THE INVERSE-CUBE CENTRAL FORCE FIELD IN QUANTUM MECHANICS*

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Abstract

The problem of the motion of a particle in an inverse-cube central force field is fully treated by quantum mechanics and the results compared with the classical theory. Taking the effective radial potential energy as S/r^2, although the solutions for negative energy for $0 \geqq S \geqq -h^2/32\pi^2\mu$ satisfy the usual boundary conditions, they can not be admitted because the Hamiltonian is not Hermitian in these solutions. This corresponds to taking $(l+\frac{1}{2})^2$ in place of $l(l+1)$ as the analogue of the square of the classical angular momentum. If we do this, we get a complete analogy between the classical and quantum mechanically allowed solutions, with no quantization. The solutions involve Bessel functions of both real and imaginary orders with both real and imaginary arguments.

1. CLASSICALLY, considerable interest has attached to the problem of the motion of a particle in a central-force field falling off inversely as the cube of the distance. This force law occupies a somewhat special position mathematically, and is one of the three for which the forms of the various possible orbits may be expressed in terms of circular functions. It was studied in particular by Roger Cotes, and the orbits are sometimes known as Cotes' spirals.[1] Quantum mechanically, this problem is of particular interest because of the complete lack of quantization, the variety of Bessel functions to which the solution leads, the peculiar rôle played by the angular momentum value $(l+\frac{1}{2})^2$, and the necessity for careful consideration of the conditions which an allowed solution must satisfy.

Let a particle of mass μ be acted on by a radial force of $2S'/r^3$, so that the potential energy is

$$V = \frac{S'}{r^2},$$

where S' is negative for an attractive force, positive for a repulsive.

We have the Schrödinger equation

$$\Delta\psi + \frac{8\pi^2\mu}{h^2}\left[W - \frac{S'}{r^2}\right]\psi = 0,$$

which, on being separated in polar coördinates, yields, as in any central-force problem

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[1] Roger Cotes, Harmonia Mensurarum, Cambridge, 1722, pp. 31–35, 98. For a modern discussion of this problem see, for example, Lamb's Dynamics, p. 266 ff.

$$\psi = \left(\frac{(2l+1)(l-|m|)!}{4\pi(l+|m|)!}\right)^{1/2} \frac{R(r)}{r} \sin^{|m|}(\theta) P_l^{|m|}(\cos\theta) e^{im\phi},$$

where $mh/2\pi$ specifies the z component of angular momentum; $l(l+1)h^2/4\pi^2$ the square of the total angular momentum, and $R(r)$ satisfies the equation

$$R'' + \frac{8\pi^2\mu}{h^2}\left[W - \frac{S'}{r^2} - \frac{h^2}{8\pi^2\mu}\frac{l(l+1)}{r^2}\right]R = 0.$$

This is the equation for one-dimensional motion in the r-coördinate under a potential energy $V_r = S/r^2$, where the effective radial force constant

$$S = S' + \frac{1}{2\mu} l(l+1) \frac{h^2}{4\pi^2} \cdot \tag{1}$$

We then have the radial equation

$$R'' + k[W - S/r^2]R = 0, \qquad \text{where } k = 8\pi^2\mu/h^2. \tag{2}$$

In this the change of variable

$$\rho = (kW)^{1/2} r \tag{3}$$

and the substitution

$$R(r) = |\rho|^{1/2} Z_\nu(\rho) \tag{4}$$

give for $Z_\nu(\rho)$ the standard form of Bessel's equation

$$\rho^2 Z_\nu''(\rho) + \rho Z_\nu'(\rho) + (\rho^2 - \nu^2) Z_\nu(\rho) = 0, \tag{5}$$

where the order ν is related to S by

$$\nu = (\tfrac{1}{4} + kS)^{1/2}. \tag{6}$$

The boundary conditions which must be satisfied[2] are that at the origin ψ shall not become infinite so rapidly as $1/r$, and that it shall remain at infinity. This requires $R(r)$ to be zero at the origin and allows it to become infinite at a rate r at infinity.

We see that since the energy W occurs only in the argument of the Bessel function we have no quantization, but only continuous spectra of energy levels.

