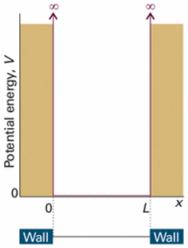
Summary for Chapter 9 Application of Quantum Mechanism

<table>
<tr><th>Motion Mode</th><th>Schrodinger equation</th><th>Wave function</th><th>Energy</th><th>Energy level</th><th>Energy properties</th></tr>
<tr>
<td rowspan="5">

Translation

Quantum number

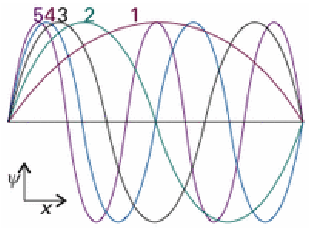
n=1,2,



</td>
<td>$\hat{\mathrm{H}}\psi = E\psi$
$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$</td>
<td rowspan="2">

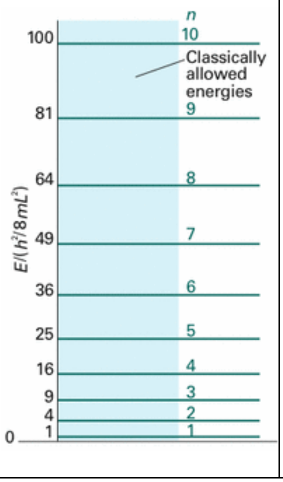
$\psi_n(x) = \left(\frac{2}{L}\right)^2 \sin\left(\frac{n\pi x}{L}\right)$

$0 \le x \le l$; n= 1, 2 …

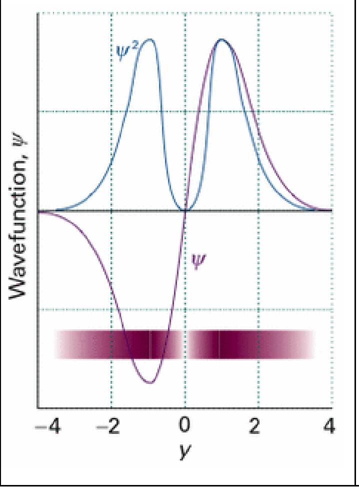
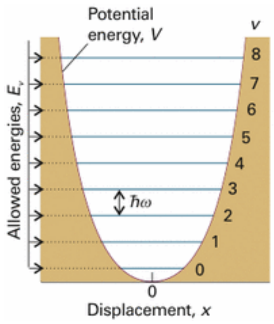


The first five normalized wavefunctions of a particle in a box.

</td>
<td rowspan="2">$E_n = \frac{n^2h^2}{8mL^2}$
n= 1, 2 …</td>
<td rowspan="2">



</td>
<td rowspan="2">(1) $E_n = \frac{n^2h^2}{8mL^2}$ n= 1, 2 …
(2) $E_{n+1} - E_n = \frac{(n+1)^2h^2}{8mL^2} - \frac{n^2h^2}{8mL^2} = (2n+1)\frac{h^2}{8mL^2}$
(3) $E_1 = \frac{h^2}{8mL^2}$</td>
</tr>
<tr>
<td>$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = E\psi$</td>
</tr>
<tr><td colspan="5">Probability</td></tr>
<tr>
<td colspan="2">The probability of finding the particle in a region between x = 0 and x = l
$P = \int_0^l \psi_n^2\,\mathrm{d}x = \frac{2}{L}\int_0^l \sin^2\frac{n\pi x}{L}\,\mathrm{d}x = \frac{l}{L} - \frac{1}{2n\pi}\sin\frac{2\pi nl}{L}$</td>
<td colspan="3">The probability of finding the particle in a region between x = a and x = b
$P = \frac{b-a}{L} - \frac{1}{2\pi}\left(\sin\frac{2\pi b}{L} - \sin\frac{2\pi a}{L}\right)$</td>
</tr>
<tr>
<td colspan="5">Expectation value
the average value of the linear momentum of a particle in a box: $\langle p\rangle = 0$
the average value of p^2 : $\langle p^2\rangle = n^2h^2/4L^2$</td>
</tr>
</table>

