (depending on the angular momentum $L = L_z$), is

$$M \frac{d^2 \rho}{dt^2} = -\frac{d}{d\rho} \left(\frac{\kappa}{\rho^2} + \frac{L^2}{2M\rho^2} \right) \quad (7)$$

$$= \frac{2\kappa + L^2/M}{\rho^3}. \quad (8)$$

This is clearly just as solvable with $\kappa \neq 0$ as it is for the free particle ($\kappa = 0$) case. The equation for the orbital curve is correspondingly

$$\frac{d^2 u}{d\phi^2} = -\left(1 + \frac{2\kappa M}{L^2}\right) u. \quad (9)$$

The full solutions in three dimensions are simply the two-dimensional (ρ, ϕ) motion superimposed upon uniform motion in the z -direction, $z(t) = z(0) + \dot{z}(0)t$. The classical approach we are using corresponds to the solution of the Schrödinger problem in cylindrical coordinates.

The nature of the solutions for $\rho(\phi) = [u(\phi)]^{-1}$ depends on the sign of $1 + 2\kappa M/L^2$, and thus on the sign of κ . If $\kappa > 0$, the coefficient in parentheses on the right-hand side of (9) is automatically positive. The only possible trajectories in this repulsive potential are scattering orbits

$$\rho = A \sec \left(\sqrt{1 + 2\kappa M/L^2} \phi + \delta \right). \quad (10)$$

In a coordinate system with the phase angle $\delta = 0$, the radial coordinate diverges at $\phi = \pm \pi/2\sqrt{1 + 2\kappa M/L^2}$, corresponding to a classical scattering angle

$$\varphi_{\text{scat}} = \pi \left| 1 - \frac{1}{\sqrt{1 + 2\kappa M/L^2}} \right|, \quad (11)$$

which depends on the angular momentum, but not separately on the energy—a consequence of the scale invariance of the problem. This expression can also be cast in terms of the impact parameter b in the xy -plane, via $L = \sqrt{2M\mathcal{E}'}b$, where $\mathcal{E}' > 0$ is the energy of the in-plane motion (so that the total energy is $\mathcal{E} = \mathcal{E}' + \frac{1}{2}M\dot{z}^2$). For attractive potentials with $\kappa < 0$, there are similar scattering orbits when the energy is positive (which means $L^2 > 2|\kappa|M$). The scattering angle is again given by (11); the absolute value present in that formula, which was superfluous for the repulsive potential, is needed in the attractive case to give a non-negative φ_{scat} .

The angle φ_{scat} represents the scattering angle in the xy -plane. When the uniform motion in the third dimension is included, it is also possible to describe the total scattering angle ϑ_{scat} . As the potential in three dimensions is not spherically symmetric, the scattering behavior does not depend solely on an impact parameter (or equivalently, for fixed energy, on an angular momentum). Instead, we shall describe the incoming trajectory of a particle by a direction $\hat{\Theta}$, together with the angular momentum component $L = L_z$. Choosing an appropriate orientation for the x and y coordinates, $\hat{\Theta}$ is

$$\hat{\Theta} = \frac{1}{\sqrt{2\mathcal{E}'/M + \dot{z}^2}} \left(\sqrt{2\mathcal{E}'/M} \hat{x} + \dot{z} \hat{z} \right). \quad (12)$$

The z -axis around which the potential $V(\rho)$ is symmetric and the incoming trajectory (along which the particle would travel if it were not deflected) are generally skew lines. Their distance of closest approach to one another is given by the in-plane impact parameter $b = L/\sqrt{2M\mathcal{E}'}$. After the scattering, the in-plane component of the velocity has been rotated through an angle $\pm\varphi_{\text{scat}}$, making the outgoing direction vector

$$\hat{\Theta}' = \frac{1}{\sqrt{2\mathcal{E}'/M + \dot{z}^2}} \left(\sqrt{2\mathcal{E}'/M} \cos \varphi_{\text{scat}} \hat{x} \pm \sqrt{2\mathcal{E}'/M} \sin \varphi_{\text{scat}} \hat{y} + \dot{z} \hat{z} \right). \quad (13)$$

Therefore, the three-dimensional scattering angle ϑ_{scat} is

$$\vartheta_{\text{scat}} = \cos^{-1} (\hat{\Theta} \cdot \hat{\Theta}') = \cos^{-1} \left(\cos \varphi_{\text{scat}} + \frac{2\dot{z}^2}{2\mathcal{E}'/M + \dot{z}^2} \sin^2 \frac{\varphi_{\text{scat}}}{2} \right), \quad (14)$$

where φ_{scat} is still a function of L or b , according to (11). Naturally, when the motion is planar ($\dot{z} = 0$), this gives $\vartheta_{\text{scat}} = \varphi_{\text{scat}}$. Conversely, when the velocity in the z -direction (which does not change) predominates, $\vartheta_{\text{scat}} \rightarrow 0$.