The quantum-mechanical probability that the particle be between r and $r+dr$ is proportional to $|R(r)|^2 dr$, which may be compared with the classical radial probabilities obtained by writing

$$W = \frac{S'}{r^2} + \frac{1}{2}\mu\dot{r}^2 + \frac{M^2}{2\mu r^2} = \frac{S}{r^2} + \frac{1}{2}\mu\dot{r}^2, \tag{7}$$

where $S_c = S' + M^2/2\mu$, and the probabilities of the different values of r are proportional to

$$\frac{1}{\dot{r}} = \frac{dt}{dr} = r\left(\frac{\mu}{2(r^2W - S_c)}\right)^{1/2}. \tag{8}$$

[2] See Dirac, Quantum Mechanics, pp. 143–4.

§2. It is seen that the Bessel function of the radial factor (4) has an imaginary argument for $W<0$, and an imaginary index for $S<-1/4k$. In this case classically the particle spirals in from a maximum radius $(S_c/W)^{1/2}$ to the origin, along the path

$$\frac{1}{r} = \left(\frac{W}{S_c}\right)^{1/2} \cosh\left(\frac{(-2\mu S_c)^{1/2}}{M}\,\theta\right),$$

increasing its radial velocity to infinity at the origin, as may be readily seen from an energy diagram. If we write $\rho = i\kappa = (-kW)^{1/2}r$, we get as the normalized classical probability that ρ be between ρ and $\rho+d\rho$

$$\frac{1}{(-kS_c)^{1/2}}\,\frac{\rho}{(-kS_c - \rho^2)^{1/2}}\,d\rho. \tag{9}$$

Quantum mechanically we have, if $\nu = in$,

$$R(r) = \rho^{1/2} Z_{in}(i\rho). \tag{10}$$

Very little work has been done on such a Bessel function, but we can determine its characteristics in a manner indicated by Bôcher,[3] using a form of Bessel's equation given by Riemann-Hattendorf.[4] If we write $t = \log|\kappa|$, $Z_\nu(\kappa)$ satisfies the equation

$$\frac{d^2Z}{dt^2} + (\kappa^2 - \nu^2)Z = 0, \tag{11}$$

and so $Z_{in}(i\rho)$ satisfies

$$\frac{d^2Z}{dt^2} - (\rho^2 - n^2)Z = 0. \tag{12}$$

From this we see that for $\rho<n$, d^2Z/dt^2 has always the opposite sign from Z, so that the solution oscillates from $t=-\infty\,(\rho=0)$ to $\rho=n$. For $\rho>n$, the second derivative has the same sign as ρ and by proper choice of the phase near $t=-\infty$, we can find one solution which falls exponentially to zero as $\rho\to\infty$. Since $\rho=n$ is the classical limit of motion for $S_c=S+1/4k$, this is just as expected. For $\rho\to 0$, $t\to-\infty$, the equation becomes that for $\sin(nt-\text{const.})$ $=\sin(n\log\rho-\text{const.})$. This gives an infinity of oscillations near the origin of constant amplitude at the start; making the average probability start as ρ, as does the classical probability. Further, the de Broglie wave-length of $\sin(n\log\rho)$ for small ρ is $2\pi\rho/n$, or, in ordinary units, $2\pi r/n$. This is seen to correspond exactly with the classical $h/\mu\dot{r} = 2\pi r/(-kS_c)^{1/2}$ for $S_c=S+1/4k$. Although we cannot ascertain the quantum mechanical probabilities in more detail than this, it is quite certain that the average of the normalized probability curve will follow the classical probability curve (9) closely almost to the classical limit where the classical probability becomes infinite and the

[3] Bôcher, Annals of Math. **6**, 137 (1891–2).

[4] Riemann-Hattendorf, Partielle Differentialgleichung, Braunschweig, 1876, p. 266 ff.

quantum mechanical curve starts falling exponentially to zero. This is probably the first instance which has been pointed out of the occurrence of a continuity of energy levels with a closed orbit and quadratically integrable ψ function.

