電子が満たすべき：運動方程式：Schrödinger方程式

波動関数： $\varphi = A\sin\left(2\pi\frac{x}{\lambda}\right), A\cos\left(2\pi\frac{x}{\lambda}\right)$

（波動方程式） $\frac{\partial}{\partial x}\varphi = Ak_x\cos(k_x x)$

$$\frac{\partial^2}{\partial x^2}\varphi = -Ak_x{}^2 sin(k_x x) = -k_x{}^2\varphi$$

$$\frac{\partial^2}{\partial x^2}\varphi + \frac{\partial^2}{\partial y^2}\varphi + \frac{\partial^2}{\partial z^2}\varphi = -A\mathbf{k}^2 sin(\mathbf{k}\cdot\mathbf{r})$$

$$= -\mathbf{k}^2\varphi = -\frac{2m}{\hbar^2}(E+V)\varphi$$

$-\frac{\hbar^2}{2m}\nabla^2\varphi - V\varphi = E\varphi$ ：Schrödinger方程式

波数ベクトル $\mathbf{k}$：

$$|\mathbf{k}| = \frac{2\pi}{\lambda}$$

量子論：物質波
（ド・ブロイ波）

$$p = \frac{h}{\lambda} = \frac{hk}{2\pi} = \hbar k$$

運動エネルギー

$$E - V = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$$

等価演算子

$p = -i\hbar\nabla$

中心力場中のSchrödinger方程式

$$\hat{H}\Psi(x,y,z) = E\Psi(x,y,z)$$

$$\hat{H} = -\frac{\hbar^2}{2m}\hat{\nabla}^2 - \frac{Ze^2}{4\pi\varepsilon_0 r}$$

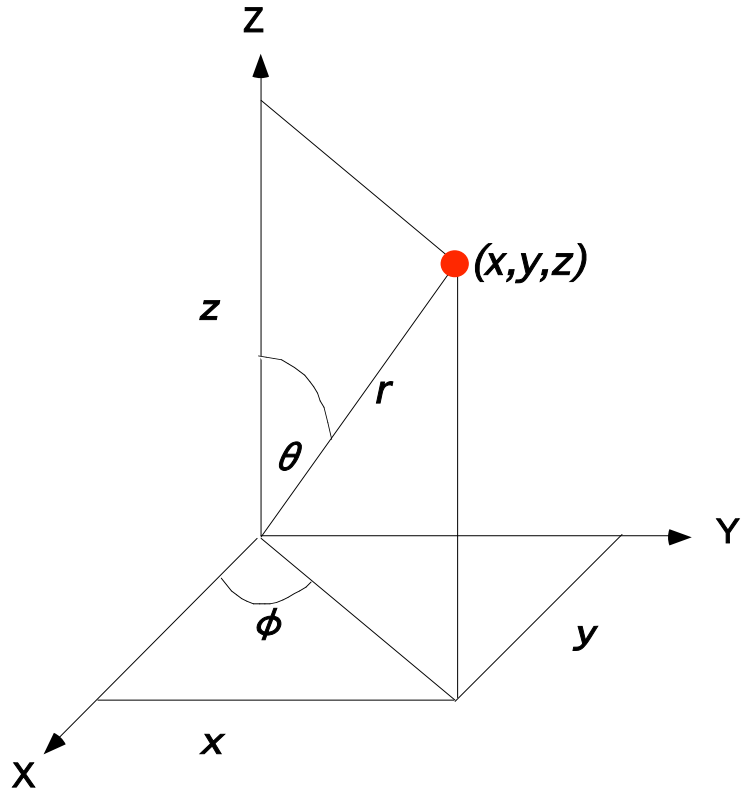
$$\hat{\nabla}^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

$$(x,y,z) \rightarrow (r,\theta,\phi)$$

$$\Psi(r,\theta,\phi) = R_{n,l}(r)\cdot\Theta_{l,m_l}(\theta)\cdot\Phi_{m_l}(\phi)$$

