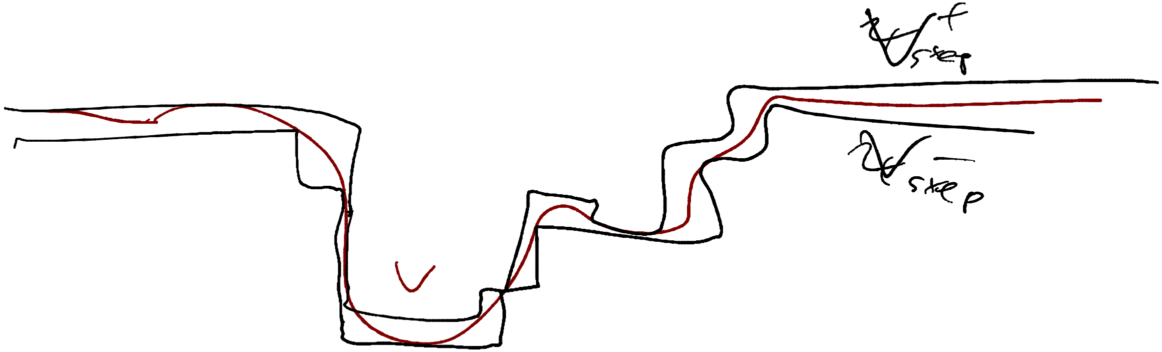
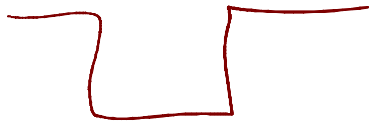
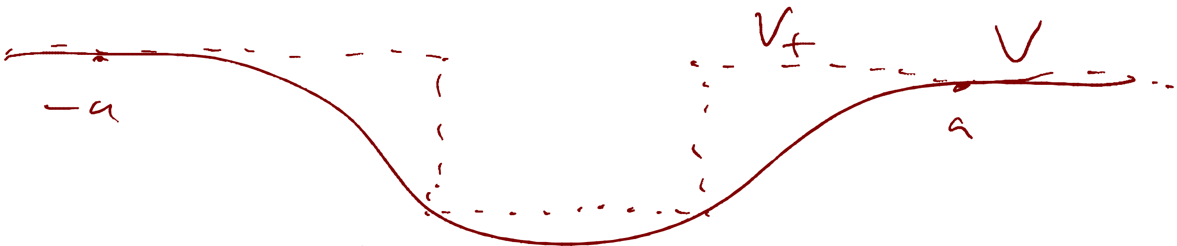


$$\lim V^{\pm}_{step} \to V$$





V_+ is a square well st $V_+(x) = 0$ for $|x| \geq a$

$V_+(x) \geq V(x) \quad (\forall x)$

There is at least one -ve energy bound state ψ_0 for the SE with potential $V_+(x)$

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V_+(x)\right)\psi_0(x) = E\,\psi_0(x)$$

$$E < 0.$$

Suppose all energy eigenvalues for SE with pot $V(x)$ are <u>positive</u>.

Then we can expand $\psi_0(x)$ as a superposition $\sum_{i=1}^{\infty} c_i \psi_i'(x)$ (or continuous sum) of eigenstates ψ_i' with eigenvalues $E_i > 0$.

Now $0 > E = \langle \hat{H} \rangle_{\psi_0} < 0$ where $\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V_+(x)$.

$$= \int \psi_0^*(x)\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V_+(x)\right)\psi(x)\,dx$$

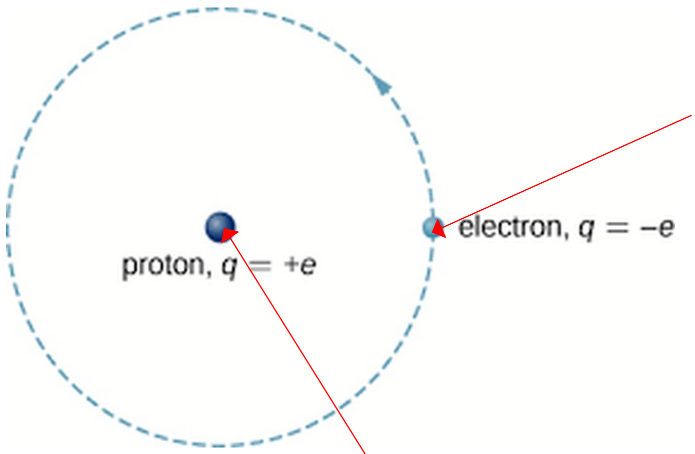
$$> \int \psi_0^*(x)\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right)\psi(x)\,dx = \langle \hat{H}' \rangle_{\psi_0}$$

where $\hat{H}' = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)$.