For positive energies in this case $(S < -1/4k)$, classically the particle spirals in from infinity to the origin, with its radial velocity asymptotically constant for large distances, but increasing to infinity at the origin, along the path

$$\frac{1}{r} = \left(-\frac{W}{S_c}\right)^{1/2} \sinh\left(\frac{(-2\mu S_c)^{1/2}}{M}\,\theta\right).$$

The clasical probabilities of being between $\textsc{r}$ and $\textsc{r}+d\textsc{r}$ are proportional to

$$\frac{\textsc{r}}{(\textsc{r}^2 - kS_c)^{1/2}}\,d\textsc{r}. \tag{13}$$

Quantum mechanically, our solution takes the form

$$R(r) = \textsc{r}^{1/2}Z_{in}(\textsc{r}) \tag{14}$$

with $\textsc{r}$ real. This Bessel function $Z_{in}(\textsc{r})$ satisfies

$$\frac{d^2Z}{dt^2} + (\textsc{r}^2 + n^2)Z = 0, \tag{15}$$

from which we see that d^2Z/dt^2 and Z always have opposite signs, so that the solution oscillates all the way from $t = -\infty$ to $+\infty$. Near $\textsc{r}=0$ we get exactly the same behavior as for solution (10) above, but for $\textsc{r} \gg n$, Eq. (15) becomes the equation for $\textsc{r}^{-1/2}$ sin $(\textsc{r}+\text{const.})$, whereas Eq. (12) became that for $\rho^{-1/2}e^{-\rho}$. This makes the radial factor (14) approach sin $(\textsc{r}+\text{const.})$ for large $\textsc{r}$, giving a constant average probability and a proper de Broglie wave-length exactly to correspond with the constant classical velocity. Here we should expect that in the whole range from 0 to ∞, the average of $R^2(r)$ will follow closely the classical probability curve (13) and that $R(r)$ will have approximately the proper de Broglie wave length to correspond to the classical velocity, just as we have seen these conditions to hold at both ends of the range.

The case $S < -1/4k$, $W = 0$ demands special consideration. Here classically we get the equiangular spiral

$$\frac{1}{r} = \exp\left\{\frac{(-2\mu S_c)^{1/2}}{M}\,\theta\right\},$$

with a radial probability proportional to r(since $\dot{r} \propto 1/r$). Quantum mechanically Eq. (2) becomes $r^2R'' - kSR = 0$, giving the solutions

$$R(r) = r^{1/2} \sin(n \log r + \text{const.}), \tag{16}$$

whose square increases as r, agreeing with the classical probability, and whose de Broglie wave-length as calculated from the slope of the $n \log r$ curve is $2\pi r/n$, agreeing exactly with the classical $h/\mu\dot{r}$ for $S_c = S + 1/4k$.

So for all W, with $S < -1/4k$, we get solutions oscillating infinitely rapidly near the origin to correspond to the classical infinite velocity, and good probability and wave-length agreements with the classical theory throughout if we compare S with $S_c - 1/4k$. We further can obtain from these solutions a good approximation to the amplitude and rate of oscillation of a Bessel function of imaginary index throughout its range.

§3. When we consider the range of S between 0 and $-1/4k$ for negative W, we have the well-known Bessel function of real order ν between 1/2 and 0, and imaginary argument. The particular solution[5] $K_\nu(\rho)$ falling exponentially to zero at infinity starts at the origin as $\rho^{-\nu}$ (as $\log \rho$ for $\nu = 0$), and so because of the factor $\rho^{1/2}$,

$$R(r) = \rho^{1/2} K_\nu(\rho) \tag{17}$$

is zero at the origin and formally satisfies all the boundary conditions. However, these solutions remain everywhere positive, and so neither they nor the eigendifferentials $\int_W^{W+\Delta W} R_W(r) dW$ are orthogonal for different W. For this reason their physical significance as stationary states is questionable, although from considerations purely of the Schrödinger equation the probability of the particle's being at each point is definitely specified for every W. Because of this non-orthogonality the matrix of H in these solutions is neither diagonal nor Hermitian.

The theory of the eigenvalues of Hermitian operators has been completely investigated by von Neumann.[6] Let H be a linear operator which can be applied to a number of functions

$$\psi_1, \psi_2, \psi_3 \cdots \tag{18}$$

and their linear combinations in such a way that the Hermitian condition

$$\int \bar{\psi}_1 H \psi_2 = \int \overline{\bar{\psi}_2 H \psi_1} = \int \overline{H\psi_1} \psi_2 \tag{19}$$

is satisfied. In general, the field of operation of H can be extended to other functions

$$\psi_1', \psi_2', \psi_3' \cdots \tag{20}$$

and their linear combinations, so that (19) holds for the total set (18), (20). If the field of operation of H is extended in this way as far as possible, one obtains a set of functions which is everywhere dense, and H has[7] a spectrum whose eigenfunctions and eigendifferentials are *included* in (18), (20), and which form a *complete* set of functions. These eigenfunctions or eigendifferentials are therefore orthogonal in the usual way, so the usual statistical interpretations may be made.