$$Y_{l,m_l}(\theta,\phi) = \Theta_{l,m_l}(\theta)\cdot\Phi_{m_l}(\phi)$$

$$\Psi(r,\theta,\phi) = R_{n,l}(r)\cdot Y_{l,m_l}(\theta,\phi)$$



$$E_n = -R_\infty \cdot \frac{ch}{n^2}$$

$$R_\infty = \frac{Z^2 me^4}{8ch^3\varepsilon_0^2} = 1.097\times 10^7 (m^{-1})$$

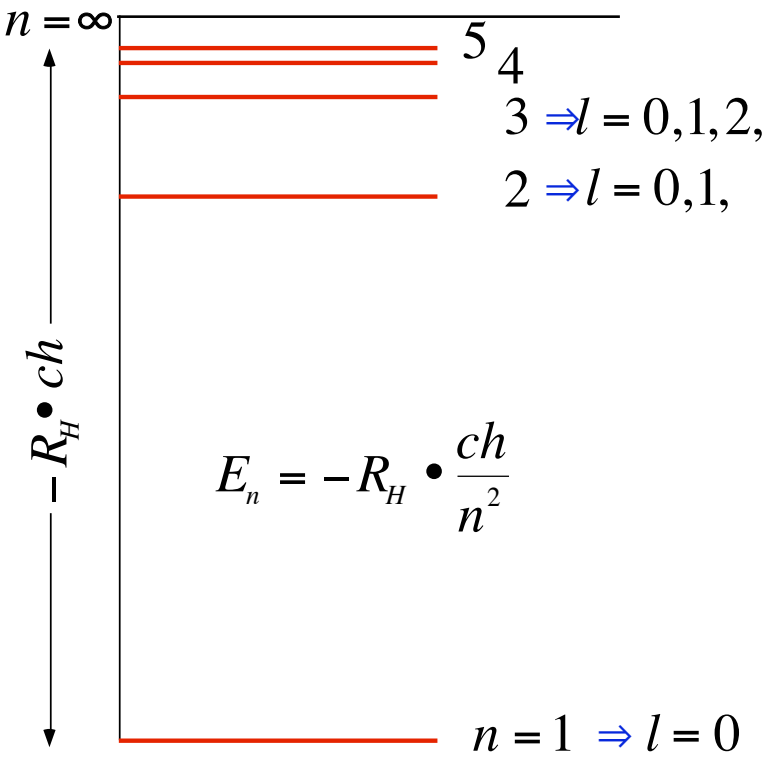
水素類似原子（モデル）のエネルギー

水素原子のエネルギーレベル

$n = 1,2,3,...$

$l = 0,1,2,3,...(n-1)$

$m_l = -l, -l+1, -l+2, ...0, 1, ...l-1, l$



水素原子のエネルギレベル

$$l_z = \hbar \cdot m_l$$

$$l^2 = \hbar^2 l(l+1)$$

n	l	m_l	電子軌道
1	0(*s*)	0	$1s^2$
2	0(*s*)	0	$2s^2$
	1(*p*)	-1,0,1	$2p^6$
3	0(*s*)	0	$3s^2$
	1(*p*)	-1,0,1	$3p^6$
	2(*d*)	-2,-1,0,1,2	$3d^{10}$