However $\langle \hat{H}' \rangle_{\psi_0} = \left(\sum c_i \psi_i'(x), \hat{H}' \sum c_i \psi_i(x)\right) = \sum |c_i|^2 E_i > 0.$

Spherically symmetric bound states of the hydrogen atom

We model the hydrogen atom by treating the proton as infinitely massive and at rest.



modelled as single particle wave function in Coulomb potential

modelled by Coulomb potential

m_p ~ 1836 m_e
so this is a pretty good approximation

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Try the ansatz

$$\psi(r) \approx \exp(-br)\,, \tag{7.26}$$

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our ansatz has $\psi(r)$ continuous at $r=0$

Is that justified?

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$-\frac{\hbar^2}{2m} \nabla^2 \psi + V\psi = E\psi$.

ψ discontinuous $\sim A\,\theta(x)$ at $x=0$.

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I.e. $\psi(r) = \left(\sum_{n=0}^{\infty} a_n r^n \right) e^{-br}$

(not $n=-1$)

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Taking the coefficient of r^{n-2} we have

$$a_n n(n-1) + 2a_n n - 2ba_{n-1}(n-1) + (a-2b)a_{n-1} = 0 \text{ for } n \geq 1\,. \tag{7.29}$$

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This gives

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$$e^{2br} = \sum \frac{1}{n!}(2br)^n = \sum c_n r^n$$

$$\frac{c_n}{c_{n-1}} = \frac{2b}{n}.$$

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Then $a_{N-1} \neq 0$, so that $a_N = 0$ implies $2bN = a$ or $b = a/2N$,

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and generally $f(r) = L^1_{N-1}(2br)$ where L^1_{N-1} is one of the *associated Laguerre polynomials*.

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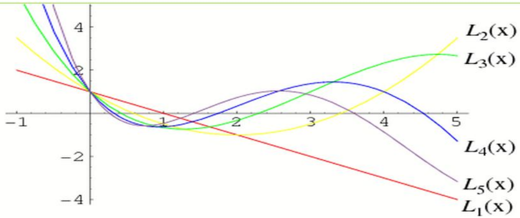
Laguerre Polynomial



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The corresponding wavefunctions are
$\psi(r) = C L_{N-1}^1(2br) \exp(-br)$, where the constant C is determined by normalisation.

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By calculating the action on a general wavefunction as before, we obtain

$$[\hat{x}_i, \hat{x}_j] = 0 = [\hat{p}_i, \hat{p}_j] \tag{7.37}$$

Canonical Commutation Relations in 3D

From (7.2) we have

$$\hat{x}_i = x_i \qquad (\text{ multiplication by } x_i)\,, \tag{7.35}$$

$$\hat{p}_i = -i\hbar\frac{\partial}{\partial x_i}\,. \tag{7.36}$$

By calculating the action on a general wavefunction as before, we obtain

$$[\hat{x}_i, \hat{x}_j] = 0 = [\hat{p}_i, \hat{p}_j] \tag{7.37}$$

$$[\hat{x}_i, \hat{p}_j] = i\hbar\delta_{ij}\,. \tag{7.38}$$

Orbital Angular Momentum

In classical mechanics we define the angular momentum vector

$$\underline{L} = \underline{x} \wedge \underline{p} \, ,$$

Orbital Angular Momentum

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$$\underline{L} = \underline{x} \wedge \underline{p}\,, \qquad L_i = \epsilon_{ijk} x_j p_k\,, \tag{7.39}$$

Orbital Angular Momentum

In classical mechanics we define the angular momentum vector

$$\underline{L} = \underline{x} \wedge \underline{p}\,, \qquad \hat{L}_i = \epsilon_{ijk} x_j \hat{p}_k\,, \tag{7.39}$$

$$\hat{L}_1 = \hat{x}_2 \hat{p}_3 - \hat{x}_3 \hat{p}_2$$

and $\underline{L}$ is conserved in a spherically symmetric potential $V(r)$.