[5] See Watson, Theory of Bessel Functions, p. 78.

[6] J. v. Neumann, Math. Ann. **102**, 49 (1929).

[7] von Neumann finds one exception.

Now it is clear in our case that the field of operation of H can be extended at most to *one* of the functions (17), because (19) does not hold for *two* of them or their eigendifferentials. Hence the rest of our solutions must form a complete set, and solutions (17) must be linear combinations of our other solutions, and therefore not stationary states of energy.

This means that we must be able to express the solutions

$$r^{1/2}K_\nu(\rho) = r^{1/2}K_\nu([-kW_1]^{1/2}r), \qquad 0 \leqq \nu < \tfrac{1}{2}$$

for negative W_1 as combinations of the eigendifferentials

$$\int_W^{W+\Delta W} r^{1/2}J_\nu([kW]^{1/2}r)dW$$

arising from the solutions $r^{1/2}J_\nu(R)$ which hold for positive W (see §4). This expansion is known[8]:

$$r^{1/2}K_\nu([-kW_1]^{1/2}r) = \int_0^\infty \frac{1}{2(W-W_1)}\left(-\frac{W}{W_1}\right)^{\nu/2}\cdot r^{1/2}J_\nu([kW]^{1/2}r)dW \qquad (21)$$

and so bears out the theory completely.[9]

This situation is related in an interesting fashion to the question of the quantum mechanical analogue of resultant angular momentum. The value $S=0$ corresponds, from Eq. (1), to the force constant

$$S' = -\frac{1}{2\mu}l(l+1)\frac{h^2}{4\pi^2}, \qquad (S=0) \qquad (22)$$

[8] See Watson, Reference 5, p. 425.

[9] The algebra of the general theory contains inherently the requirement that all operators be Hermitian, and so the general theory eliminates these eigenvalues in the following way: Making use of the commutator $(1/r)p_r - p_r(1/r) = h/2\pi i r^2$, we may write the Hamiltonian in the form

$$H = \bar{A}A = \left(\frac{p_r}{(2\mu)^{1/2}} + \frac{i\alpha}{r}\right)\left(\frac{p_r}{(2\mu)^{1/2}} - \frac{i\alpha}{r}\right) = \frac{1}{2\mu}p_r^2 + \frac{S}{r^2},$$

where α is real and $S=\alpha^2+\alpha/k^{1/2}$. This form for the Hamiltonian is possible only for $S \geqq -1/4k$, since the expression $\alpha^2+\alpha/k^{1/2}$ has an absolute minimum at $-1/4k$ for α real. Now since $H\psi(W)=W\psi(W)$, we have

$$\int\bar{\psi}(W)H\psi(W) = W\int\bar{\psi}\psi = \int\bar{\psi}\bar{A}A\psi = \int\overline{A\psi}A\psi > 0$$

since the integral of a function times its complex conjugate is necessarily positive. Hence W is necessarily positive whenever H can be written in this form, that is, for $S \geqq = 1/4k$. Thus we see that in terms of the general theory the usual boundary conditions on Schrödinger's ψ are necessary but not sufficient, and must be supplemented by an orthogonality requirement.

Langer and Rosen, Phys. Rev. **37,** 658 (1931), conclude that the fundamental requirement for an allowed solution is the equality of the "Hamiltonian Integral" $J=\int[(h^2/4\pi^2)T(q, \partial\psi/\partial q) + V\psi^2]d\tau$ and the energy. This is equivalent to the introduction of the Hermitian requirement and accomplishes the elimination of this band of energies since J here is divergent at the origin.