量子数と電子軌道

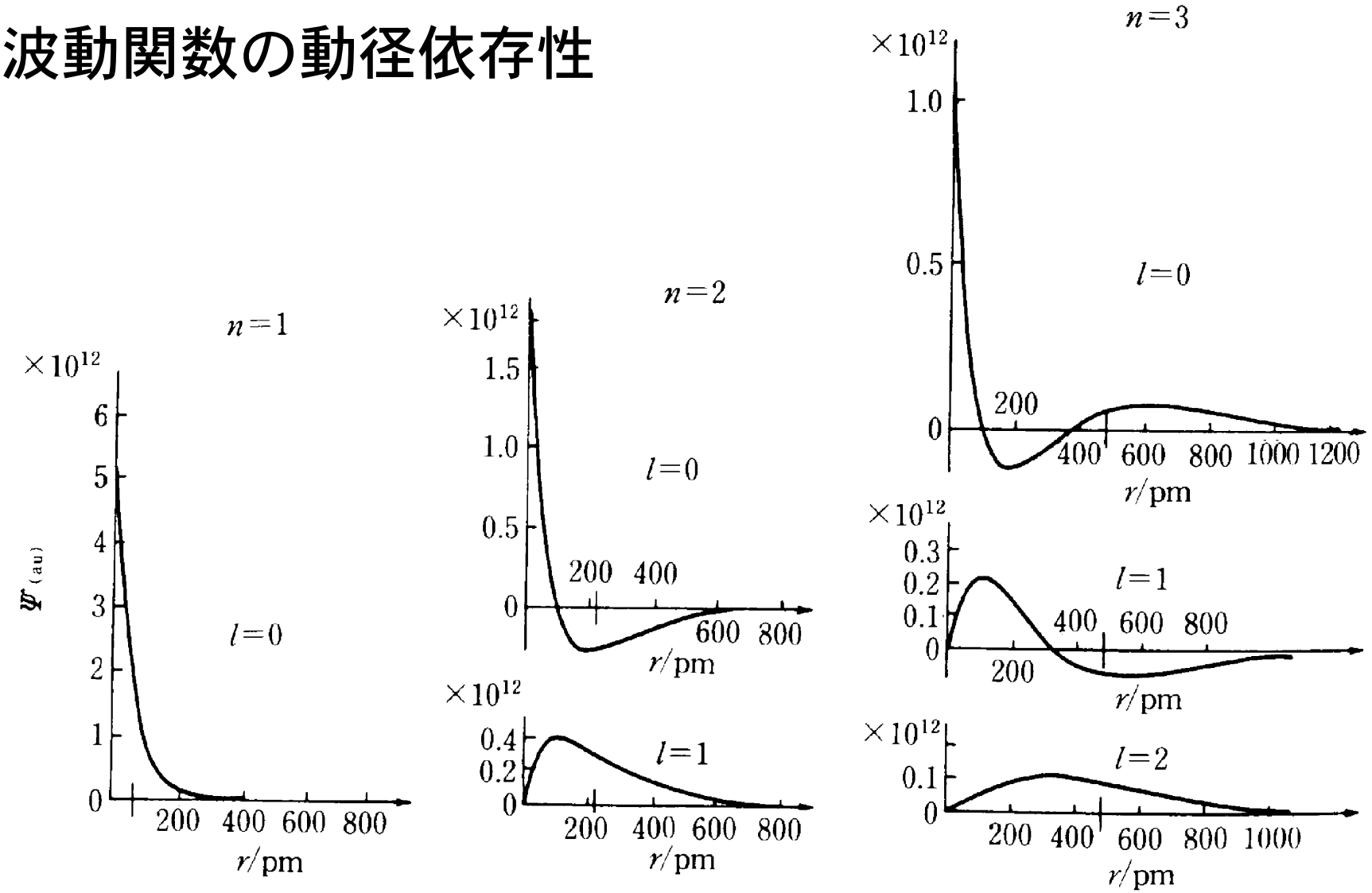
水素様原子の原子軌道の動径部分 $R_{nl}(r)$ と角度部分 $Y_{lm}(\theta,\phi)$

n	l	m	$R_{nl}(r)$	$Y_{lm}(\theta,\phi)$
1	0	0	$2Z^{3/2}\exp(-Zr)$	$1/2\sqrt{\pi}$
2	0	0	$(1/2\sqrt{2})Z^{3/2}(2-Zr)\exp(-Zr/2)$	$1/2\sqrt{\pi}$
2	1	0	$(1/2\sqrt{6})Z^{5/2}r\exp(-Zr/2)$	$(\sqrt{3}/2\sqrt{\pi})\cos\theta$
2	1	1		$(\sqrt{6}/4\sqrt{\pi})\sin\theta\exp(i\phi)$
2	1	−1		$(\sqrt{6}/4\sqrt{\pi})\sin\theta\exp(-i\phi)$
3	0	0	$(2/81\sqrt{3})Z^{3/2}(27-18Zr+2Z^2r^2)\exp(-Zr/3)$	$1/2\sqrt{\pi}$
3	1	0	$(4/81\sqrt{6})Z^{5/2}(6-Zr)r\exp(-Zr/3)$	$(\sqrt{3}/2\sqrt{\pi})\cos\theta$
3	1	1		$(\sqrt{6}/2\sqrt{\pi})\sin\theta\exp(i\phi)$
3	1	−1		$(\sqrt{6}/2\sqrt{\pi})\sin\theta\exp(-i\phi)$
3	2	0	$(4/81\sqrt{30})Z^{7/2}r^2\exp(-Zr/3)$	$(\sqrt{5}/4\sqrt{\pi})(3\cos^2\theta-1)$
3	2	1		$(\sqrt{30}/4\sqrt{\pi})\sin\theta\cos\theta\exp(i\phi)$
3	2	−1		$(\sqrt{30}/4\sqrt{\pi})\sin\theta\cos\theta\exp(-i\phi)$
3	2	2		$(\sqrt{30}/8\sqrt{\pi})\sin^2\theta\exp(i2\phi)$
3	2	−2		$(\sqrt{30}/8\sqrt{\pi})\sin^2\theta\exp(-i2\phi)$