<table>
<tr><th>Motion Mode</th><th>Schrodinger equation</th><th>Wave function</th><th>Energy</th><th>Energy level</th><th>Energy properties</th></tr>
<tr>
<td rowspan="2">Vibration
Quantum number
$v = 0,\ 1,\ 2\ ...$</td>
<td>$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}+\frac{1}{2}kx^2\psi=E\psi$
k : force constant</td>
<td>$\psi_v(x)=N_vH_v(y)e^{-y^2/2}$
$y=\frac{x}{\alpha};\quad \alpha=\left(\frac{\hbar^2}{mk}\right)^{1/2}$
 </td>
<td>$E_v=\left(v+\frac{1}{2}\right)\hbar\omega$
$\omega=\left(\frac{k}{m}\right)^{1/2}$
$v=0,1,2...$</td>
<td> </td>
<td>(1)
$E_v=\left(v+\frac{1}{2}\right)\hbar\omega$
(2)
$E_{v+1}-E_v=\hbar\omega$
(3)
$E_0=\frac{1}{2}\hbar\omega$</td>
</tr>
<tr>
<td colspan="5">$\langle x\rangle=0\qquad \langle x^2\rangle=(v+\frac{1}{2})\frac{\hbar}{(mk)^{1/2}}$
$\langle V\rangle=\langle\frac{1}{2}kx^2\rangle=\frac{1}{2}(v+\frac{1}{2})\hbar\left(\frac{k}{m}\right)^{1/2}=\frac{1}{2}(v+\frac{1}{2})\hbar\omega\qquad \langle V\rangle=\frac{1}{2}E_v\ \ \langle E_K\rangle=\frac{1}{2}E_v$</td>
</tr>
</table>

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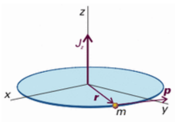
<tr><th>Motion Mode</th><th>Schrodinger equation</th><th>Wave function</th><th>Angular momentum</th><th>Energy</th><th>Energy properties</th></tr>
<tr><td rowspan="2">Rotation
Quantum number
$m_l = 0, \pm 1, \pm 2 \ldots$
 </td>
<td>$\frac{d^2\psi}{d\phi^2} = -\frac{2IE}{\hbar^2}\psi$
$\hat{H} = -\frac{\hbar^2}{2I}\frac{d^2}{d\phi^2}$</td>
<td>$\psi_{m_l}(\phi) = \frac{e^{im_l\phi}}{(2\pi)^{1/2}}$
$\Psi_0(\varphi) = 1/(2\pi)^{1/2}$</td>
<td>$J_Z = m_l\hbar$
$\hat{l}_z = \frac{\hbar}{i}\frac{\partial}{\partial\phi}$</td>
<td>$E = \frac{J_z^2}{2I} = \frac{m_l^2\hbar^2}{2I}$</td>
<td>Degeneracy
states with a given value of $|m_l|$ are doubly degenerate, except for $m_l = 0$, which is non-degenerate.</td></tr>
<tr><td colspan="5">(1) cyclic boundary condition: $\Psi(\varphi + 2\pi) = \Psi(\varphi)$
$\psi_{m_l}(\phi + 2\pi) = \frac{e^{im_l(\phi+2\pi)}}{(2\pi)^{1/2}} = \frac{e^{im_l\phi}e^{2\pi i m_l}}{(2\pi)^{1/2}} = \psi_{m_l}(\phi)e^{2\pi i m_l}$
$(-1)^{2m_l} = 1,\ m_l = 0, \pm1, \pm2, \ldots$
(2) Probability density
$\psi_{m_l}^{*}\psi_{m_l} = \left(\frac{e^{im_l\phi}}{(2\pi)^{1/2}}\right)^{*}\left(\frac{e^{im_l\phi}}{(2\pi)^{1/2}}\right) = \left(\frac{e^{-im_l\phi}}{(2\pi)^{1/2}}\right)\left(\frac{e^{im_l\phi}}{(2\pi)^{1/2}}\right) = \frac{1}{2\pi}$
(3) Angular momentum
$\hat{l}_z\psi_{m_l} = \frac{\hbar}{i}\frac{d\psi_{m_l}}{d\phi} = im_l\frac{\hbar}{i}e^{im_l\phi} = m_l\hbar\psi_{m_l}$</td></tr>
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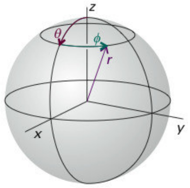
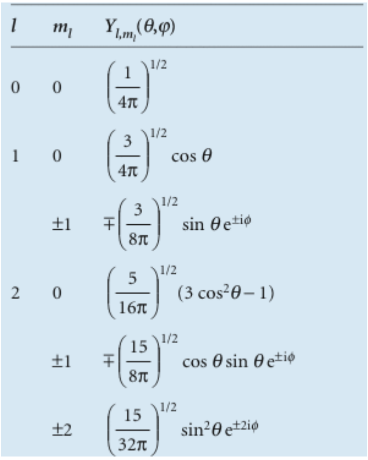
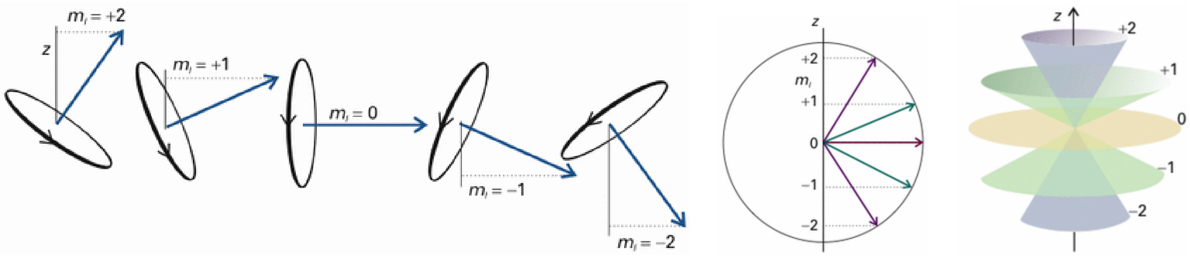
<tr><th>Motion Mode</th><th>Schrodinger equation</th><th>Wave function</th><th>Angular momentum</th><th>Energy</th><th>Energy properties</th></tr>
<tr><td rowspan="3">Particle on a Sphere


