Central potentials

Sourendu Gupta

TIFR, Mumbai, India

Quantum Mechanics 1 2013
3 October, 2013

Outline

Outline

Conventions

1. From now on we will use units with $\hbar = 1$. As discussed in the previous lecture this will mean $[E] = T^{-1}$, $[J] = 1$ and $[e^2] = LT^{-1}$.
2. We shall understand the difference between operators and eigenvalues in context. The notation with the hat over a symbol will not be used.
3. Instead we will use the notation $\hat{\mathbf{x}}$ to mean the unit vector in the direction of the vector $\mathbf{x}$.
4. For the Coulomb problem we will use the definition of the Bohr radius $a_0 = 1/Me^2$ and the Rydberg, $R = Me^4/2$.

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

Use $\mathbf{L} = \mathbf{r} \times \mathbf{p}$, then H_{cm}, H, L^2 and L_z commute with each other. (check) The states $H_{cm}\,|E_{cm}\rangle = E_{cm}\,|E_{cm}\rangle$, are free particle states, since there is no potential in the coordinate conjugate to $\mathbf{P}$. Also

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

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 a hidden symmetry.

Since $[\mathbf{P}, \mathbf{p}] = [\mathbf{P}, \mathbf{r}] = 0$, the basis of states is the direct product $|E_{cm}\rangle \otimes |Elm\rangle$. 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 radial momentum

Define the radial momentum

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

Note also that

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

so writing $\Psi_{El}(r) = u_{El}(r)/r$, the kinetic energy term becomes

$$-\frac{p_r^2}{2M}\Psi_{El}(r) = -\frac{1}{2M}\frac{d^2}{dr^2}u_{El}(r).$$

Clearly, one must have $u_{El}(0) = 0$ in order to have a normalizable wavefunction $\Psi_{El}(r)$.

The effective potential

It is 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 $H = (p_r^2 + L^2/r^2)/(2M) + V(r)$. The differential equation satisfied by the radial part of the wave function is then

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

In this form the equation looks like a quasi-one-dimensional equation with an effective potential which is

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

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

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

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

$$u_{El}(r) = r^{l+1} y_{El}(r), \quad \text{where} \quad y_{El}(0) \neq 0.$$

With $\Psi_{El}(r) = r^l y_{El}(r)$, the equation for $y(r)$ becomes

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

Outline

The free particle equation

For a free particle $V(r) = 0$. Set $k^2 = 2ME$, then

$$y'' + \frac{2(l+1)}{r} y' + k^2 y = 0.$$

The solution for $l = 0$ is $y(r) = (\sin kr)/r$.
The derivative of the equation is

$$y''' + \frac{2(l+1)}{r} y'' - \frac{2(l+1)}{r^2} y' + k^2 y' = 0.$$

With the definition $w = y'/r$, it is easy to check that this equation can be rewritten as

$$w'' + \frac{2(l+2)}{r} w' + k^2 w = 0.$$

So, starting from the solution for $l = 0$, we can generate the remainder by a recursion.

Free particle wavefunctions

As a result, one has

$$y_{k,l}(r) = \frac{2}{(-k)^l}\left(\frac{1}{r}\frac{d}{dr}\right)^l \frac{\sin kr}{r},$$
$$\Psi_{k,l}(r) = 2\frac{(-r)^l}{k^l}\left(\frac{1}{r}\frac{d}{dr}\right)^l \frac{\sin kr}{r}.$$

As $r \to \infty$, the slowest falling part of the wavefunction is when the derivatives act on $\sin kr$, *i.e.*, $\Psi(r) \simeq \sin(kr - l\pi/2)/r$. One also writes

$$\Psi_{k,l}(r) = \sqrt{\frac{2\pi k}{r}} J_{l+1/2}(kr) = 2kj_l(kr).$$

Clearly, these are expansion coefficients when $\exp(i\mathbf{k}\cdot\mathbf{r})$ is written as a series in Y^l_m.

Problem 12.1: Phase shifts

A short-ranged potential is one in which the dominant long-distance part of the equation is the centrifugal term. The Coulomb potential is not short distance. Any potential which falls faster than $1/r^2$, or goes to zero outside some range, is short-ranged.

For such a potential $V(r)$, the radial wavefunction must asymptotically go to

$$\Psi_{k,l}(r) \simeq \frac{1}{r} \sin\left[kr - \frac{l\pi}{2} + \delta_l(k)\right],$$

where the phase shifts $\delta_l(k)$ can be obtained by matching the wavefunction in the interior region ($V \neq 0$) to that in the exterior region ($V = 0$).

Solve the problem of a spherical "square" well, *i.e.*, $V(r) = -V_0$ for $0 < r < a$ and zero elsewhere. Using this solution find the phase shifts, $\delta_l(k)$, for this potential.

Outline

The scaled Coulomb problem

For the Coulomb potential $V(r) = \pm e^2/r$. Multiplying the radial equation by $2M$ and then again by a_0^2, one has

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

where $\rho = r/a_0$ and $\lambda^2 = E/R$.
In the classical problem, when $E < 0$ the motion is Keplerian, with elliptic orbits; when $E > 0$ the orbits are unbounded and hyperbolic. Quantum solutions fall into the same classes. We expect that energies of the bounded orbits are quantized, through impositiion of the boundary condition $u(r \to \infty) = 0$, but 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 $\lambda^2 = -E/R > 0$, *i.e.*, flip the sign of the term λ^2. We make the ansatz

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

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

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

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.