4	0	0	$(1/768)Z^{3/2}(192-144Zr+Z^2r^2-Z^3r^3)\exp(-Zr/4)$	$1/2\sqrt{\pi}$
4	1	0	$(1/256\sqrt{15})Z^{5/2}(80-20Zr+Z^2r^2)r\exp(-Zr/4)$	$(\sqrt{3}/2\sqrt{\pi})\cos\theta$
4	1	1		$(\sqrt{6}/4\sqrt{\pi})\sin\theta\exp(i\phi)$
4	1	−1		$(\sqrt{6}/4\sqrt{\pi})\sin\theta\exp(-i\phi)$
4	2	0	$(1/768\sqrt{5})Z^{7/2}(12-Zr)r^2\exp(-Zr/4)$	$(\sqrt{5}/4\sqrt{\pi})(3\cos^2\theta-1)$
4	2	1		$(\sqrt{30}/4\sqrt{\pi})\sin\theta\cos\theta\exp(i\phi)$
4	2	−1		$(\sqrt{30}/4\sqrt{\pi})\sin\theta\cos\theta\exp(-i\phi)$
4	2	2		$(\sqrt{30}/8\sqrt{\pi})\sin^2\theta\exp(i2\phi)$
4	2	−2		$(\sqrt{30}/8\sqrt{\pi})\sin^2\theta\exp(-i2\phi)$
4	3	0	$(1/768\sqrt{35})Z^{9/2}r^3\exp(-Zr/4)$	$(\sqrt{7}/4\sqrt{\pi})(5\cos^3\theta-3\cos\theta)$
4	3	1		$(\sqrt{21}/8\sqrt{\pi})\sin\theta(5\cos^2\theta-1)\exp(i\phi)$
4	3	−1		$(\sqrt{21}/8\sqrt{\pi})\sin\theta(5\cos^2\theta-1)\exp(-i\phi)$
4	3	2		$(\sqrt{210}/8\sqrt{\pi})\sin^2\theta\cos\theta\exp(i2\phi)$
4	3	−2		$(\sqrt{210}/8\sqrt{\pi})\sin^2\theta\cos\theta\exp(-i2\phi)$
4	3	±3		$\frac{\sqrt{35}}{8\sqrt{\pi}}\sin^3\theta\cdot\exp(\pm 3i\phi)$