The solution of the central field problem for non-integral l, which led Jaffé (Zeits. f. Physik **66,** 770 (1931)) to conclude that ψ must be finite and continuous, may be eliminated on the same grounds of non-orthogonality as our solutions above. Requiring $\psi(=R(r)/r)$ to be finite at the origin would eliminate almost all of our solutions!

while the value $S=-1/4k$ corresponds to

$$S' = -\frac{1}{2\mu}\,(l+\tfrac{1}{2})^2\frac{h^2}{4\pi^2}. \qquad (S=-1/4k) \tag{23}$$

Now classically, the force constant

$$S' = -\frac{1}{2\mu}\,M^2 \qquad (S_c=0)$$

divides those values of S_c for which all values of W are allowed from those for which only positive values of W are allowed, and quantum mechanically, this same rôle is played by (23), so in the sense of comparing the allowed energy ranges with classical theory, $(l+\frac{1}{2})^2h^2/4\pi^2$ is to be taken as the

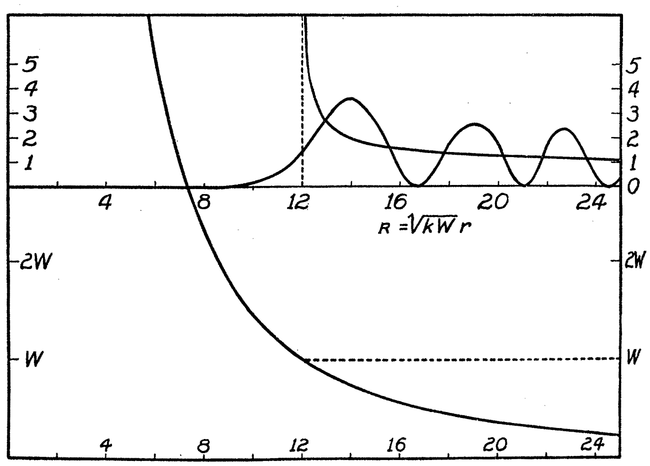

Fig. 1. Probability curves for $\nu=12$. Lower curve is the radial potential energy $S/r^2\approx 144W/R^2$. Upper curves compare the quantum mechanical probability $\pi R J^2_{12}(R)$ with the classical $R/(R^2-144)^{1/2}$.

analogue of the square of the angular momentum. So we should compare $S+1/4k$ with the classical S_c, in which case our correspondence is complete in every respect.

§4. For positive S_c and W, classically the particle moves from $R=(kS)^{1/2}$ to ∞, rapidly approaching a constant velocity, along the path

$$\frac{1}{r} = \left(\frac{W}{S_c}\right)^{1/2}\cos\left(\frac{(2\mu S_c)^{1/2}}{M}\,\theta\right),$$

with radial probabilities given by Eq. (13), which has an average value one.

Quantum-mechanically for $S \geqq -1/4k$, $W>0$, we get

$$R(r) = \pi^{1/2}R^{1/2}J_\nu(R), \qquad 0 \leqq \nu \tag{24}$$

with the ordinary Bessel functions whose properties are well known.[10] This solution remains very small almost until $R=\nu$, the classical limit for $S_c = S+1/4k$, after which it oscillates to infinity, approaching $2^{1/2} \sin (R+\text{const.})$, with the proper de Broglie wave-length and average probability one. The average of this probability curve follows the classical curve very closely as expected. One point of interest is that the case $S_c=0$, giving a constant radial velocity, would seem to correspond better to $S=0$, which gives $R(r)= \pi^{1/2}R^{1/2}J_{1/2}(R)=2^{1/2}\sin R$, than to $S=-1/4k$, which involves $J_0(R)$; however, for these small values of S one cannot expect too good a comparison. Fig. 1 shows the good agreement between the probability curves for $\nu=12$, and it is just such an agreement, for large $|S|$, that we would expect with the solutions involving the imaginary Bessel functions previously discussed.

As in the classical case, these results are only as yet of academic interest; it would be pleasing if such pretty mathematical results were to find an application to atomic physics. I wish to thank Professors Condon, Wigner, and Robertson of Princeton University for helpful discussions concerning this problem.

[10] For the limited range $0 \leqq \nu < \frac{1}{2}$, the solution with the Bessel function of the second kind, $Y_\nu(R)$, also formally satisfies the boundary conditions, since it starts as $R^{-\nu}$. We might expect this solution to be eliminated just as was the quadratically-integrable solution for negative energies which started in the same way in the same band of S. Orthogonality considerations are rather difficult, but the reasonable requirement that the Hamiltonian integral J converge in any finite range—in particular in a range about a singularity or infinity of the potential function—would eliminate these solutions, since for the solution $R^{1/2}Y_\nu(R)$, J does not converge at the origin, whereas for $R^{1/2}J_\nu(R)$ it does. See footnote (9).