Apart from the sign difference inside the absolute value in (11), there is another important difference between the attractive and repulsive regimes. When $\kappa > 0$, the scattering angle is limited to the range $0 \leq \varphi_{\text{scat}} < \pi$; the trajectory never crosses itself. In contrast, when $\kappa < 0$, the angle φ_{scat} may be arbitrarily large. When the potential is attractive, the particle may orbit around the center any number of times before it escapes again to infinity. The resulting two-dimensional trajectories cross over themselves repeatedly. This is quite different than the behavior seen in classical Rutherford scattering, in which the trajectories for attractive and repulsive potentials are represented by the two

disjoint branches of the same hyperbola. However, this behavior, with the number of times the orbital curve intersects itself increasing as the total energy approaches zero, is by no means unique to the attractive $1/\rho^2$ potential, but is in fact fairly generic.

The $\kappa < 0$ scattering orbits, with more and more revolutions around the origin as the energy decreases, are approaching the limit of perfectly circular orbits, which occur when the energy vanishes at $L^2 = -2\kappa M$. Any attractive potential will have classical circular orbits. However, for the potential we are interested in, it turns out that these circular orbits are actually the only persistent bound orbits. If the total energy is negative, then the quantity in parentheses in (9) is negative, and the orbital solution $u(\phi)$ becomes a linear combination of equiangular spirals, so that

$$\rho(\phi) = A \operatorname{sech} \left(\sqrt{2|\kappa|M/L^2 - 1} \phi + \delta \right), \quad (15)$$

or

$$\rho(\phi) = A \operatorname{csch} \left(\sqrt{2|\kappa|M/L^2 - 1} \phi + \delta \right), \quad (16)$$

where depending on whether the both endpoints lie at $\rho = 0$ or one at $\rho = 0$ and the other at $\rho = \infty$. Note that all the bound orbits in two dimensions do therefore (in a certain sense) close, because the circular orbits are the only persistent bound orbits.

Alternatively, taking the negative-energy solutions of (9) as linear combinations

$$u(\phi) = B \cosh \left(\sqrt{2|\kappa|M/L^2 - 1} \phi \right) + C \sinh \left(\sqrt{2|\kappa|M/L^2 - 1} \phi \right), \quad (17)$$

$\rho(\phi)$ has the form (15), with both endpoints at the center, if $|B| > |C|$; it has the form (16) if $|B| < |C|$. The intermediate cases, with $B = \pm C$, yields pure inward or outward equiangular spirals. The spirals are also limiting forms of the other expressions, with $\delta \rightarrow \infty$ while $Ae^{-\delta}$ is held finite.

Most generally, for states with $\kappa + L^2/2M < 0$, energy $\mathcal{E}' < 0$, and initial radial velocity inward ($\dot{\rho}(0) \leq 0$ at time $t = 0$), the equation of motion (7) has the implicit solution

$$t = \frac{\rho}{2|\mathcal{E}'|} \sqrt{\frac{2\kappa M + L^2}{\rho^2} - 2M|\mathcal{E}'|} + \frac{M\rho(0)\dot{\rho}(0)}{2|\mathcal{E}'|}. \quad (18)$$

In this regime, the time t_f required for the particle to reach $\rho = 0$ is

$$t_f = \frac{\sqrt{2\kappa M + L^2}}{2|\mathcal{E}'|} - \frac{M\rho(0)|\dot{\rho}(0)|}{2|\mathcal{E}'|} \quad (19)$$

This behavior is known as “falling to the center”. Note that making $\dot{\rho}(0)$ more negative while keeping $\rho(0)$ fixed decreases t_f , which is clearly correct.

3. Two Separations of the Schrödinger Equation

We now turn our attention to the quantum theory. The classical theory with an attractive potential was dominated by the falling to the center. The quantum mechanical wave functions in the presence of the $\kappa < 0$ potential exhibit their own manifestation of this phenomenon. If $\psi(\vec{\rho})$ is an eigenfunction of the two-dimensional time-independent Schrödinger equation (with energy eigenvalue \mathcal{E}'_0), then for any real number α , $\psi(\alpha\vec{\rho})$ is also an eigenfunction, with energy $\alpha^2\mathcal{E}'_0$. Thus, if there is a normalizable eigenstate with energy $\mathcal{E}'_0 < 0$, then there must be eigenstates with arbitrarily negative energies. By compressing the wave function closer to the attractive singularity at $\rho = 0$, the energy may be made as negative as we wish, meaning that there cannot be a stable Hilbert space of quantum states; the energy is not bounded below.