水素様原子の原子軌道

1s	$(1/\sqrt{\pi})Z^{3/2}\exp(-Zr)$
2s	$(1/4\sqrt{2\pi})Z^{3/2}(2-Zr)\exp(-Zr/2)$
$2p_x$	$(1/4\sqrt{2\pi})Z^{5/2}\exp(-Zr/2)x$
$2p_y$	$(1/4\sqrt{2\pi})Z^{5/2}\exp(-Zr/2)y$
$2p_z$	$(1/4\sqrt{2\pi})Z^{5/2}\exp(-Zr/2)z$
3s	$(1/81\sqrt{3\pi})Z^{3/2}(27-18Zr+2Z^2r^2)\exp(-Zr/3)$
$3p_x$	$(2/81\sqrt{2\pi})Z^{5/2}(6-Zr)\exp(-Zr/3)x$
$3p_y$	$(2/81\sqrt{2\pi})Z^{5/2}(6-Zr)\exp(-Zr/3)y$
$3p_z$	$(2/81\sqrt{2\pi})Z^{5/2}(6-Zr)\exp(-Zr/3)z$
$3d_{3z^2-r^2}$	$(1/81\sqrt{6\pi})Z^{7/2}\exp(-Zr/3)(3z^2-r^2)$
$3d_{zx}$	$(2/81\sqrt{2\pi})Z^{7/2}\exp(-Zr/3)zx$
$3d_{zy}$	$(2/81\sqrt{2\pi})Z^{7/2}\exp(-Zr/3)zy$
$3d_{xy}$	$(2/81\sqrt{2\pi})Z^{7/2}\exp(-Zr/3)xy$
$3d_{x^2-y^2}$	$(1/81\sqrt{2\pi})Z^{7/2}\exp(-Zr/3)(x^2-y^2)$
4s	$(1/1536\sqrt{\pi})Z^{3/2}(192-144Zr+24Z^2r^2-Z^3r^3)\exp(-Zr/4)$
$4p_x$	$(1/512\sqrt{5\pi})Z^{5/2}(80-20Zr+Z^2r^2)\exp(-Zr/4)x$
$4p_y$	$(1/512\sqrt{5\pi})Z^{5/2}(80-20Zr+Z^2r^2)\exp(-Zr/4)y$
$4p_z$	$(1/512\sqrt{5\pi})Z^{5/2}(80-20Zr+Z^2r^2)\exp(-Zr/4)z$
$4d_{3z^2-r^2}$	$(1/3072\sqrt{\pi})Z^{7/2}(12-Zr)\exp(-Zr/4)(3z^2-r^2)$
$4d_{zx}$	$(1/512\sqrt{3\pi})Z^{7/2}(12-Zr)\exp(-Zr/4)zx$
$4d_{zy}$	$(1/512\sqrt{3\pi})Z^{7/2}(12-Zr)\exp(-Zr/4)zy$
$4d_{xy}$	$(1/512\sqrt{3\pi})Z^{7/2}(12-Zr)\exp(-Zr/4)xy$
$4d_{x^2-y^2}$	$(1/1024\sqrt{3\pi})Z^{7/2}(12-Zr)\exp(-Zr/4)(x^2-y^2)$
$4f_{5z^3-3zr^2}$	$(1/3072\sqrt{5\pi})Z^{9/2}\exp(-Zr/4)z(5z^2-3r^2)$
$4f_{5xz^2-xr^2}$	$(1/1024\sqrt{30\pi})Z^{9/2}\exp(-Zr/4)x(5z^2-r^2)$
$4f_{5yz^2-yr^2}$	$(1/1024\sqrt{30\pi})Z^{9/2}\exp(-Zr/4)y(5z^2-r^2)$
$4f_{zx^2-zy^2}$	$(1/1024\sqrt{3\pi})Z^{9/2}\exp(-Zr/4)z(x^2-y^2)$
$4f_{xyz}$	$(1/512\sqrt{3\pi})Z^{9/2}\exp(-Zr/4)xyz$
$4f_{x^3-3xy^2}$	$(1/3072\sqrt{2\pi})Z^{9/2}\exp(-Zr/4)x(x^2-3y^2)$
$4f_{y^3-3yx^2}$	$(1/3072\sqrt{2\pi})Z^{9/2}\exp(-Zr/4)y(y^2-3x^2)$