Coulomb bound state solutions

The Coulomb bound state energies and radial wavefunctions are

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

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

The state with $n = 1$ should then be non-degenerate. However, spectroscopic measurements found a doublet state (W. V. Houston: 1926). This is connected to the observation that isolated electrons come in two states (S. Goudsmit and G. E. Uhlenbeck: 1926). We now understand that pointlike particles may carry angular momentum spin $S^2 = 0$, $3/4$ or 2. The electron has $s = \pm 1/2$. States of the Hydrogen atom are labelled by $|Elms\rangle$, which gives rise to such doubling. The degeneracy of levels should then be $2n^2$.

Scaling the solutions

Particles	M (MeV)	a_0	R	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
$p\bar{p}$	470	0.6 fm	12.5 KeV	0.3 fm
$c\bar{c}$	750	0.4 fm	20.0 KeV	0.2 fm
$b\bar{b}$	2500	0.1 fm	66.7 KeV	0.05 fm

Which of these systems do not have doubled energy levels? The strength of the potential is given by the dimensionless product of the size of the system and the binding. Try to find this for different physical systems and check whether this is universal, or whether non-electromagnetic interactions can be seen in two-body states.

Problem 12.2: the Runge-Lenz vector

$$\mathcal{A} = \hat{\mathbf{r}} - \frac{a_0}{2}(\mathbf{p} \times \mathbf{L} - \mathbf{L} \times \mathbf{p})$$

is a vector operator, therefore $[L_j, \mathcal{A}_k] = i\epsilon_{jkl}\mathcal{A}_l$. Also, one can check that

$$[\mathcal{A}_j, \mathcal{A}_k] = -2iMa_0^2 H \epsilon_{jkl} L_l.$$

Finally, this is a symmetry generator, $[\mathcal{A}_j, H] = 0$. This vector operator can be used to ladder between states $|nlm\rangle$ for varying l. For the bound states, it is more convenient to define

$$A_j = \frac{\mathcal{A}_j}{\sqrt{-2Ma_0^2 E}}, \quad \text{so} \quad [L_j, A_k] = i\epsilon_{jkl}A_l, \quad [A_j, A_k] = i\epsilon_{jkl}L_l.$$

These are the commutation relations for the generators of the group of rotations in 4 (Euclidean) dimensions, *i.e.*, SO(4).

Four dimensional rotations

Define the generators of rotations in 4-dimensions through the operators $L_{ab} = r_a p_b - r_b p_a$ where $a \neq b$ and both indices run from 1 to 4. Then it is a straightforward check that the canonical commutation relations give rise to $[L_{ab}, L_{bc}] = -iL_{ac}$ (when $a \neq b \neq c$).

Now make the identification

$$L = \begin{pmatrix} 0 & L_3 & -L_2 & A_1 \\ & 0 & L_1 & A_2 \\ & & 0 & A_3 \\ & & & 0 \end{pmatrix}.$$

Then with this identification of the components L_{ab} it is clear that the previously computed commutators become exactly those for the generators of SO(4).

For $E > 0$ the definition of $\mathbf{A}$ contains an extra factor of i. The group of symmetries is then the Lorentz group SO(3,1).

Pauli's solution

Define $\mathbf{J}^{\pm} = (\mathbf{L} \pm \mathbf{A})/2$. Then the previous commutators can be written as $[J_j^{\pm}, J_k^{\pm}] = i\epsilon_{jkl} J_l^{\pm}$ and $[J_j^{+}, J_k^{-}] = 0$. Therefore, the bound eigenstates of the Coulomb Hamiltonian can be specified by the eigenvalues of $(J^+)^2$ and $(J^-)^2$. One can easily check that

$$\mathbf{L} \cdot \mathbf{A} = \mathbf{A} \cdot \mathbf{L} = 0, \qquad \text{and} \qquad L^2 + A^2 = -\frac{1}{2Ma_0^2 E} - 1.$$

From these it follows that

$$(J^+)^2 = (J^-)^2 = j(j+1), \qquad \text{and} \qquad 4Ma_0^2 E = -\frac{1}{n^2},$$

where $n = 2j + 1$. Clearly the degeneracy of each level is $(2j_1 + 1)(2j_2 + 1) = n^2$. Since $\mathbf{L} = \mathbf{J}^+ + \mathbf{J}^-$, the allowed values of l are those obtained by a coupling of two angular momenta of magnitude $(n-1)/2$, *i.e.*, $0 \leq l \leq n-1$.

Finding simultaneous eigenvectors of H, A_z and L_z correspond to diagonalizing the Coulomb Hamiltonian in parabolic coordinates.

Problem 12.3: Coulomb scattering states

The Coulomb problem is not short ranged, so the $E > 0$ states are not phase shifted plane waves. Instead they are special functions which are called Coulomb wave functions.

How does the full quantum treatment of Coulomb scattering states differ from the classical phenomena?

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—

$$u_{\lambda,l}(\rho) = \rho^{l+1} e^{\pm i\lambda\rho} y_{\lambda,l}(\rho),$$

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?

Outline

Keywords and References

Keywords

Rotationally invariant potential, reduced mass, hidden symmetry, radial momentum, effective potential, centrifugal barrier, free particle, short-ranged potential, phase shifts, spherical square well, elliptic orbits, hyperbolic orbits, Laguerre polynomials, spin, Lorentz group, Coulomb scattering states, The Runge-Lenz vector,

References

Quantum Mechanics (Non-relativistic theory), by L. D. Landau and E. M. Lifschitz, chapter 5.
Quantum Mechanics (Vol 1), C. Cohen-Tannoudji, B. Diu and F. Laloë, chapter 7.
Classical Mechanics, J. Goldstein.
A Handbook of Mathematical Functions, by M. Abramowicz and I. A. Stegun.