In contrast, when $\kappa > 0$, the energy eigenvalues are always positive. We may still dilate the wave function to decrease its energy, but the energies remain bounded from below by zero; and it is, of course, no surprise that all positive energies are allowed in this scattering system.

It is possible, via one of several renormalization procedures, to let the strength of the attractive $1/r^2$ potential go to zero, in such a way that there is a reasonable physical spectrum (with exactly one bound state) [21–23]. However, the resulting Hamiltonian is not self-adjoint, in spite of it having a naively Hermitian appearance [24]; moreover, the scale invariance of the solutions is broken by an anomaly. Most analyses of the regularized Hamiltonian have focused on the three-dimensional $1/r^2$ potential, although the general character of the solutions appears to be independent of the dimensionality [21,25–27]. Our results in this paper might be extended to this renormalized regime; in fact, it would be very interesting to see how the renormalization would interact with the separation of the Schrödinger equation in parabolic coordinates. However, this regime lies beyond the scope of the present work.

We shall now present separation of variables solutions to the Schrödinger equation for the $1/\rho^2$ potential in both cylindrical and parabolic coordinates. The solution in cylindrical coordinates is quite conventional. It represents a straightforward application of well-known techniques, and the solutions involve the same families of special functions that are commonplace in two-dimensional problems. However, the solution in parabolic coordinates is completely new. It may be surprising that the Schrödinger equation involved is separable in parabolic coordinates at all, particularly as the use of parabolic coordinates breaks the translational symmetry—which plays such an important role in cylindrical coordinates—of the problem. Moreover, the separation solution in parabolic coordinates will also provide insight into an alternative method for solving the classical problem that was considered in Section 2.

3.1. Cylindrical Coordinates

In order to have a quantum theory with well-defined wave functions, without additional regularization of the potential in the vicinity of $\rho = 0$, the potential we shall consider in the remainder of our analysis is

$$V(\vec{r}) = \frac{\hbar^2 K}{2M} \frac{1}{\rho^2}, \quad (20)$$

with repulsive $K > 0$. (The potential strength κ has been rescaled to avoid unnecessary factors of \hbar and M .) With this potential, the Schrödinger equation in cylindrical coordinates is

$$\left[-\frac{1}{\rho} \frac{\partial}{\partial \rho} \left(\rho \frac{\partial}{\partial \rho} \right) - \frac{1}{\rho^2} \frac{\partial^2}{\partial \phi^2} - \frac{\partial^2}{\partial z^2} + \frac{K}{\rho^2} \right] \psi = E \psi, \quad (21)$$

where $E = 2M\mathcal{E}/\hbar^2$, with \mathcal{E} being the total energy. With a separable ansatz,

$$\psi = P(\rho) e^{ikz} e^{im\phi}, \quad (22)$$

this reduces to a single-variable Schrödinger equation for $P(\rho)$,

$$\left[-\frac{1}{\rho} \frac{d}{d\rho} \left(\rho \frac{d}{d\rho} \right) + \frac{m^2 + K}{\rho^2} \right] P = (E - k^2) P. \quad (23)$$

This is just the usual Bessel's equation that arises for a free particle in two dimensions, except with the indices of the Bessel function solutions changed to $\sqrt{m^2 + K}$. (Note that $m^2 + K$ just corresponds to the classical quantity $L_z^2 + 2M\kappa$, measured in units of \hbar^2 .) The general solution is thus

$$P(\rho) = A J_{\sqrt{m^2 + K}}(\sqrt{E - k^2} \rho) + B J_{-\sqrt{m^2 + K}}(\sqrt{E - k^2} \rho). \quad (24)$$

If the Bessel function index $\sqrt{m^2 + K}$ happens to be an integer, the usual replacement of the linearly dependent $J_{-\sqrt{m^2 + K}}$ by the Neumann function $N_{\sqrt{m^2 + K}}$ is required. However, only the Bessel function with positive index is regular at $\rho = 0$ (and thus permitted).

The scattering theory of these solutions is straightforward. The scattering by a three-dimensional $1/\rho^2$ potential is worked out in [28]. One surprising result is that the classical limit only exists for strong potentials, as the classical scattering cross section is linear (never quadratic) in the strength of the potential. The two-dimensional $1/\rho^2$ version is completely analogous, merely using the formalism for partial wave scattering in two dimensions [29]. The partial wave expansion for an incoming plane wave is

$$e^{iqx} = J_0(q\rho) + 2 \sum_{m=1}^{\infty} i^m \cos(m\phi) J_m(q\rho), \quad (25)$$

in terms of the free wave radial functions. The Bessel functions have the limiting behavior $J_\nu(s) = \sqrt{\frac{2}{\pi s}} \cos\left(s - \frac{\nu\pi}{2} - \frac{\pi}{4}\right)$, and the scattering state wave function may be written