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$$\underline{\hat{L}} = -i\hbar \underline{\hat{x}} \wedge \underline{\nabla}\,, \qquad \hat{L}_i = -i\hbar \epsilon_{ijk} \hat{x}_j \frac{\partial}{\partial x_k}\,, \tag{7.40}$$

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and the total angular momentum

$$\hat{L}^2 = \hat{\underline{L}}.\hat{\underline{L}}$$

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and the total angular momentum

$$\hat{L}^2 = \hat{\underline{L}}.\hat{\underline{L}} = \hat{L}_1^2 + \hat{L}_2^2 + \hat{L}_3^2\,. \tag{7.41}$$

Orbital Angular Momentum

$$[\hat{L}_i, \hat{L}_j] = -\hbar^2 \epsilon_{ilm}\epsilon_{jnp}[\hat{x}_l \frac{\partial}{\partial x_m}, \hat{x}_n \frac{\partial}{\partial x_p}]$$

Orbital Angular Momentum

$$
\begin{aligned}
[\hat{L}_i, \hat{L}_j] &= -\hbar^2 \epsilon_{ilm}\epsilon_{jnp}[\hat{x}_l \frac{\partial}{\partial x_m}, \hat{x}_n \frac{\partial}{\partial x_p}] \\
&= -\hbar^2 \epsilon_{ilm}\epsilon_{jnp}([\hat{x}_l \frac{\partial}{\partial x_m}, \hat{x}_n] \frac{\partial}{\partial x_p} + \hat{x}_n [\hat{x}_l \frac{\partial}{\partial x_m}, \frac{\partial}{\partial x_p}])
\end{aligned}
$$

Orbital Angular Momentum

$$
\begin{aligned}
[\hat{L}_i, \hat{L}_j] &= -\hbar^2 \epsilon_{ilm}\epsilon_{jnp}[\hat{x}_l \frac{\partial}{\partial x_m}, \hat{x}_n \frac{\partial}{\partial x_p}] \\
&= -\hbar^2 \epsilon_{ilm}\epsilon_{jnp}([\hat{x}_l \frac{\partial}{\partial x_m}, \hat{x}_n]\frac{\partial}{\partial x_p} + \hat{x}_n[\hat{x}_l \frac{\partial}{\partial x_m}, \frac{\partial}{\partial x_p}]) \\
&= -\hbar^2 \epsilon_{ilm}\epsilon_{jnp}(\hat{x}_l[\frac{\partial}{\partial x_m}, \hat{x}_n]\frac{\partial}{\partial x_p} + \hat{x}_n[\hat{x}_l, \frac{\partial}{\partial x_p}]\frac{\partial}{\partial x_m})
\end{aligned}
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[\hat{L}_i, \hat{L}_j] &= -\hbar^2 \epsilon_{ilm}\epsilon_{jnp}[\hat{x}_l \frac{\partial}{\partial x_m}, \hat{x}_n \frac{\partial}{\partial x_p}] \\
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&= -\hbar^2 \epsilon_{ilm}\epsilon_{jnp}(\hat{x}_l[\frac{\partial}{\partial x_m}, \hat{x}_n]\frac{\partial}{\partial x_p} + \hat{x}_n[\hat{x}_l, \frac{\partial}{\partial x_p}]\frac{\partial}{\partial x_m}) \\
&= -\hbar^2 \epsilon_{ilm}\epsilon_{jnp}(\hat{x}_l \delta_{mn}\frac{\partial}{\partial x_p} - \hat{x}_n \delta_{lp}\frac{\partial}{\partial x_m})
\end{aligned}
$$

