

Chemická struktura B

Elektronová struktura molekul

Lubomír Rulíšek, Martin Srnec

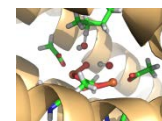
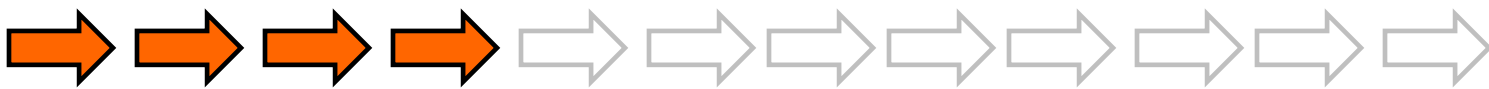
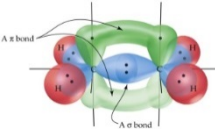
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ÚOCHB ^{AV}_{ČR}
IOCB PRAGUE



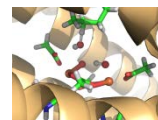
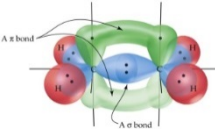
(2016/17: pondělí CH3 8:10–9:40, CH3 9:50–10:35)



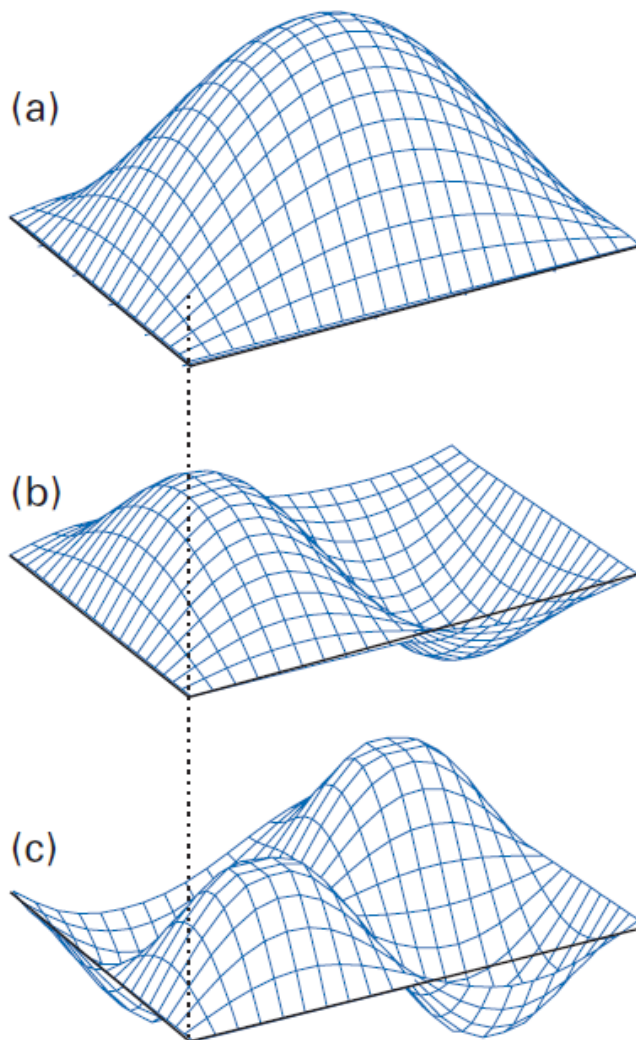
Přednáška 4: Shrnutí a obrázky

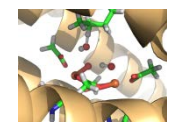
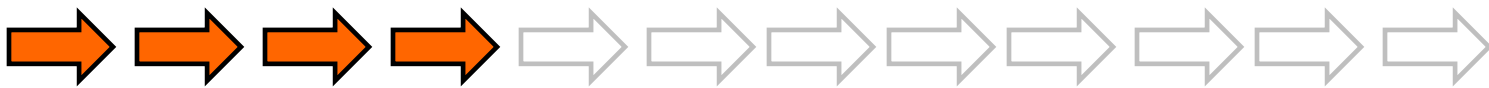
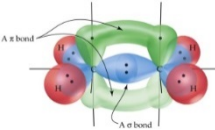
(podrobnější materiál: Atkins, *Molecular Quantum Mechanics*, kapitola 3)

- Harmonický oscilátor
- Částice na kruhu
- Moment hybnosti (úvod)
- Částice na kouli
- Tuhý rotor – zmínka
- **Atom vodíku**