$l= 0, 1,2 \ldots$
$m_l= l, l-1, \ldots, -l$</td><td rowspan="2">$\Lambda^2\psi=-\varepsilon\psi \qquad \varepsilon=\frac{2IE}{\hbar^2}$
$\Lambda^2=\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}+\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta}$</td><td rowspan="2">spherical harmonics
$Y_{l},m_{l}(\theta,\varphi)$
<table><tr><th>l</th><th>m_l</th><th>$Y_{l,m_l}(\theta,\varphi)$</th></tr><tr><td>0</td><td>0</td><td>$\left(\frac{1}{4\pi}\right)^{1/2}$</td></tr><tr><td>1</td><td>0</td><td>$\left(\frac{3}{4\pi}\right)^{1/2}\cos\theta$</td></tr><tr><td></td><td>±1</td><td>$\mp\left(\frac{3}{8\pi}\right)^{1/2}\sin\theta\, e^{\pm i\phi}$</td></tr><tr><td>2</td><td>0</td><td>$\left(\frac{5}{16\pi}\right)^{1/2}(3\cos^2\theta-1)$</td></tr><tr><td></td><td>±1</td><td>$\mp\left(\frac{15}{8\pi}\right)^{1/2}\cos\theta\sin\theta\, e^{\pm i\phi}$</td></tr><tr><td></td><td>±2</td><td>$\left(\frac{15}{32\pi}\right)^{1/2}\sin^2\theta\, e^{\pm 2i\phi}$</td></tr></table></td><td>magnitude of the angular momentum=
$\{l(l+1)\}^{1/2}\hbar$
l=0, 1, 2,…</td><td rowspan="2">$E=l(l+1)\frac{\hbar^2}{2I}$
$l=0,1,2\ldots$
l: orbital angular momentum quantum number</td><td rowspan="2">--</td></tr>
<tr><td>angular momentum about the z-axis=
$m_l\hbar$
$m_l= l, l-1, \ldots, -l$</td></tr>
<tr><td colspan="5">(1) permitted orientations of angular momentum when l = 2 (m_l=+2, +1, 0, -1, -2)

 </td></tr>
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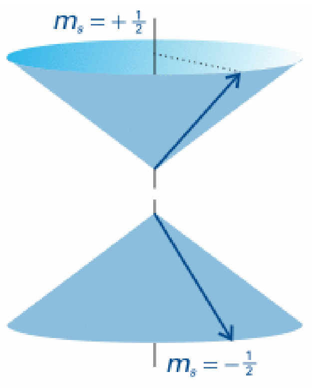
<tr><th>Motion Mode</th><th></th><th></th><th>Angular momentum</th><th></th><th></th></tr>
<tr><td rowspan="2">Spin
For electron
$s = 1/2$
m_s=+1/2, -1/2</td><td>--</td><td>--</td><td>spin angular momentum = $\{s(s + 1)\}^{1/2}\hbar$
the z-component= $m_s\hbar$</td><td>--</td><td>--</td></tr>
<tr><td colspan="5">(1) Orientation of spin
An electron spin (s = ½) can take only two orientations with respect to a specified axis.
● An α electron (top) is an electron with m_s = + ½;
● a β electron (bottom) is an electron with m_s = −½.

(2) Fermion and boson
Particles with half-integral spin (s=1/2, 3/2 …) are called fermions
Particles with integral spin (including 0) are called bosons</td></tr>
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