Snippets of Physics

18. Perturbing Coulomb to Avoid Accidents!

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The Coulomb problem, which corresponds to motion in a potential that varies as r^{-1}, has a peculiar symmetry which leads to a phenomenon known as 'accidental' degeneracy. This curious feature exists both in the classical and quantum domain and is best understood by studying a more general potential and obtaining the Coulomb problem as a limiting case.

The motion of a particle in an attractive $-(1/r)$ potential is of historical and theoretical importance. The fact that the classical bound orbits in such a potential are ellipses played a crucial role in the historical study of planetary motion and gravity. The Coulomb potential, on the other hand, played a crucial role in the early days of quantum theory in the study of hydrogen spectra. In both the cases, it was soon realized that the $(1/r)$ potential has some very special features not shared by a generic central potential. In this installment, we will investigate several aspects of this problem from both classical and quantum perspectives.

It turns out that a nice way of undersanding the peculiar features of the Coulomb problem is to start with a slightly more general potential – which does *not* have these peculiar features – and treat the Coulomb problem as a special case of this more general situation. This can be done in many different ways and I will choose to study the dynamics under the action of the potential given by

$$U(r) = -\frac{\alpha}{r} + \frac{\beta}{r^2} \, , \qquad (1)$$

Keywords
Coulomb problem, Runge–Lenz vector, accidental degeneracy.

which, of course, reduces to the attractive Coulomb potential when $\beta \to 0^+$. For the sake of definiteness, I will take $\alpha > 0$ and $\beta \geq 0$ though most of the analysis can be generalized to other cases.

Classical motion of a particle of mass m, in 3-dimensions, under the action of $U(r)$ is straightforward to analyze using the standard textbook description of a central force problem. Just for fun, I will do it in a slightly different manner. We know that, as with any central force problem, angular momentum $\mathbf{J}$ is conserved, confining the motion to a plane which we will take to be $\theta = \pi/2$. Using $J = mr^2\dot{\phi}$, the energy of the particle can be expressed as

$$E = \frac{1}{2}m\left(\dot{r}^2 + \frac{J^2}{m^2r^2}\right) - \frac{\alpha}{r} + \frac{\beta}{r^2} \; . \tag{2}$$

Combining the two terms with $(1/r^2)$ dependence into C^2/r^2, where $C^2 = (J^2/2m) + \beta$ and completing the square, we get the relation

$$E + \frac{\alpha^2}{4C^2} = \frac{1}{2}m\dot{r}^2 + \left(\frac{C}{r} - \frac{\alpha}{2C}\right)^2 \equiv \mathcal{E}^2 \; . \tag{3}$$

This suggests introducing a function $f(t)$ via the equations

$$\sqrt{\frac{m}{2}}\,\dot{r} = \mathcal{E}\sin f(t)\,; \qquad \left(\frac{C}{r} - \frac{\alpha}{2C}\right) = \mathcal{E}\cos f(t) \; . \tag{4}$$

Differentiating the second equation with respect to time and using the first equation will give you an expression for $\dot{f}$. Dividing this expression by $\dot{\phi} = J/mr^2$ leads to the simple relation $(\mathrm{d}f/\mathrm{d}\phi) = (2mC^2/J^2)^{1/2}$. Hence, f is a linear function of ϕ and from the second equation in (4) we get the equation for the trajectory to be

$$\frac{(2C^2/\alpha)}{r} = 1 + \left(\frac{2\mathcal{E}C}{\alpha}\right)\cos(\omega\phi) \; , \tag{5}$$

where

$$\omega^2 = \frac{2m}{J^2}\,C^2 = \left(1 + \frac{2m\beta}{J^2}\right) \; . \tag{6}$$

Now that we have solved the problem completely, let us look at the properties of the solution. To begin with, let us ask what kind of orbit we would expect given

the known symmetries of the problem. A particle moving in 3 space dimensions has a phase space which is 6-dimensional. For any time-independent central force, we have constancy of energy E and angular momentum $\mathbf{J}$. Conservation of these four quantities (E, J_x, J_y, J_z) confines the motion to a region of $6 - 4 = 2$ dimensions. The projection of this phase space trajectory on to xy-plane will, in general, fill a two-dimensional region of space. So you would expect the orbit to fill a finite two-dimensional region of this plane, if there are no other conserved quantities. This is precisely what happens for a generic value of the conserved quantities J and E. Because ω will not be an integer, when ϕ changes by 2π, the cosine factor will pick up a term $\cos(2\pi\omega)$ which will not be unity. In general, the orbit will fill a 2-dimensional region in the plane between two radii r_1 and r_2.