$$\begin{aligned} \psi &= e^{iq\rho} + \psi_{\text{scat}} \\ &\rightarrow e^{iq\rho} + \sqrt{\frac{2}{\pi q\rho}} \left[\cos\left(q\rho - \frac{\pi}{4} + \delta_0\right) + 2 \sum_{m=1}^{\infty} i^m \cos(m\phi) \cos\left(q\rho - \frac{m\pi}{2} - \frac{\pi}{4} + \delta_m\right) \right], \end{aligned} \quad (26)$$

where $q = \sqrt{E - k^2}$. The non-free wave functions with $J_{\sqrt{m^2 + K}}(q\rho)$ are simply phase shifted by

$$\delta_m = -\frac{\pi}{2} \left(\sqrt{m^2 + K} - |m| \right). \quad (27)$$

The fact that δ_m is independent of the energy for each partial wave is another consequence of the scale invariance. Moreover, as noted, the classical limit corresponds to $K \gg |m|$.

3.2. Parabolic Coordinates

Unlike the scattering solution in cylindrical coordinates, the solution of the $1/\rho^2$ potential in parabolic coordinates is not a standard problem. A $1/\rho^2$ potential has, however, previously been considered algebraically, as a perturbation added to the Coulomb Hamiltonian (which, as noted above, is also parabolic separable) [30,31].

In parabolic coordinates, the Laplacian is

$$\vec{\nabla}^2 = \frac{4}{\eta + \xi} \frac{\partial}{\partial \eta} \left(\eta \frac{\partial}{\partial \eta} \right) + \frac{4}{\eta + \xi} \frac{\partial}{\partial \xi} \left(\xi \frac{\partial}{\partial \xi} \right) + \frac{1}{\eta \xi} \frac{\partial^2}{\partial \phi^2}. \quad (28)$$

Whether an eigenfunction is separable in cylindrical coordinates, with $\psi = P(\rho)\Phi(\phi)Z(z)$ or in parabolic coordinates $\psi = H(\eta)\Xi(\xi)\Phi(\phi)$, we may take it to be an eigenfunction of L_z , $\Phi(\phi) = e^{im\phi}$. Noting that $\eta\xi = \rho^2$, taking this azimuthal dependence reduces the Laplacian plus potential in the parabolic coordinates to

$$-\vec{\nabla}^2 + \frac{K}{\rho^2} = -\frac{4}{\eta + \xi} \frac{\partial}{\partial \eta} \left(\eta \frac{\partial}{\partial \eta} \right) - \frac{4}{\eta + \xi} \frac{\partial}{\partial \xi} \left(\xi \frac{\partial}{\partial \xi} \right) + \frac{m^2 + K}{\eta \xi} \quad (29)$$

$$= \frac{1}{\eta + \xi} \left[-4 \frac{\partial}{\partial \eta} \left(\eta \frac{\partial}{\partial \eta} \right) - 4 \frac{\partial}{\partial \xi} \left(\xi \frac{\partial}{\partial \xi} \right) + (m^2 + K) \left(\frac{1}{\eta} + \frac{1}{\xi} \right) \right]. \quad (30)$$

Once again, and not coincidentally, the inclusion of the potential corresponds to the change $m^2 \rightarrow m^2 + K$.

With $\Phi(\phi)$ factored out, the remaining Schrödinger equation can be written in the separation form

$$\left[\frac{4}{H} \frac{\partial}{\partial \eta} \left(\eta \frac{\partial H}{\partial \eta} \right) + E\eta - (m^2 + K) \frac{1}{\eta} \right] + \left[\frac{4}{\Xi} \frac{\partial}{\partial \xi} \left(\xi \frac{\partial \Xi}{\partial \xi} \right) + E\xi - (m^2 + K) \frac{1}{\xi} \right] = 0. \quad (31)$$

Letting the first bracketed term in (31) be equal to a constant C , the ordinary differential equation for H is

$$4\eta^2 \frac{d^2 H}{d\eta^2} + 4\eta \frac{dH}{d\eta} + \eta^2 EH - \eta CH - (m^2 + K) H = 0, \quad (32)$$

and with $C \rightarrow -C$ in the equation for Ξ .

As the wave function is complex, it may not be automatically clear whether C should be real or complex. Note that a purely imaginary C gives the real and imaginary parts of the solutions to the ordinary differential equations definite behavior under inversions of the variables, $\eta \rightarrow -\eta$ or $\xi \rightarrow -\xi$. However, this behavior is not actually physically mandated by the theory, because the physical space is limited to the parameter region where both η and ξ are non-negative. It will, however, necessarily be the case that only a one-parameter family of C values will correspond to physically meaningful states. Any separable energy eigenfunction in three dimensions is determined (up to phase and normalization) by the values of the three real quantum numbers. In this system, we have the physical observables represented by m and E , so the choice of C must provide exactly one additional real degree of freedom. As with a real-valued C , the separate differential equations for H and Ξ can be cast as eigenvalue equations for Hermitian operators, a real C is a sufficient condition for having equations that yield bases of wave functions with asymptotic forms that are continuum normalizable. Thus, a real C gives the correct one-parameter family of solutions.