波動関数の動径依存性


n=1
×10^12
6
5
4
3
2
1
0
ψ(au)
l=0
200 400 600 800
r/pm
n=2
×10^12
1.5
1.0
0.5
0
l=0
200 400
600 800
r/pm
×10^12
0.4
0.2
0
l=1
200 400 600 800
r/pm
n=3
×10^12
1.0
0.5
0
l=0
200
400 600 800 1000 1200
r/pm
×10^12
0.3
0.2
0.1
0
l=1
200
400 600 800
r/pm
×10^12
0.1
0
l=2
200 400 600 800 1000
r/pm

$$\int_{\theta=0}^{\pi}\int_{\phi=0}^{2\pi}\Psi(r,\theta,\phi)^2 r^2 \sin\theta \mathrm{d}\theta\mathrm{d}\phi$$

$$R\cdot 4\pi r^2 dr$$

動径分布関数

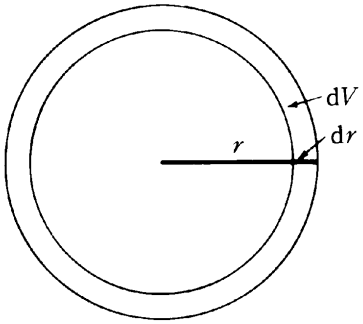
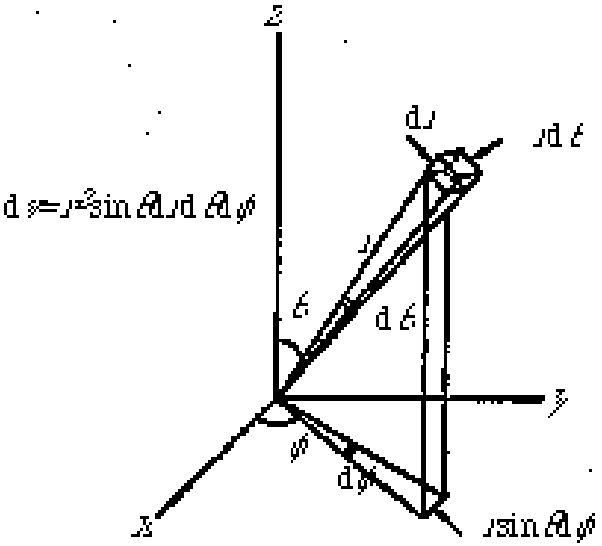
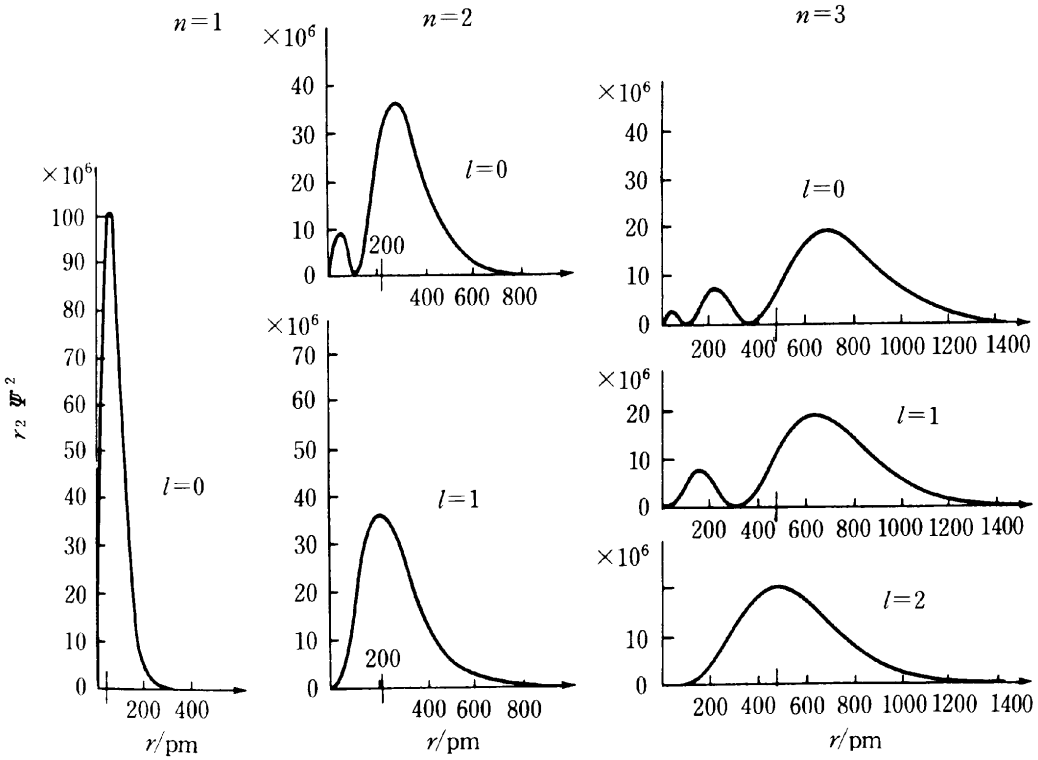
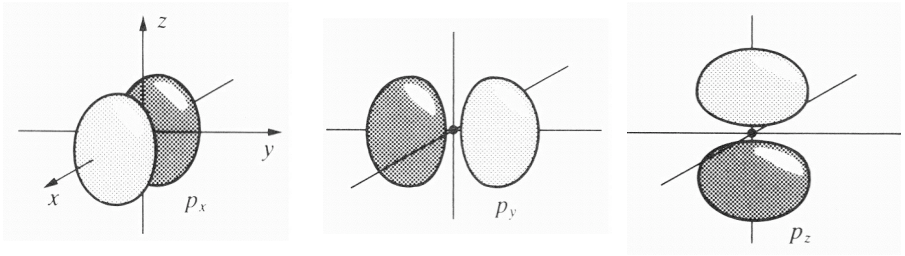