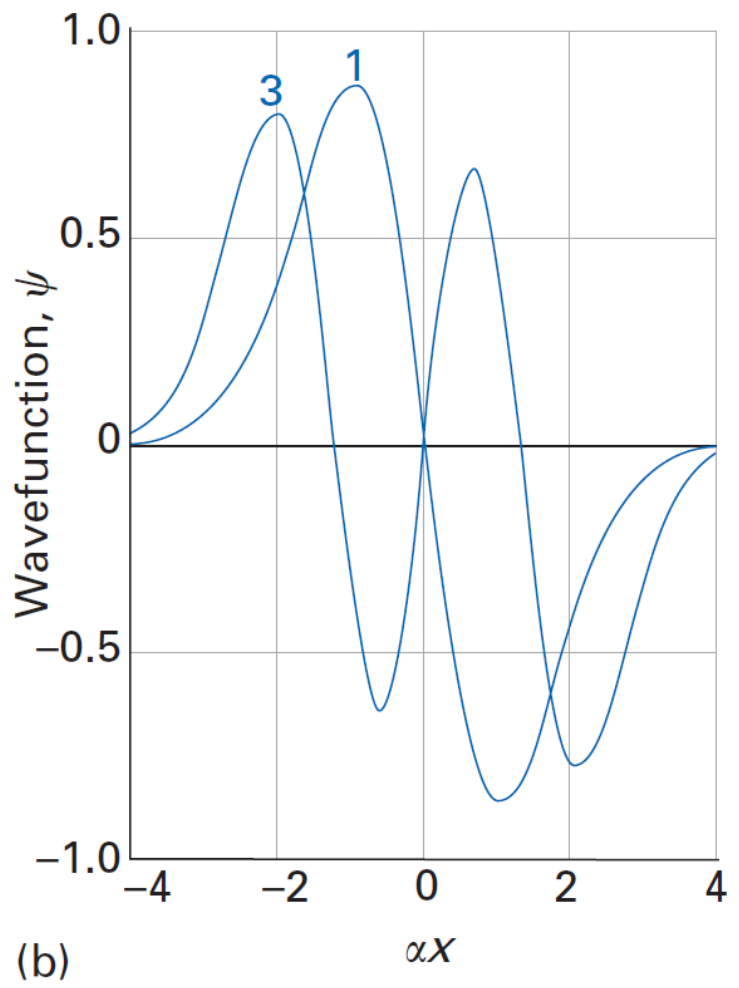
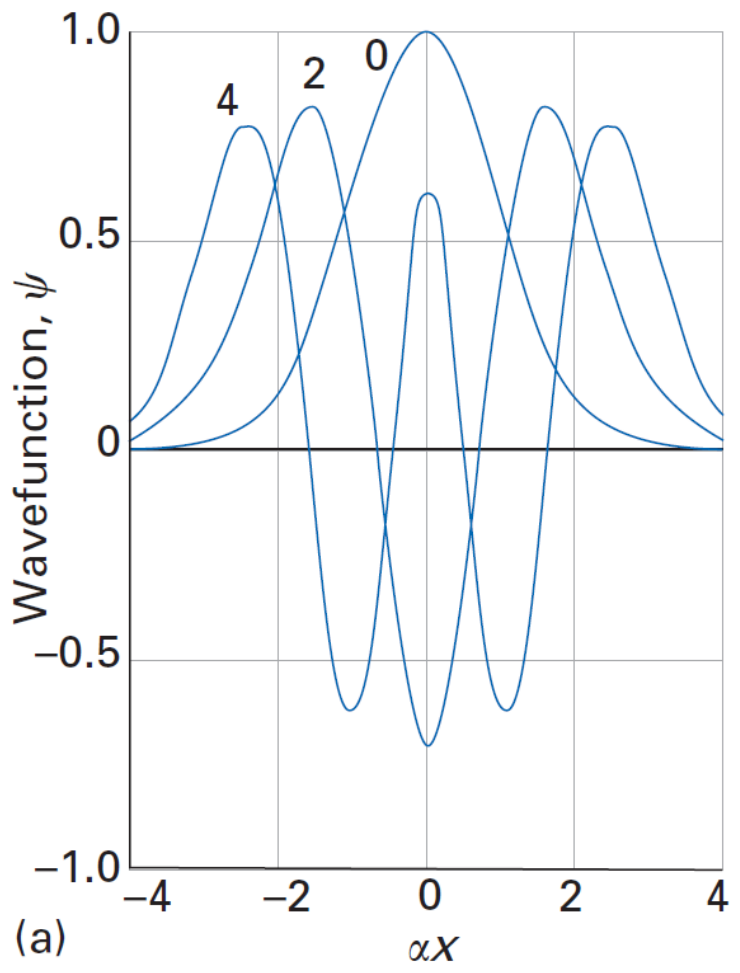