The linearly independent solutions of (32) are expressible in terms of the confluent hypergeometric functions ${}_1F_1(a; b; s)$,

$$h_{\pm}(\eta) = \eta^{\pm \frac{1}{2} \sqrt{m^2 + K}} e^{-\frac{i}{2} \sqrt{E} \eta} {}_1F_1 \left(\frac{1}{2} \pm \frac{1}{2} \sqrt{m^2 + K} - \frac{iC}{4\sqrt{E}}; 1 \pm \sqrt{m^2 + K}; i\sqrt{E} \eta \right). \quad (33)$$

In order to have regularity at the origin (where $\eta = \xi = 0$), we must have the solution $H = h_+(\eta)$, and for Ξ ,

$$\Xi = h'_+(\xi) = \xi^{\frac{1}{2} \sqrt{m^2 + K}} e^{-\frac{i}{2} \sqrt{E} \xi} {}_1F_1 \left(\frac{1}{2} + \frac{1}{2} \sqrt{m^2 + K} + \frac{iC}{4\sqrt{E}}; 1 + \sqrt{m^2 + K}; i\sqrt{E} \xi \right). \quad (34)$$

Unfortunately, the overlap integrals giving the weights needed to write the wave functions $H(\eta)\Xi(\xi)$ as superpositions of the $P(\rho)Z(z)$ in cylindrical coordinates are intractable in the general case.

The asymptotic behavior of ${}_1F_1(a; b; s)$ for $|s| \rightarrow \infty$ and $-\frac{3\pi}{2} < \arg s < \frac{\pi}{2}$ is

$${}_1F_1(a; b; s) \sim \Gamma(b) \left[\frac{e^s s^{a-b}}{\Gamma(a)} + \frac{e^{i\pi a} s^{-a}}{\Gamma(b-a)} \right]. \quad (35)$$

For the solutions h_+ and h'_+ , the relevant values of a and $b - a (= a^*)$ always have real parts $\frac{1}{2} + \frac{1}{2} \sqrt{m^2 + K}$, which means that the first and second terms in (35) are of the same magnitude when η or ξ is large. The large η behavior of the confluent hypergeometric function appearing in $h_+(\eta)$ is accordingly (using the phase convention that $s = e^{\frac{i\pi}{2}} \sqrt{E} \eta$, corresponding to that in (35)),

$${}_1F_1 \sim \Gamma\left(1 + \sqrt{m^2 + K}\right) \left(i\sqrt{E}\eta\right)^{-\left(\frac{1}{2} + \frac{1}{2}\sqrt{m^2 + K}\right)} \left[\frac{e^{i\sqrt{E}\eta} \left(e^{\frac{i\pi}{2}} \sqrt{E}\eta\right)^{-\left(\frac{iC}{4\sqrt{E}}\right)}}{\Gamma\left(\frac{1}{2} + \frac{1}{2}\sqrt{m^2 + K} - \frac{iC}{4\sqrt{E}}\right)} \right. \quad (36)$$

$$\left. + \frac{e^{i\pi\left(\frac{1}{2} + \frac{1}{2}\sqrt{m^2 + K} - \frac{iC}{4\sqrt{E}}\right)} \left(e^{\frac{i\pi}{2}} \sqrt{E}\eta\right)^{\left(\frac{iC}{4\sqrt{E}}\right)}}{\Gamma\left(\frac{1}{2} + \frac{1}{2}\sqrt{m^2 + K} + \frac{iC}{4\sqrt{E}}\right)} \right] \\ = \frac{\Gamma\left(1 + \sqrt{m^2 + K}\right) e^{\frac{\pi C}{8\sqrt{E}}} \left(i\sqrt{E}\eta\right)^{-\left(\frac{1}{2} + \frac{1}{2}\sqrt{m^2 + K}\right)}}{\left|\Gamma\left(\frac{1}{2} + \frac{1}{2}\sqrt{m^2 + K} - \frac{iC}{4\sqrt{E}}\right)\right|} \left[e^{i\left(\sqrt{E}\eta - \arg \Gamma(a) + \frac{C}{4\sqrt{E}} \log \sqrt{E}\eta\right)} \right. \quad (37)$$