We can now see how the Coulomb problem becomes rather special. In this case, we have $\beta = 0$ making $\omega = 1$. The curve in (5) closes on itself for any value of J and E and, in fact, becomes an ellipse with the latus-rectum $p = (2C^2/\alpha)$ and eccentricity $e = (2\mathcal{E}C/\alpha)$. You should verify that this is indeed the standard textbook solution to the Kepler problem. So when $\beta = 0$, $\omega = 1$, the orbit closes and becomes a one-dimensional curve rather than filling a 2-dimensional region. This analysis shows how turning on a non-zero β completely changes the topological character of the orbit.

In the argument given above, we linked the nature of the orbit to the number of conserved quantities for the motion. Given the fact that $\beta = 0$ reduces the dimension of the orbital space by one, we expect to have one more conserved quantity in the problem when $\beta = 0$ but not otherwise. To discover this constant, consider the time derivative of the quantity $(\mathbf{p} \times \mathbf{J})$ in any central force $f(r)\hat{\mathbf{r}}$. We have

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}(\mathbf{p} \times \mathbf{J}) &= \dot{\mathbf{p}} \times \mathbf{J} = \frac{f(r)}{r}\mathbf{r} \times (\mathbf{r} \times m\dot{\mathbf{r}}) \\ &= \frac{mf(r)}{r}[\mathbf{r}(\mathbf{r} \cdot \dot{\mathbf{r}}) - \dot{\mathbf{r}}r^2] \\ &= -mf(r)r^2\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\mathbf{r}}{r}\right). \end{aligned} \tag{7}$$

That is,

$$\frac{\mathrm{d}}{\mathrm{d}t}(\mathbf{p} \times \mathbf{J}) = -mf(r)r^2\frac{\mathrm{d}\hat{\mathbf{r}}}{\mathrm{d}t}\ , \tag{8}$$

where $\hat{\mathbf{r}}$ is the unit vector in the radial direction. The miracle of inverse square force is now in sight: When $f(r)r^2 = \text{constant} = -\alpha$, we find that the vector

(called *Runge–Lenz vector* though it was originally discovered by Hamilton!):

$$\mathbf{A} \equiv \mathbf{p} \times \mathbf{J} - \alpha m \hat{\mathbf{r}} \tag{9}$$

is conserved. But we needed only one constant of motion while we now have got 3 components of $\mathbf{A}$ which will prevent the particle from moving at all! Such an overkill is avoided because $\mathbf{A}$ satisfies the following two, easily verified, relations:

$$A^2 = 2mJ^2E + \alpha^2 m^2; \quad \mathbf{A}.\mathbf{J} = 0 \ , \tag{10}$$

where $E = p^2/2m - \alpha/r$ is the conserved energy for the motion. The first relation tells you that the magnitude of $\mathbf{A}$ is fixed in terms of other constants of motion and the second one shows that $\mathbf{A}$ lies in the orbital plane. These two constraints reduce the number of independent constants in $\mathbf{A}$ from 3 to 1, exactly what we needed. It is this extra constant that keeps the planet on a closed orbit.

The ultimate test of our analysis is whether we can find the orbit in (5) for the case of $\beta = 0$ without integrating any differential equation. This is, of course, true. To find the orbit, we only have to take the dot product of (9) with the radius vector $\mathbf{r}$ and use the identity $\mathbf{r}.(\mathbf{p} \times \mathbf{J}) = \mathbf{J}.(\mathbf{r} \times \mathbf{p}) = J^2$. This gives

$$\mathbf{A}.\mathbf{r} = Ar\cos\phi = J^2 - \alpha m r \ , \tag{11}$$

or, in a more familiar form, the conic section:

$$\frac{(J^2/\alpha m)}{r} = 1 + \frac{A}{\alpha m}\cos\phi. \tag{12}$$

As a bonus we see that $\mathbf{A}$ is in the direction of the major axis of the ellipse and its magnitude is essentially the eccentricity of the orbit: $e = A/\alpha m$. For this reason, $\mathbf{A}/m\alpha$ is called the eccentricity vector.

Having developed all these formalisms starting from $U(r)$ in (1) we can close the circle by asking what happens to the eccentricity vector when we add a β/r^2 term. Obviously, if you add a $1/r^3$ component to the force, (which can arise, for example, from the general relativistic corrections to Newton's law of gravitation or because the Sun is not spherical and has a small quadrupole moment) $\mathbf{J}$ and E are still conserved but not $\mathbf{A}$. If the perturbation is small, it will make the direction of $\mathbf{A}$ slowly change in space and we will get a 'precessing' ellipse, which will of course fill a 2-dimensional region. For the potential in (1) we find, using (8), that the rate of change of Runge–Lenz vector is now given by $\dot{\mathbf{A}} = -(2\beta m/r)(\mathrm{d}/\mathrm{d}t)(\mathbf{r}/r)$.

