Central forces and the Coulomb problem

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Outline

The two-body problem

Consider two particles, at positions $\mathbf{r}_1$ and $\mathbf{r}_2$, which interact through a rotationally invariant potential, $V(r)$, where $r = |\mathbf{r}|$ and $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$. The Hamiltonian is

$$H_2 = \frac{\mathbf{p}_1^2}{2m_1} + \frac{\mathbf{p}_2^2}{2m_2} + V(r),$$

where operators acting on different particles commute.
We decompose the momenta into the pieces

$$\mathbf{P} = \mathbf{p}_1 + \mathbf{p}_2 \qquad \text{and} \qquad \mathbf{p} = \frac{m_2\mathbf{p}_1 - m_1\mathbf{p}_2}{m_1 + m_2}.$$

Then, defining the reduced mass, $M = m_1 m_2/(m_1 + m_2)$, one can decompose the Hamiltonian as $H_2 = H_{cm} + H$, where

$$H_{cm} = \frac{\mathbf{P}^2}{2(m_1 + m_2)} \qquad \text{and} \qquad H = \frac{\mathbf{p}^2}{2M} + V(r).$$

Now, $\mathbf{r}$ and $\mathbf{p}$ satisfy canonical commutation relations. (**check**)

A tensor decomposition

Define $\mathbf{L} = \mathbf{r} \times \mathbf{p}$. Then H_{cm}, H, L^2 and L_z commute with each other. (**check**) Since $[\mathbf{P}, \mathbf{p}] = 0$, the basis of states can be decomposed into direct products $|E_{cm}\rangle \otimes |Elm\rangle$. This basis uses the eigenkets

$$H|Elm\rangle = E|Elm\rangle, \quad L^2|Elm\rangle = \hbar^2 l(l+1)|Elm\rangle, \quad L_z|Elm\rangle = \hbar m|Elm\rangle,$$

and $H_{cm}|E_{cm}\rangle = E_{cm}|E_{cm}\rangle$.
Since $[H, \mathbf{L}] = 0$, we find that $H\{L_+|Elm\rangle\} = E\{L_+|Elm\rangle\}$. As a result, E does not depend on m, although it can depend on j. Thus each energy level is at least $(2j+1)$-fold degenerate. If there is a higher degree of degeneracy, then there is possibly an overlooked symmetry.
Usually one is interested in the eigenvalues E and the relative wavefunction

$$\langle \mathbf{r}|Elm\rangle = \psi_{Elm}(\mathbf{r}) = \Psi_{El}(r) Y^l_m(\hat{\mathbf{r}}).$$

The state $|E_{cm}\rangle$ is a free particle state, since there is no potential in the direction conjugate to $\mathbf{P}$.

The radial part of the Hamiltonian

To solve for the radial part of the wavefunction, one needs the radial part of the Hamiltonian. Define the radial momentum

$$p_r = \frac{1}{2}(\hat{\mathbf{r}}\cdot\mathbf{p} + \mathbf{p}\cdot\hat{\mathbf{r}}) = \frac{1}{r}(\mathbf{r}\cdot\mathbf{p} - i\hbar) \to -i\hbar\left(\frac{\partial}{\partial r} + \frac{1}{r}\right).$$

One can **check** that $[p_r, r] = i\hbar$, so that $[p_r, f(r)] = -i\hbar df/dr$. It is also straightforward to show that

$$L^2 = (\mathbf{r}\times\mathbf{p})\cdot(\mathbf{r}\times\mathbf{p}) = r^2(p^2 - p_r^2).$$

Hence, the one can write

$$H = \frac{p_r^2}{2M} + \frac{L^2}{2Mr^2} + V(r).$$

The differential equation satisfied by the radial part of the wave function is then

$$\left[-\frac{\hbar^2}{2M}\left(\frac{d}{dr} + \frac{1}{r}\right)^2 + \frac{\hbar^2 l(l+1)}{2Mr^2} + V(r) - E\right]\Psi_{El}(r) = 0.$$

The radial differential equation

Since

$$\left(\frac{d}{dr}+\frac{1}{r}\right)\frac{u(r)}{r}=\frac{1}{r}\frac{du}{dr},$$