$$\left. + e^{i\left(\frac{\pi}{2} + \frac{\pi}{2}\sqrt{m^2 + K} + \arg \Gamma(a) - \frac{C}{4\sqrt{E}} \log \sqrt{E}\eta\right)} \right] \\ = \frac{2\Gamma\left(1 + \sqrt{m^2 + K}\right) e^{\frac{\pi C}{8\sqrt{E}}} \left(\sqrt{E}\eta\right)^{-\left(\frac{1}{2} + \frac{1}{2}\sqrt{m^2 + K}\right)}}{\left|\Gamma\left(\frac{1}{2} + \frac{1}{2}\sqrt{m^2 + K} - \frac{iC}{4\sqrt{E}}\right)\right|} e^{\frac{i}{2}\sqrt{E}\eta} \cos\left[\frac{1}{2}\sqrt{E}\eta \right. \quad (38)$$

$$\left. + \frac{C}{8\sqrt{E}} \log\left(\sqrt{E}\eta\right) - \frac{1}{2} \arg \Gamma\left(\frac{1}{2} + \frac{1}{2}\sqrt{m^2 + K} - \frac{iC}{4\sqrt{E}}\right) - \frac{\pi}{4} \sqrt{m^2 + K} - \frac{\pi}{4} \right].$$

In the intermediate formula (37), $\arg \Gamma(a)$ has been used to abbreviate the complex argument of $\Gamma\left(\frac{1}{2} + \frac{1}{2}\sqrt{m^2 + K} - \frac{iC}{4\sqrt{E}}\right)$.

It follows that the asymptotic behavior of the wave function ($r \rightarrow \infty$, but away from the z -axis, where η or ξ will vanish) is

$$H(\eta)\Xi(\xi) \propto \frac{1}{\sqrt{\eta\xi}} \cos\left[\frac{1}{2}\sqrt{E}\eta + \frac{C}{8\sqrt{E}} \log\left(\sqrt{E}\eta\right) - \frac{1}{2} \arg \Gamma(a) - \frac{\pi}{4} \sqrt{m^2 + K} - \frac{\pi}{4} \right] \\ \times \cos\left[\frac{1}{2}\sqrt{E}\xi + \frac{C}{8\sqrt{E}} \log\left(\sqrt{E}\xi\right) - \frac{1}{2} \arg \Gamma(a^*) - \frac{\pi}{4} \sqrt{m^2 + K} - \frac{\pi}{4} \right] \quad (39)$$

$$= \frac{1}{2\rho} \left\{ \cos\left[\sqrt{E}r + \frac{C}{8\sqrt{E}} \log\left(\cot^2 \frac{\theta}{2}\right) - \frac{\pi}{2} \sqrt{m^2 + K} - \frac{\pi}{2} \right] \right. \quad (40)$$

$$\left. + \cos\left[\sqrt{E}z + \frac{C}{8\sqrt{E}} \log\left(E\rho^2\right) - \arg \Gamma(a) \right] \right\},$$

using $\eta\xi = \rho^2$ and $\frac{\eta}{\xi} = \cot^2 \frac{\theta}{2}$.

The limiting form (40) away from the z -axis is clearly normalizable as a continuum state. On the other hand, in the vicinity of the z -axis, either $h_+(\eta)$ or $h'_+(\xi)$ is close to 1, while the other function—and the wave function ψ as a whole—scale as $\sim 1/\sqrt{|z|}$, which is again normalizable behavior. This confirms that our earlier choice of a real separation constant C was the correct one for the physical wave function solutions.

4. Special Features

Remarkably, the separated Equation (32) for H can actually be cast in nearly the same form as the radial Schrödinger equation for a Coulomb potential. Letting $U_1(\eta) = \sqrt{\eta}H(\eta)$, (32) becomes

$$-\frac{d^2 U_1}{d\eta^2} + \frac{C}{4\eta} U_1 + \frac{m^2 + K - 1}{4\eta^2} U_1 = \frac{E}{4} U_1. \quad (41)$$

The ordinary differential equation of $U_2(\xi) = \sqrt{\xi}\Xi(\xi)$ is identical, except for the switch $C \rightarrow -C$, equivalent to interchanging an attractive Coulomb potential with a repulsive one. Moreover, the normalization condition for the wave function,

$$\frac{1}{4} \int_0^\infty d\xi \int_0^\infty d\eta (\eta + \xi) |H(\eta)\Xi(\xi)|^2 = \frac{1}{4} \int_0^\infty d\xi \int_0^\infty d\eta \left(\frac{1}{\eta} + \frac{1}{\xi} \right) |U_1(\eta)U_2(\xi)|^2 = \frac{1}{2\pi}, \quad (42)$$

sets the same kinds of constraints on how quickly the functions U_1 and U_2 must decay at spatial infinity as in the Coulomb problem. The equivalence also immediately explains the presence of the $\log(\sqrt{E}\eta)$ and $\arg \Gamma(a)$ terms in the argument of the cosine in (38), as these same kinds of terms appear in the phases of Coulomb waves.