The change $\Delta\mathbf{A}$ per orbit is obtained by integrating $\dot{\mathbf{A}}\mathrm{d}t$ over the range $(0, T)$, where T is the period of the original orbit. Doing one integration by parts and changing the variable of integration from t to the polar angle ϕ, we get $\Delta\mathbf{A}$ per orbit to be

$$\Delta\mathbf{A}\big|_{\text{orbit}} = -2\beta m \int_0^{2\pi} \frac{\mathbf{r}}{r^3}\frac{\mathrm{d}r}{\mathrm{d}\phi}\mathrm{d}\phi. \tag{13}$$

Let us take the coordinate system such that the unperturbed orbit originally had $\mathbf{A}$ pointing along the x-axis. After one orbit, a ΔA_y component will be generated and the major axis of the ellipse would have precessed by an amount $\Delta\phi = \Delta A_y/A$. The ΔA_y can be easily obtained from (13) by using $y = r\sin\phi$, converting the dependent variable from r to $u = (1/r)$ and substituting $(\mathrm{d}u/\mathrm{d}\phi) = -(A/J^2)\sin\phi$ (which comes from (12)). This gives the angle of precession per orbit to be

$$\Delta\phi = \frac{\Delta A_y}{A} = \frac{2\beta m}{A}\int_0^{2\pi} \sin\phi\frac{\mathrm{d}u}{\mathrm{d}\phi}\mathrm{d}\phi = -\frac{2\pi\beta m}{J^2}. \tag{14}$$

Since we have the exact solution in (5), you can easily verify that this is indeed the precession of the orbit when β/r^2 is treated as a perturbation. The Runge–Lenz vector not only allows us to solve the $(1/r)$ problem, but even tells us how an r^{-2} perturbation makes the orbit precess!

We will next consider the quantum version of the same problem. In this case, we first need to solve the Schrödinger equation for the potential in (1). It turns out that this is indeed possible and the analysis proceeds exactly as in the case of normal hydrogen atom problem. Once the angular dependence is separated out using the standard spherical harmonics $Y_{\ell m}(\theta,\phi)$, the radial part of the wavefunction $R(r)$ will satisfy the differential equation

$$R'' + \frac{2}{r}R' + \frac{2m}{\hbar^2}\left\{E - \frac{\hbar^2}{2mr^2}\,\ell(\ell+1) - \frac{\beta}{r^2} + \frac{\alpha}{r}\right\}R = 0\ , \tag{15}$$

where the prime denotes derivative with respect to r and $E(<0)$ is the energy eigenvalue. Introducing a new variable ρ by $\rho = 2(-2mE)^{1/2}r/\hbar$ and two new constants s and n by

$$s(s+1) \equiv \frac{2m\beta}{\hbar^2} + \ell(\ell+1); \qquad n \equiv \frac{\alpha}{\hbar}\left(\frac{m}{-2E}\right)^{1/2}\ , \tag{16}$$

the radial equation can be rewritten as:

$$\frac{\mathrm{d}^2R}{\mathrm{d}\rho^2} + \frac{2}{\rho}\frac{\mathrm{d}R}{d\rho} + \left(-\frac{1}{4} + \frac{n}{\rho} - \frac{s(s+1)}{\rho^2}\right) R = 0 \ . \tag{17}$$

This equation is *identical* to the standard radial equation for the hydrogen atom as you can ascertain by checking it up in any standard textbook. The quantization condition for energy levels now follows in a straightforward manner and you will find that $p \equiv (n - s - 1)$ must be a positive integer or zero for well-behaved solutions to exist. (The s is taken to be the positive root of the quadratic equation in (16).) This allows us to obtain the energy levels to be

$$-E = \frac{2\alpha^2 m}{\hbar^2}\left\{2p + 1 + \left[(2\ell+1)^2 + \frac{8m\beta}{\hbar^2}\right]^{1/2}\right\}^{-2} \ . \tag{18}$$

In the quantum mechanical case, this is the key result we are after since there are no orbits to be determined.

It is again clear that the nature of energy levels changes depending on whether $\beta = 0$ or $\beta \neq 0$. When $\beta \neq 0$ we find that the energy levels depend both on p and ℓ. That is, if we keep p fixed and change ℓ, the energy of the state changes because it depends on both the quantum numbers. On the other hand, when $\beta = 0$, (16) tells us that $s = \ell$. Therefore, the factor inside the curly bracket in (18) reduces to

$$(2n - 2l - 2) + 1 + (2\ell + 1) = 2n \ . \tag{19}$$

In this limit, the energy depends only on the principle quantum number n and becomes independent of the angular quantum number ℓ. The states with same n and different ℓ become degenerate which is the origin of the phrase 'accidental degeneracy of the Coulomb potential'. In a way, this is similar to the classical orbits closing in the case of $\beta = 0$. As I said before, starting from the potential in (1), solving the problem completely and then taking the limit of $\beta \to 0$ helps us to distinguish such 'accidental' results from more generic results.