Orbital Angular Momentum

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\begin{aligned}
[\hat{L}_i, \hat{L}_j] &= -\hbar^2 \epsilon_{ilm}\epsilon_{jnp}[\hat{x}_l \frac{\partial}{\partial x_m}, \hat{x}_n \frac{\partial}{\partial x_p}] \\
&= -\hbar^2 \epsilon_{ilm}\epsilon_{jnp}([\hat{x}_l \frac{\partial}{\partial x_m}, \hat{x}_n]\frac{\partial}{\partial x_p} + \hat{x}_n[\hat{x}_l \frac{\partial}{\partial x_m}, \frac{\partial}{\partial x_p}]) \\
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&= -\hbar^2 \epsilon_{ilm}\epsilon_{jnp}(\hat{x}_l \delta_{mn}\frac{\partial}{\partial x_p} - \hat{x}_n \delta_{lp}\frac{\partial}{\partial x_m}) \\
&= -\hbar^2 \epsilon_{mil}\epsilon_{mpj}\hat{x}_l \frac{\partial}{\partial x_p} - \hbar^2 \epsilon_{pjn}\epsilon_{pmi}\hat{x}_n \frac{\partial}{\partial x_m})
\end{aligned}
$$

Orbital Angular Momentum

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\begin{aligned}
[\hat{L}_i, \hat{L}_j] &= -\hbar^2 \epsilon_{ilm}\epsilon_{jnp}[\hat{x}_l \frac{\partial}{\partial x_m}, \hat{x}_n \frac{\partial}{\partial x_p}] \\
&= -\hbar^2 \epsilon_{ilm}\epsilon_{jnp}([\hat{x}_l \frac{\partial}{\partial x_m}, \hat{x}_n] \frac{\partial}{\partial x_p} + \hat{x}_n [\hat{x}_l \frac{\partial}{\partial x_m}, \frac{\partial}{\partial x_p}]) \\
&= -\hbar^2 \epsilon_{ilm}\epsilon_{jnp}(\hat{x}_l [\frac{\partial}{\partial x_m}, \hat{x}_n] \frac{\partial}{\partial x_p} + \hat{x}_n [\hat{x}_l, \frac{\partial}{\partial x_p}] \frac{\partial}{\partial x_m}) \\
&= -\hbar^2 \epsilon_{ilm}\epsilon_{jnp}(\hat{x}_l \delta_{mn} \frac{\partial}{\partial x_p} - \hat{x}_n \delta_{lp} \frac{\partial}{\partial x_m}) \\
&= -\hbar^2 \epsilon_{mil}\epsilon_{mpj} \hat{x}_l \frac{\partial}{\partial x_p} - \hbar^2 \epsilon_{pjn}\epsilon_{pmi} \hat{x}_n \frac{\partial}{\partial x_m}) \\
&= -\hbar^2 (\delta_{ip}\delta_{lj} - \delta_{ij}\delta_{lp}) \hat{x}_l \frac{\partial}{\partial x_p} - (\delta_{jm}\delta_{ni} - \delta_{ji}\delta_{nm})(\hat{x}_n \frac{\partial}{\partial x_m})
\end{aligned}
$$

Orbital Angular Momentum

$$
\begin{aligned}
[\hat{L}_i, \hat{L}_j] &= -\hbar^2 \epsilon_{ilm}\epsilon_{jnp}[\hat{x}_l \frac{\partial}{\partial x_m}, \hat{x}_n \frac{\partial}{\partial x_p}] \\
&= -\hbar^2 \epsilon_{ilm}\epsilon_{jnp}([\hat{x}_l \frac{\partial}{\partial x_m}, \hat{x}_n] \frac{\partial}{\partial x_p} + \hat{x}_n [\hat{x}_l \frac{\partial}{\partial x_m}, \frac{\partial}{\partial x_p}]) \\
&= -\hbar^2 \epsilon_{ilm}\epsilon_{jnp}(\hat{x}_l [\frac{\partial}{\partial x_m}, \hat{x}_n] \frac{\partial}{\partial x_p} + \hat{x}_n [\hat{x}_l, \frac{\partial}{\partial x_p}] \frac{\partial}{\partial x_m}) \\
&= -\hbar^2 \epsilon_{ilm}\epsilon_{jnp}(\hat{x}_l \delta_{mn} \frac{\partial}{\partial x_p} - \hat{x}_n \delta_{lp} \frac{\partial}{\partial x_m}) \\
&= -\hbar^2 \epsilon_{mil}\epsilon_{mpj} \hat{x}_l \frac{\partial}{\partial x_p} - \hbar^2 \epsilon_{pjn}\epsilon_{pmi} \hat{x}_n \frac{\partial}{\partial x_m}) \\
&= -\hbar^2 (\delta_{ip}\delta_{lj} - \delta_{ij}\delta_{lp}) \hat{x}_l \frac{\partial}{\partial x_p} - (\delta_{jm}\delta_{ni} - \delta_{ji}\delta_{nm})(\hat{x}_n \frac{\partial}{\partial x_m}) \\
&= -\hbar^2 (\hat{x}_j \frac{\partial}{\partial x_i} - \delta_{ij} \hat{x}_l \frac{\partial}{\partial x_l} - \hat{x}_i \frac{\partial}{\partial x_j} + \delta_{ij} \hat{x}_l \frac{\partial}{\partial x_l}
\end{aligned}
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Orbital Angular Momentum