The transformation of the separated parts of the Schrödinger equation into Coulomb-like forms opens up a number of tools that can be used to further analyze the wave function solutions. However, those tools may play different roles in the analysis of the $1/\rho^2$ potential than in the study of the $1/r$ potential. For example, there are $(0+1)$ -dimensional supersymmetry transformations that carry solutions of the radial Schrödinger equation in the Coulomb problem to other radial solutions with the same energies but different values of the angular momentum (changing $l \leftrightarrow l+1$) [13,14]. Applied to (41), these transformations would still leave the energy unaffected (and also the separation constant C unchanged), but the strength of the potential would be modified through a change to the quantity $m^2 + K$, which combines the z -component of angular momentum with the strength of the repulsive potential. This is analogous to the situation with the one-dimensional $\text{sech}^2 ax$ potential, where the supersymmetry transformations connect potentials with the same functional form, but of different depths.

Another interesting feature of the solution in parabolic coordinates stems from the fact that the choice of coordinate system breaks the translation invariance along the z -direction. This symmetry is manifestly present in the equations of motion in a cylindrical coordinate system, where z is a cyclic coordinate. As z never enters the dynamics explicitly, there is nothing special about the location of $z = 0$. The translation symmetry is obscured somewhat in the parabolic coordinates, but it must still exist. If $\psi_1 = H(\eta)\Xi(\xi)e^{im\phi}$ is a solution of the Schrödinger equation, then

$$\psi_2 = H \left[\sqrt{\rho^2 + (z-a)^2} + (z-a) \right] \Xi \left[\sqrt{\rho^2 + (z-a)^2} - (z-a) \right] e^{im\phi} \quad (43)$$

must also be a solution, as it is simply a translate of ψ_1 along the z -direction. The degeneracy of these states is analogous to the energy degeneracy of the Landau levels for a charged particle moving in the plane perpendicular to a constant magnetic field. The magnitude of the degeneracy is proportional to the area of the plane, as the origin of the coordinates may be located anywhere in the plane.

The presence of C in the eigenfunction Equation (41) also appears to break the scale invariance of the problem, as the Hermitian operator on the left-hand side contains C , which has units of $(\text{length})^{-1}$. However, as C is merely a separation constant, which can take any real value, a rescaling $\vec{\rho} \rightarrow \alpha\vec{\rho}$ (and thus $\eta \rightarrow \alpha\eta$, $\xi \rightarrow \alpha\xi$) may be accompanied by $C \rightarrow \alpha^{-1}C$. As the same C appears in the equations for H and Ξ , this restores the physical scaling invariance.

Finally, the separation of the quantum-mechanical problem in parabolic coordinates can give some insight about the classical behavior in that coordinate system. Because the η and ξ portions of the Schrödinger equation are the same as those for two Coulomb problems, one attractive and the other equally repulsive, we can apply the normal methods for solving the Kepler problem to the classical time evolution of a particle's (η, ξ, ϕ) coordinates. Recalling that the classical limit applies when K is large, we may neglect the -1 in the $m^2 + K - 1$ appearing in (41). Then, restoring the factors of $\hbar^2/2M$, (41) corresponds to a classical limit of

$$\frac{1}{2}M\dot{\eta}^2 + \frac{C}{4\eta} + \frac{L^2 + 2M\kappa}{4\eta^2} = \frac{\mathcal{E}}{4}, \quad (44)$$

where $C = 2MC/\hbar^2$. There is no orbital equation that is directly analogous to the one for $r(\phi)$ in the normal Kepler problem, as the relationship between the angular velocity $\dot{\phi}$ and $L = L_z = M\rho^2\dot{\phi} = M\eta\dot{\xi}\dot{\phi}$ is determined by both η and ξ together. However, (44) may be solved implicitly for the time t as a function of the coordinate η ,

$$t = \sqrt{\frac{M}{2}} \int_{\eta_{\min}}^{\eta} \frac{d\eta'}{\sqrt{\frac{\mathcal{E}}{4} - \frac{C}{4\eta'} - \frac{L^2 + 2M\kappa}{8(\eta')^2}}} \quad (45)$$

$$= \frac{\sqrt{2M\mathcal{E}\eta^2 - 2MC\eta - L^2 - 2M\kappa}}{\mathcal{E}} + \frac{\sqrt{MC}}{\sqrt{2}\mathcal{E}^{\frac{3}{2}}} \log \left[2\sqrt{\mathcal{E} \left(\mathcal{E}\eta^2 - C\eta - \frac{L^2}{2M} - \kappa \right) + 2\mathcal{E}\eta - C} \right] - \frac{\sqrt{MC}}{2\sqrt{2}\mathcal{E}^{\frac{3}{2}}} \log \left[C^2 + 4\mathcal{E} \left(\frac{L^2}{2M} + \kappa \right) \right]. \quad (46)$$

