Simple rotationally symmetric potentials

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Quantum Mechanics 1
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1. The free particle
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The free particle equation

The radial differential equation for a free particle is

$$\left[\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + k^2\right] u_{k,l}(r) = 0, \qquad u_{k,l}(r) = r^{l+1} y_{k,l}(r),$$

where $k^2 = 2ME/\hbar^2$, and $\Psi_{k,l}(r) = u_{k,l}(r)/r$. The solution for $l = 0$ is $u_{k,0}(r) = \sin kr$. The equation for $y_{k,l}$ is

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

where we have dropped the subscripts on y to lighten the notation. The derivative of this 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

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

Free particle wavefunctions

As a result, one has

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

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.

Finite range potentials

- For any spherically symmetric potential $V(r)$ which is zero outside some range, 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 ($V = 0$).
- The Coulomb potential is not finite ranged.
- **A problem**: 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.

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The radial equation

The radial differential equation for an isotropic harmonic oscillator is

$$\left[\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} - \frac{M^2\omega^2}{\hbar^2}r^2 + \frac{2ME}{\hbar^2}\right] u_{k,l}(r) = 0, \qquad u_{k,l}(r) = r^{l+1} y_{k,l}(r),$$

where $\Psi_{k,l}(r) = u_{k,l}(r)/r$. Now defining the intrinsic length $a_0 = \sqrt{\hbar/M\omega}$ and defining the dimensionless variables $\rho = r/a_0$ and $\lambda = 2E/\hbar\omega$, we find that the equation becomes

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

At long distances the centrifugal term and λ are sub-dominant. Then the dominant part of the solution is clearly $y \simeq \exp(-\rho^2/2)$. Using this, an appropriate ansatz for the solution would be to write $y_{\lambda,l}(\rho) = p_{\lambda,l}(\rho)\exp(-\rho^2/2)$, where p grows slower than the inverse of the exponential. We insert this ansatz into the radial equation.

The radial solution

The equation for p is found to be

$$\left[\frac{d^2}{d\rho^2} - 2\left(\rho + \frac{l+1}{\rho}\right)\frac{d}{d\rho} - (2l+3-\lambda)\right] p = 0.$$

The radial equation determines that the is even under the (unphysical) transformation $\rho \to -\rho$. As a result, $p(\rho)$ must be either even or odd. However, $c_0 \neq 0$, otherwise the solution at small ρ would have wrong behaviour. Hence, the solutions have only even powers of ρ. Using the Taylor expansion $p = \sum_j c_j \rho^j$, we get a recurrence relation for the coefficients

$$(j+2)(j-2l-1)c_{j+2} = (2j+2l+3-\lambda)c_j.$$

The non-terminating solution grows too fast, and must be discarded. When $\lambda = 2n+3$, solutions terminate at the $(n-l)$-th term, which is even. The ground state, $n=0$ (hence $E = 3\hbar\omega/2$) has $l=0$; the first excited state, $n=1$, *i.e.*, $E = 5\hbar\omega/2$, has $l=1$; the second excited state, $n=2$, *i.e.*$E = 7\hbar\omega/2$, has $l=0$ and 2.

The complete symmetry of the problem

Write the Hamiltonian for the isotropic harmonic oscillator in the form

$$H = \hbar\omega \left[\frac{3}{2} + \sum_{j=1}^{3} a_j^\dagger a_j \right],$$

where $a_j = (M\omega r_j + ip_j)/\sqrt{2M\hbar\omega}$ are lowering operators. The eigenstates are $|n_x, n_y, n_z\rangle$, and they form an alternate basis on the space spanned by $|nlm\rangle$ with $n = n_x + n_y + n_z$. Now construct the operators

$$T_{ij} = \frac{1}{2}(a_i^\dagger a_j + a_j^\dagger a_i), \qquad [T_{ij}, T_{kl}] = \delta_{jk} T_{il} - \delta_{il} T_{jk}.$$

They do not change n, and hence commute with H. Only eight of these are independent, and they form the algebra called su(3). Exponentials of these operators are the symmetry group of the problem, and is called SU(3).

A problem

Check that $L_j = -i\hbar\epsilon_{jkl}T_{kl}$. Also, define the operators

$$A_{ij} = \frac{1}{2}\hbar\omega(T_{ij} + T_{ji}) = \frac{1}{2M}(p_i p_j + M^2\omega^2 r_i r_j).$$

Note that the corresponding classical operators are conserved. Explicitly construct the eigenvectors of the classical tensor **A** (considered as a 3×3 matrix) and find the relation between the orbit of oscillator and these eigenvectors.
Define the quantities $a_\pm = a_1 \pm ia_2$, $a_0 = a_3$ and their Hermitean conjugate operators. Find the commutators of these operators with L_j. Using these raising and lowering operators, construct

$$\begin{aligned} Q_0 &= \hbar[2a_0^\dagger a_0 - \frac{1}{2}(a_-^\dagger a_+ + a_+^\dagger a_-)], \\ Q_{\pm 1} &= \mp\hbar[a_0^\dagger a_\pm + a_\pm^\dagger a_0], \\ Q_{\pm 2} &= \hbar a_\pm^\dagger a_\pm. \end{aligned}$$

Find the commutators of the Q_λ with each other and with the L_i. How are they related to T_{ij}? Compute $Q_\lambda|nlm\rangle$.

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The Runge-Lenz vector

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

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

$$[\mathcal{A}_j, \mathcal{A}_k] = -i\frac{2Ma_0^2 H}{\hbar^2}\epsilon_{jkl}L_l.$$

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

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

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 $[L_{ab}, L_{bc}] = -i\hbar L_{ac}$ (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 $[J_j^{\pm}, J_k^{\pm}] = i\hbar\epsilon_{jkl}J_l^{\pm}$ 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

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

From these it follows that

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

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.*, $0 \le l \le n-1$.
Finding simultaneous eigenvectors of H, A_z and L_z correspond to diagonalizing the Coulomb Hamiltonian in parabolic coordinates.

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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 for the Coulomb potential are solved. The solution in parabolic coordinates is also given.
2. Quantum Mechanics (Vol 1), C. Cohen-Tannoudji, B. Diu and F. Laloë. Chapter 7 of this book discusses central potentials.
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. Classical groups for Physicists, by B. G. Wybourne. This book is highly recommended for a good exposition of Lie groups, and contains material of direct relevance to this lecture.
5. 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.