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\begin{aligned}
[\hat{L}_i, \hat{L}_j] &= -\hbar^2 \epsilon_{ilm}\epsilon_{jnp}[\hat{x}_l \frac{\partial}{\partial x_m}, \hat{x}_n \frac{\partial}{\partial x_p}] \\
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&= -\hbar^2 \epsilon_{ilm}\epsilon_{jnp}(\hat{x}_l[\frac{\partial}{\partial x_m}, \hat{x}_n]\frac{\partial}{\partial x_p} + \hat{x}_n[\hat{x}_l, \frac{\partial}{\partial x_p}]\frac{\partial}{\partial x_m}) \\
&= -\hbar^2 \epsilon_{ilm}\epsilon_{jnp}(\hat{x}_l \delta_{mn}\frac{\partial}{\partial x_p} - \hat{x}_n \delta_{lp}\frac{\partial}{\partial x_m}) \\
&= -\hbar^2 \epsilon_{mil}\epsilon_{mpj}\hat{x}_l \frac{\partial}{\partial x_p} - \hbar^2 \epsilon_{pjn}\epsilon_{pmi}\hat{x}_n \frac{\partial}{\partial x_m}) \\
&= -\hbar^2(\delta_{ip}\delta_{lj} - \delta_{ij}\delta_{lp})\hat{x}_l \frac{\partial}{\partial x_p} - (\delta_{jm}\delta_{ni} - \delta_{ji}\delta_{nm})(\hat{x}_n \frac{\partial}{\partial x_m}) \\
&= -\hbar^2(\hat{x}_j \frac{\partial}{\partial x_i} - \delta_{ij}\hat{x}_l \frac{\partial}{\partial x_l} - \hat{x}_i \frac{\partial}{\partial x_j} + \delta_{ij}\hat{x}_l \frac{\partial}{\partial x_l} \\
&= i\hbar\epsilon_{ijk}\hat{L}_k\,. \qquad (7.42)
\end{aligned}
$$

Orbital Angular Momentum

$$[\hat{L}^2, \hat{L}_i] \quad = \quad [\hat{L}_j \hat{L}_j, \hat{L}_i]$$

Orbital Angular Momentum

$$
\begin{aligned}
[\hat{L}^2, \hat{L}_i] &= [\hat{L}_j \hat{L}_j, \hat{L}_i] \\
&= [\hat{L}_j, \hat{L}_i]\hat{L}_j + \hat{L}_j[\hat{L}_j, \hat{L}_i]
\end{aligned}
$$

Orbital Angular Momentum

$$\begin{aligned}
[\hat{L}^2, \hat{L}_i] &= [\hat{L}_j \hat{L}_j, \hat{L}_i] \\
&= [\hat{L}_j, \hat{L}_i]\hat{L}_j + \hat{L}_j[\hat{L}_j, \hat{L}_i] \\
&= i\hbar(\epsilon_{jik}(\hat{L}_k \hat{L}_j + \hat{L}_j \hat{L}_k))
\end{aligned}$$

Orbital Angular Momentum

$$\begin{aligned}
[\hat{L}^2, \hat{L}_i] &= [\hat{L}_j \hat{L}_j, \hat{L}_i] \\
&= [\hat{L}_j, \hat{L}_i]\hat{L}_j + \hat{L}_j[\hat{L}_j, \hat{L}_i] \\
&= i\hbar(\epsilon_{jik}(\hat{L}_k \hat{L}_j + \hat{L}_j \hat{L}_k)) \\
&= 0 \,. \qquad (7.43)
\end{aligned}$$

Orbital Angular Momentum

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\begin{aligned}
[\hat{L}^2, \hat{L}_i] &= [\hat{L}_j \hat{L}_j, \hat{L}_i] \\
&= [\hat{L}_j, \hat{L}_i]\hat{L}_j + \hat{L}_j[\hat{L}_j, \hat{L}_i] \\
&= i\hbar(\epsilon_{jik}(\hat{L}_k \hat{L}_j + \hat{L}_j \hat{L}_k)) \\
&= 0\,. \qquad (7.43)
\end{aligned}
$$

Since the $\hat{L}_i$ do not commute, they are not simultaneously diagonalisable.