The origin of the time coordinate has been chosen in this case so that $t = 0$ occurs at the turning point

$$\eta(0) = \eta_{\min} = \frac{C + \sqrt{C^2 + 4\mathcal{E} \left(\frac{L^2}{2M} + \kappa \right)}}{2\mathcal{E}} \quad (47)$$

for η . As the condition for η_{\min} is $\sqrt{2M\mathcal{E}\eta_{\min}^2 - 2MC\eta_{\min} - L^2 - 2M\kappa} = 0$, both square roots in (46) vanish at $\eta = \eta_{\min}$, and just the last term comes from the lower limit of the integration.

Simultaneously, the ξ coordinate is evolving independently. The time is once again given implicitly, in this instance by

$$t = \frac{\sqrt{2M\mathcal{E}\xi^2 + 2MC\xi - L^2 - 2M\kappa}}{\mathcal{E}} - \frac{\sqrt{2M\mathcal{E}\xi(0)^2 + 2MC\xi(0) - L^2 - 2M\kappa}}{\mathcal{E}} - \frac{\sqrt{MC}}{\sqrt{2}\mathcal{E}^{\frac{3}{2}}} \log \left\{ \frac{2\sqrt{\mathcal{E} \left(\mathcal{E}\xi^2 + C\xi - \frac{L^2}{2M} - \kappa \right) + 2\mathcal{E}\xi + C}}{2\sqrt{\mathcal{E} \left[\mathcal{E}\xi(0)^2 + C\xi(0) - \frac{L^2}{2M} - \kappa \right] + 2\mathcal{E}\xi(0) + C}} \right\}. \quad (48)$$

$\xi(0)$ is the value of ξ when $\eta = \eta_{\min}$. If $\eta(t)$ and $\xi(t)$ are determined, then the remaining angular behavior can be found from

$$\phi(t) = \phi(0) + \frac{L}{M} \int_0^t \frac{dt'}{\eta(t')\xi(t')}, \quad (49)$$

completing the classical solution.

5. Conclusions

Hamiltonians that are amenable to separation of variables methods in more than one coordinate system have a number of important properties. These include accidental degeneracies in their bound state spectra, and classical behavior that typically involves bound orbits that always close. The nonrelativistic Hamiltonians for a number of important physical systems, such as the hydrogen atom and the charged particle in a constant magnetic field, are multiply separable in this way. These features are also tied to the usefulness of operator methods in solving these Hamiltonians.

The z -independent $1/\rho^2$ potential in three dimensions is obviously separable in cylindrical coordinates (ρ, ϕ, z) , and we have shown that it is also separable in parabolic coordinates (η, ξ, ϕ) . Although parabolic coordinates are not used nearly as frequently as rectangular, spherical, and cylindrical coordinate systems, they were already known to be useful for addressing certain aspects of the Coulomb problem. The attractive $1/\rho^2$ potential is too strong to support a stable set of

bound states, but the repulsive version is well behaved. When separated in parabolic coordinates, the one-dimensional Schrödinger equations for the component functions $H(\eta)$ and $\Xi(\xi)$ have the same forms as the radial Schrödinger equation in the Coulomb problem, although the strength of the Coulomb-like term is set by the separation constant C , so that one equation features the effective equivalent of an attractive potential, which the other has a repulsive potential of equal magnitude.

The asymptotic behavior of the full wave function $\psi(\eta, \xi, \phi)$ in parabolic coordinates is thus determined by the limiting behavior of a product of Coulomb waves, albeit ones that typically have non-integral values for what would normally be the angular momentum parameter ℓ . Moreover, although we have focused on the scattering states of a repulsive $1/\rho^2$ potential, it is clear that for sufficiently large values of $L_z = m\hbar$, the scattering wave function in an attractive $1/\rho^2$ potential will have essentially the same structures. They will still be products of Coulomb radial functions in η and ξ , with unconventional values of ℓ and equal and opposite effective potential strengths.

While the separation of variables in cylindrical coordinates keeps the translation symmetry along the z -direction and the scale invariance of the problem manifest, both of these invariances are obscured in the parabolic coordinate system, which picks a particular $z = 0$ location about which the η and ξ coordinate surfaces are focused. The fact that these important features are hidden in the parabolic coordinates formalism suggests that there may be yet other interesting features of these potentials still to be uncovered. In any case, the planar $1/\rho^2$ potential, as well as being a system of real physical significance [17–19], appears to be a fruitful theoretical laboratory for understanding the structure of mechanics in parabolic coordinates and the behavior of multiply separable quantum systems.

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