By introducing the change of notation $\Psi(r)=u(r)/r$, the differential equation for the radial part of the wavefunction becomes

$$\left[-\frac{\hbar^2}{2M}\frac{d^2}{dr^2}+\frac{\hbar^2 l(l+1)}{2Mr^2}+V(r)-E\right]u_{El}(r)=0,\qquad u_{El}(0)=0.$$

The last condition ensures that the wavefunction remains normalizable. In this form the equation looks like a quasi-one-dimensional equation with an effective potential which is

$$V_{eff}(r)=V(r)+\frac{\hbar^2 l(l+1)}{2Mr^2}.$$

The extra term is positive, and infinite as $r\to 0$. It acts like a barrier, for $l>0$, and prevents particles from probing the region near $r=0$. It is sometimes called the centrifugal barrier.

The radial solution

Since $u(r)$ is regular as $r \to 0$, it must vanish as some positive power of r, *i.e.*, $u(r) \to Cr^z$. This is just that part of the solution which has the slowest approach to zero. Substituting this into the radial differential equation, one finds

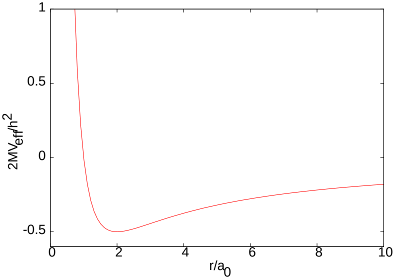
$$-\frac{\hbar^2}{2M}\left\{z(z-1) - l(l+1)\right\} r^{z-2} + \mathcal{O}(r^z) = 0.$$

The coefficient of each power of r has to be equated to zero, and hence $z(z-1) = l(l+1)$. The only positive solution is $z = l + 1$.
Hence, the regularity condition at $r = 0$ reduces to the condition that

$$\overset{\text{Lim}}{r \to 0}\ u_{El}(r) = r^{l+1}.$$

Outline

Scales of the Coulomb problem



For the Coulomb interactions between an electron and a proton (or two electrons, or two protons) $V(r) = \pm e^2/r$. Since $\alpha = e^2/\hbar c$ is dimensionless, we have a fundamental velocity, a fundamental length (Bohr radius), and hence a fundamental frequency (energy, the Rydberg energy) in this problem—

$$v_0 = e^2/\hbar, \qquad a_0 = \frac{\hbar^2}{Me^2}, \qquad E_0 = \frac{Me^4}{2\hbar^2}.$$

For the ep system, the reduced mass $M \simeq m_e$, and hence $E_0 = 13.6$ eV.

The scaled Coulomb problem

Multiplying the radial equation by $2M/\hbar^2$ and then again by a_0^2, one has

$$\left[-\frac{d^2}{d\rho^2} + \frac{l(l+1)}{\rho^2} \pm \frac{2}{\rho} - \lambda^2\right] u_{\lambda,l}(\rho) = 0, \qquad \operatorname*{Lim}_{\rho \to 0} u_{\lambda,l}(\rho) = \rho^{l+1},$$

where $\rho = r/a_0$ and $\lambda^2 = E/E_0$. The sign of the $1/\rho$ term is negative for the Hydrogen atom problem.

There are two types of solutions for the classical problem: when $E < 0$ the motion is bounded, consisting of Keplerian elliptic orbits; when $E > 0$ the motion is unbounded, the orbits being hyperbolae. Solutions of the quantum problem fall into the same classes. From previous experience we expect that energy eigenvalues for the bounded orbits will be quantized, through impositiion of the boundary condition $u(r \to \infty) = 0$, whereas the unbounded orbits will have a continuous energy spectrum.

In the limit $\rho \to \infty$ the potential terms can be neglected. When λ is real (*i.e.*, $E < 0$) one gets the solutions $u \simeq \exp(\pm\lambda\rho)$. Only the decaying exponential is acceptable.