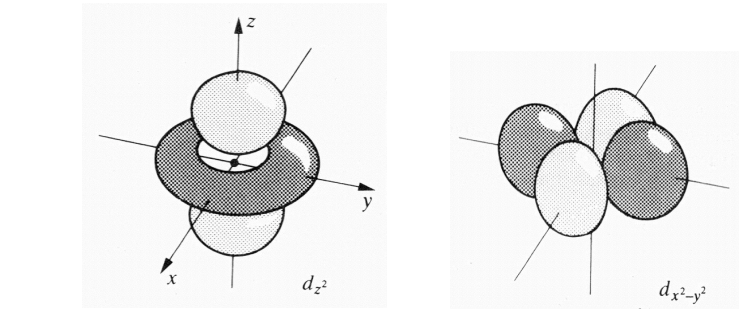
図 2・4　厚さ dr の殻の体積

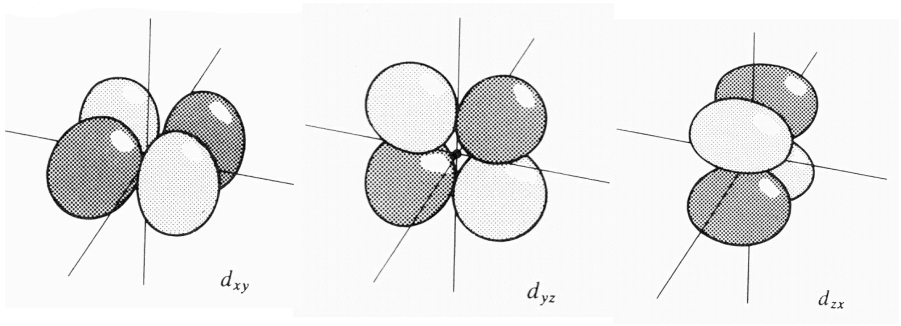


波動関数の動径分布

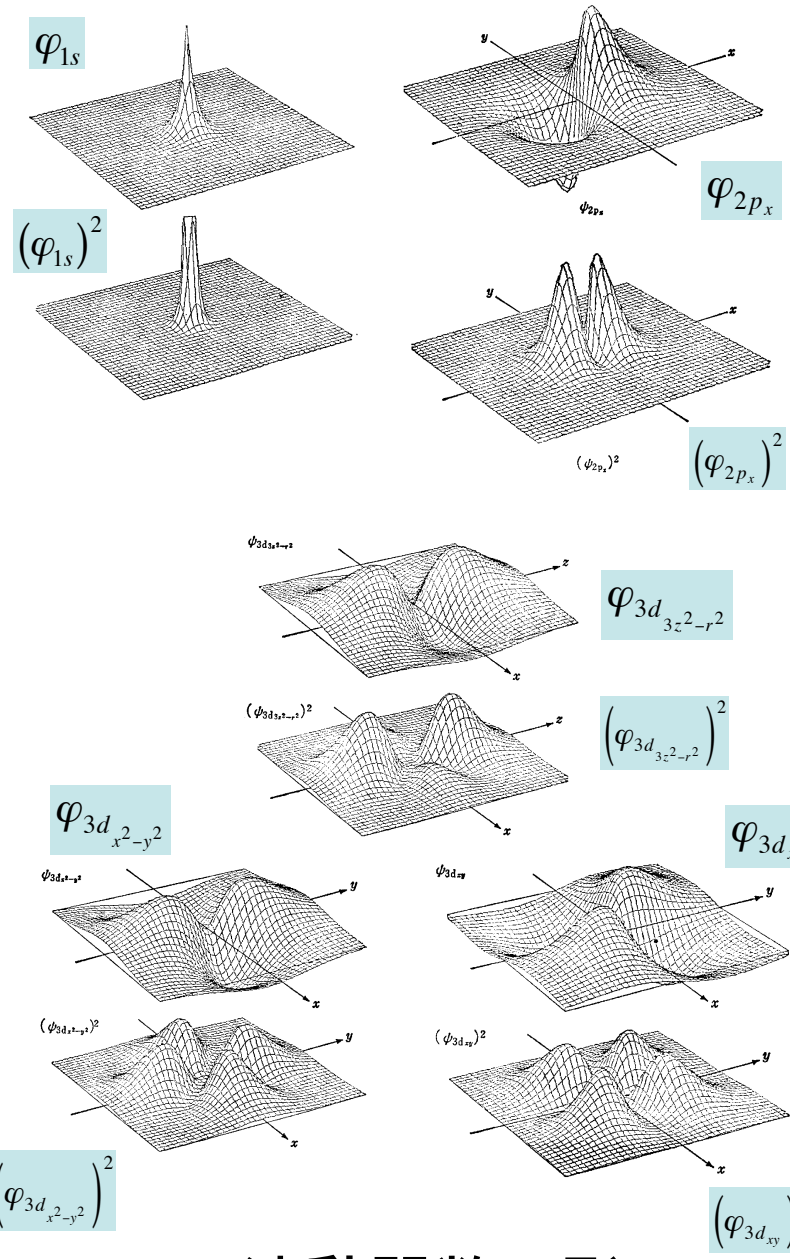