In the classical Coulomb problem, we could find the orbit purely algebraically using the Runge–Lenz vector without solving a differential equation. Can we do the same thing in the case of quantum mechanics? Can we find the energy levels of the hydrogen atom without explicitly solving the Schrödinger equation? It turns out that this is indeed possible as was first shown by Pauli in 1926.

Unfortunately, the operator algebra which is involved is fairly intense and hence I will just indicate the flow of logic. (One good place to look up the details of the algebra is in [1].)

We begin by defining an operator $\mathbf{M} = \mathbf{A}/m$ corresponding to the classical Runge–Lenz vector (divided by m for convenience). Classically $\mathbf{p} \times \mathbf{J} = -\mathbf{J} \times \mathbf{p}$; but this is not true in quantum mechanics because of the nontrivial commutation relation. Hence the appropriate operator needs to be defined as

$$\mathbf{M} = \frac{1}{2m} (\mathbf{p} \times \mathbf{J} - \mathbf{J} \times \mathbf{p}) - \alpha \frac{\mathbf{r}}{r} , \tag{20}$$

where each term is now an operator. By explicit computation, you can verify that the following identities are satisfied:

$$[\mathbf{M}, H] = 0; \qquad \mathbf{J} \cdot \mathbf{M} = \mathbf{M} \cdot \mathbf{J} \tag{21}$$

and

$$M^2 = \alpha^2 + \frac{2H}{m}(\hbar^2 + J^2) . \tag{22}$$

You can easily see the correspondence between these operator relations and the classical properties of the Runge–Lenz vector given by (10). Further we have the commutation rules, which can be directly obtained from the definition:

$$[J_i, J_j] = i\hbar\epsilon_{ijk}J_k; \quad [M_i, J_j] = i\hbar\epsilon_{ijk}M_k; \quad [M_i, M_j] = -2i(\hbar/m)H\epsilon_{ijk}J_k . \tag{23}$$

The first one is standard; the second reflects the fact that the components of $\mathbf{M}$ behave as a vector under spatial rotations. The really nontrivial one is the third commutation rule which – by a series of manipulations – allows us to deduce the eigen values of H. I will now outline this procedure.

We first note that, since $H, \mathbf{M}, \mathbf{J}$ are constants (in the sense that they all commute with the Hamiltonian), we can confine ourselves to a sub-space of a Hilbert space that corresponds to a particular eigenvalue $E(< 0)$ of the Hamiltonian H. In that case we can replace H by its eigenvalue in the third commutation relations in (23). We then rescale $\mathbf{M}$ by $\mathbf{M}' \equiv (-m/2E)^{1/2}\mathbf{M}$ so that the last two commutation relations in (23) can be expressed in the form

$$[M_i, J_j] = i\hbar\epsilon_{ijk}M_k; \qquad \left[M'_i, M'_j\right] = i\hbar\epsilon_{ijk}J_k , \tag{24}$$

showing that they constitute a closed set. This set can be separated by the usual trick of defining two other operators $\mathbf{I} = (1/2)(\mathbf{J} + \mathbf{M}'), \mathbf{K} = (1/2)(\mathbf{J} - \mathbf{M}')$ which will satisfy the commutation relations:

$$[I_i, I_j] = i\hbar\epsilon_{ijk}I_k; \qquad \left[K_i', K_j'\right] = i\hbar\epsilon_{ijk}K_k \ , \tag{25}$$

with other commutators vanishing. From our knowledge of the angular momentum operators, we know that the spectra of I^2 and K^2 are given by $j(j+1)\hbar^2, k(k+1)\hbar^2$ where $(j,k) = 0, 1/2, 1....$ But since $I^2 - K^2 = \mathbf{J} \cdot \mathbf{M} = 0$, we only need to consider the subspace with $j = k$. Then the operator

$$(1/2)(J^2 + M'^2) = (1/2)(J^2 - (m/2E)M^2) = -m\alpha^2/4E - (1/2)\hbar^2 \ , \tag{26}$$

(where the last relation arises from (22)) will have the spectrum $2k(k+1)\hbar^2$. We thus see that E is quantized in the form:

$$E = -\frac{m\alpha^2}{2\hbar^2(2k+1)^2} \ , \tag{27}$$

which is the standard result.(I will leave it to you to prove that we also get the standard result for the spectrum of J^2.) So, once again, the existence of an extra conserved quantity allows us to solve the problem completely.

Suggested Reading

[1] W Greiner and B Muller, *Quantum Mechanics – Symmetries*, Springer, Chapter 14, 1992.

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