Coulomb bound states

We choose the negative sign for the $1/\rho$ term, and take $\lambda^2 = -E/E_0 > 0$, *i.e.*, flip the sign of the term λ^2. We make the ansatz

$$u_{\lambda,l}(\rho) = \rho^{l+1} \mathrm{e}^{-\lambda\rho} p_{\lambda,l}(\rho), \qquad p_{\lambda,l}(\rho) = \sum_{i=0} c_i \rho^i,$$

where $p(\rho)$ is bounded as $\rho \to 0$ and grows slower than the exponential as $\rho \to \infty$. The differential equation for bound states is

$$\left[-\frac{d^2}{d\rho^2} + 2\left\{\lambda - \frac{l+1}{\rho}\right\}\frac{d}{d\rho} - \frac{2}{\rho}\left\{\lambda(l+1) - 1\right\}\right] p_{\lambda,l}(\rho) = 0.$$

Substituting the series into the equation, one finds a relation between the successive coefficients—

$$i[(i+1) + 2(l+1)]c_{i+1} = 2[\lambda(i+l+1) - 1]c_i.$$

For large i one finds $c_{i+1} \simeq 2\lambda c_i/(i+1)$. Hence, any infinite series solution sums up to $\exp(2\lambda\rho)$, giving $u(\rho)$ which diverges with ρ. Acceptable solutions are, therefore, polynomials. Clearly when $\lambda = 1/n$, c_i vanishes for $i > n - l - 1$. These are the Laguerre polynomials. Normalization fixes c_0.

Coulomb bound state solutions

The Coulomb bound state energies and radial wavefunctions are

$$E(n) = -\frac{E_0}{n^2} \qquad u_{nl}(r) = \left(\frac{r}{a_0}\right)^{l+1} L^{n-l-1}\left(\frac{r}{a_0}\right) \mathrm{e}^{-r/(na_0)}.$$

States n contain $0 \leq l < n$, and hence are n^2-fold degenerate.

Particles	M (MeV)	a_0	E_0	Size
ep	0.51	5.3 nm	13.6 eV	5.3 nm
μp	106	2.8 fm	2.5 KeV	2.5 fm
πp	121	2.2 fm	3.2 KeV	1.9 fm
Kp	323	0.8 fm	8.6 KeV	5.5 fm
e^+e^-	0.25	10.6 nm	6.8 eV	5.3 nm
$\mu^+\mu^-$	53	5.1 fm	1.4 KeV	2.5 fm
$\mathrm{p\bar{p}}$	470	0.6 fm	12.5 KeV	0.3 fm
$\mathrm{c\bar{c}}$	750	0.4 fm	20.0 KeV	0.2 fm
$\mathrm{b\bar{b}}$	2500	0.1 fm	66.7 KeV	0.05 fm

Two problems

1. **Coulomb scattering states**: When $E > 0$, the quantity $\lambda^2 > 0$. Then the asymptotic solutions of the Coulomb radial equation can be taken to be $\exp(\pm i\lambda\rho)$ (either sign is allowed). Now construct the ansatz for the radial part of the wavefunction—
$$u_{\lambda,l}(\rho) = \rho^{l+1} \mathrm{e}^{\pm i\lambda\rho} y_{\lambda,l}(\rho),$$
and examine the solutions of the differential equation for $y_{\lambda,l}(\rho)$. What is the form of y at large ρ? For a given λ what values of l can one have?
2. **The Runge-Lenz vector**: In the classical Coulomb problem the Runge-Lenz vector
$$\mathcal{A} = \hat{\mathbf{r}} - \frac{1}{2} (\mathbf{p} \times \mathbf{L} - \mathbf{L} \times \mathbf{p})$$
is conserved. Check that this remains true in the quantum problem, *i.e.*, $[\mathcal{A}, H] = 0$. Find also the commutators $[L_j, \mathcal{A}_k]$ and $[\mathcal{A}_j, \mathcal{A}_k]$.

Outline

References

1. Quantum Mechanics (Non-relativistic theory), by L. D. Landau and E. M. Lifschitz. The material in this lecture can be found in chapter 5. Both the bound state and scattering state problem are solved.
2. Quantum Mechanics (Vol 1), C. Cohen-Tannoudji, B. Diu and F. Laloë. Chapter 7 of this book discusses angular momentum. The presentation in these lectures follow this chapter occassionally.
3. Classical Mechanics, J. Goldstein. The material on central forces in this book is a pre-requisite for understanding this part of the course.
4. A Handbook of Mathematical Functions, by M. Abramowicz and I. A. Stegun. This is a handy place to look up useful things about various classes of functions.