Orbital Angular Momentum

$$
\begin{aligned}
[\hat{L}^2, \hat{L}_i] &= [\hat{L}_j \hat{L}_j, \hat{L}_i] \\
&= [\hat{L}_j, \hat{L}_i]\hat{L}_j + \hat{L}_j[\hat{L}_j, \hat{L}_i] \\
&= i\hbar(\epsilon_{jik}(\hat{L}_k \hat{L}_j + \hat{L}_j \hat{L}_k)) \\
&= 0\,. \qquad (7.43)
\end{aligned}
$$

Since the $\hat{L}_i$ do not commute, they are not simultaneously diagonalisable.However, $\hat{L}^2$ and any one of the $\hat{L}_i$ can be simultaneously diagonalised, since $[\hat{L}^2, \hat{L}_i] = 0$.

eg $\hat{L}_3$

S.t. $[\hat{L}_3, \hat{L}_2] \neq 0$

so not $\hat{L}_3$ and $\hat{L}_2$.

Orbital Angular Momentum

We also have

$$[\hat{L}_i, \hat{x}_j] = i\hbar\epsilon_{ijk}\hat{x}_k\,, \qquad (7.44)$$

Orbital Angular Momentum

We also have

$$[\hat{L}_i, \hat{x}_j] = i\hbar\epsilon_{ijk}\hat{x}_k \,, \quad (7.44)$$

$$[\hat{L}_i, \hat{p}_j] = i\hbar\epsilon_{ijk}\hat{p}_k \,, \quad (7.45)$$

Orbital Angular Momentum

We also have

$$[\hat{L}_i, \hat{x}_j] = i\hbar\epsilon_{ijk}\hat{x}_k\,, \tag{7.44}$$

$$[\hat{L}_i, \hat{p}_j] = i\hbar\epsilon_{ijk}\hat{p}_k\,, \tag{7.45}$$

$$[\hat{L}_i, \sum_j \hat{x}_j^2] = 2i\hbar\epsilon_{ijk}\hat{x}_j\hat{x}_k = 0\,, \tag{7.46}$$

Orbital Angular Momentum

We also have

$$[\hat{L}_i, \hat{x}_j] = i\hbar\epsilon_{ijk}\hat{x}_k \,, \tag{7.44}$$

$$[\hat{L}_i, \hat{p}_j] = i\hbar\epsilon_{ijk}\hat{p}_k \,, \tag{7.45}$$

$$[\hat{L}_i, \sum_j \hat{x}_j^2] = 2i\hbar\epsilon_{ijk}\hat{x}_j\hat{x}_k = 0\,, \tag{7.46}$$

$$[\hat{L}_i, \sum_j \hat{p}_j^2] = 2i\hbar\epsilon_{ijk}\hat{p}_j\hat{p}_k = 0\,. \tag{7.47}$$

Orbital Angular Momentum

Now we have that $\hat{r} = \sqrt{\sum_j \hat{x}_j^2}$.

Orbital Angular Momentum

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Orbital Angular Momentum

Now we have that $\hat{r} = \sqrt{\sum_j \hat{x}_j{}^2}$. We also have that $[\hat{L}_i, \sum_j \hat{x}_j{}^2] = 0$. One can show from this that $[\hat{L}_i, \hat{r}] = 0$.

Orbital Angular Momentum

Now we have that $\hat{r} = \sqrt{\sum_j \hat{x}_j{}^2}$. We also have that $[\hat{L}_i, \sum_j \hat{x}_j{}^2] = 0$. One can show from this that $[\hat{L}_i, \hat{r}] = 0$. More generally, one can show that $[\hat{L}_i, V(r)] = 0$ for any spherically symmetric potential $V(r)$.