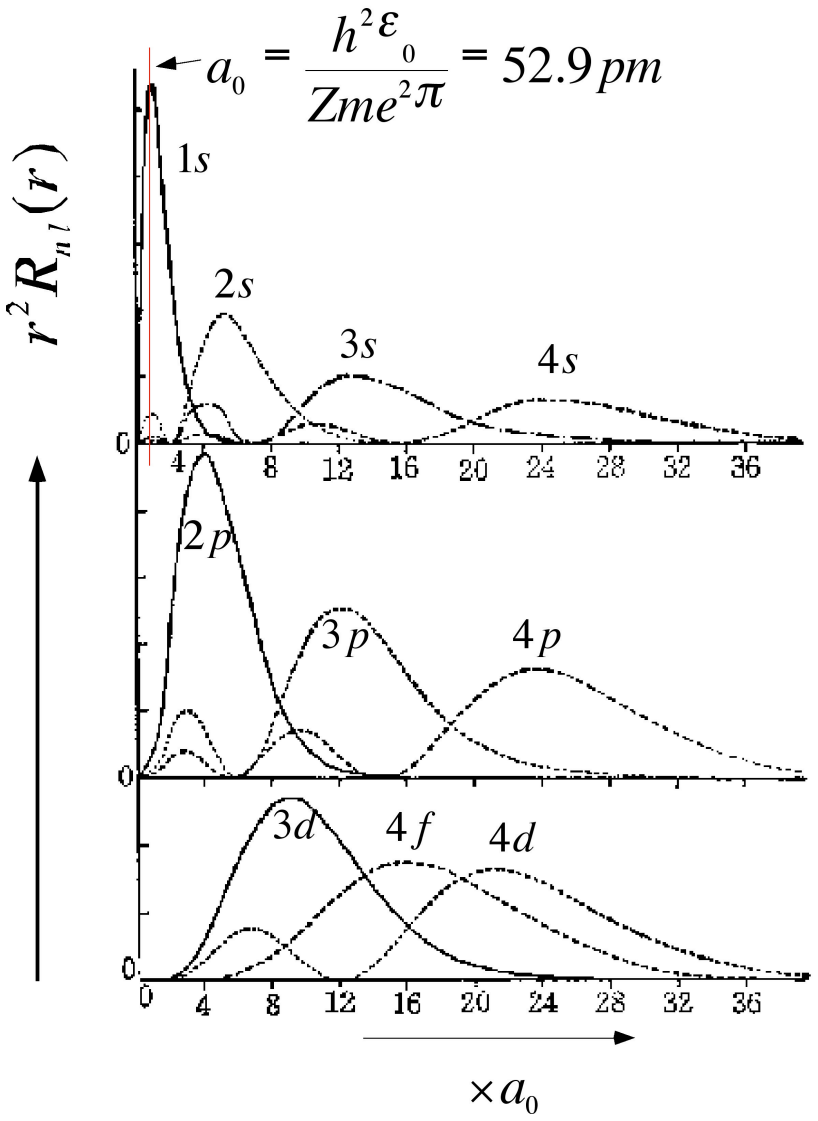


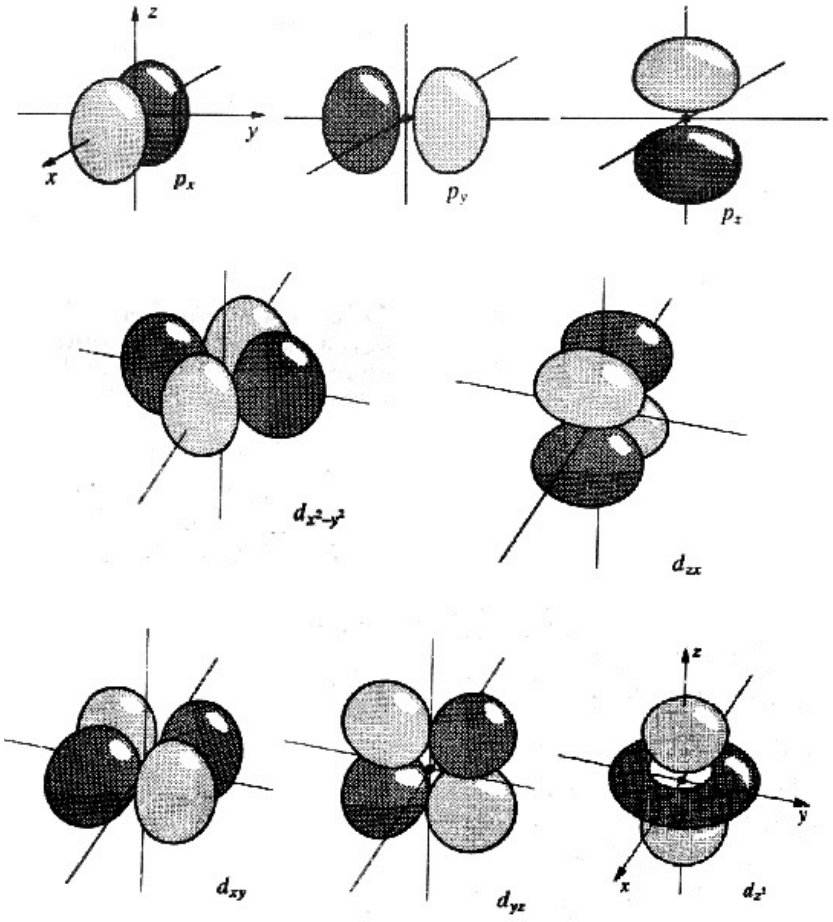
波動関数の角度依存



波動関数の形

水素の波動関数の形（1）





水素波動関数の形（２）