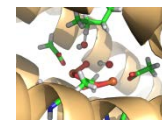
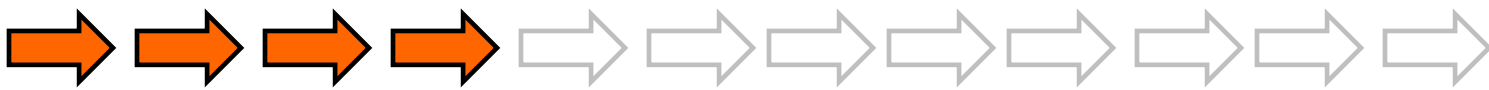
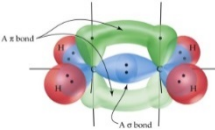
Částice ve 2D krabici, vlnové funkce pro $|1,1\rangle$; $|2,1\rangle$; $|2,2\rangle$



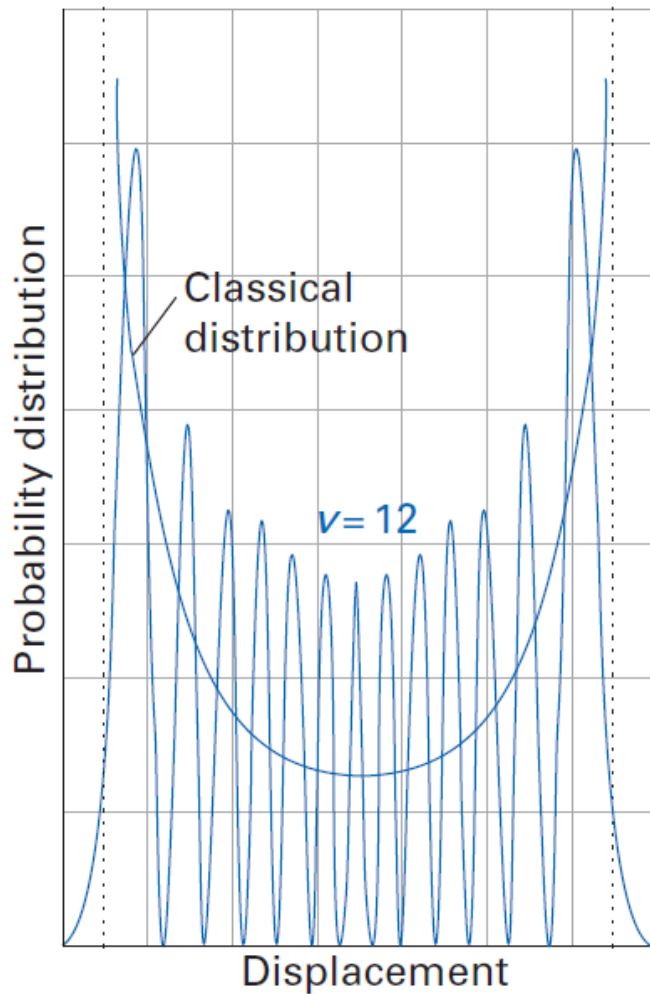


Harmonický oscilátor – vlnové funkce





Porovnání klasického a kvantového HO



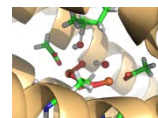
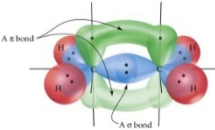


Table 2.1 Hermite polynomials

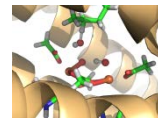
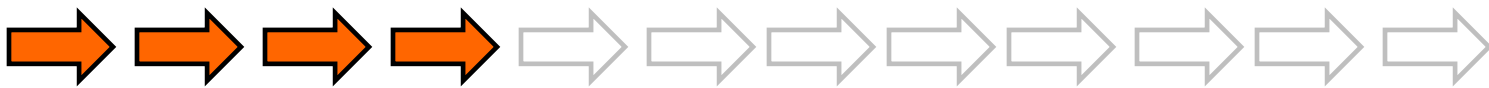
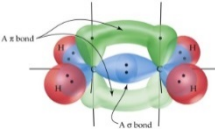
ν	$H_\nu(z)$
0	1
1	$2z$
2	$4z^2 - 2$
3	$8z^3 - 12z$
4	$16z^4 - 48z^2 + 12$
5	$32z^5 - 160z^3 + 120z$
6	$64z^6 - 480z^4 + 720z^2 - 120$
7	$128z^7 - 1344z^5 + 3360z^3 - 1680z$
8	$256z^8 - 3584z^6 + 13440z^4 - 13440z^2 + 1680$

Differential equation: $H_\nu'' - 2zH_\nu' + 2\nu H_\nu = 0$

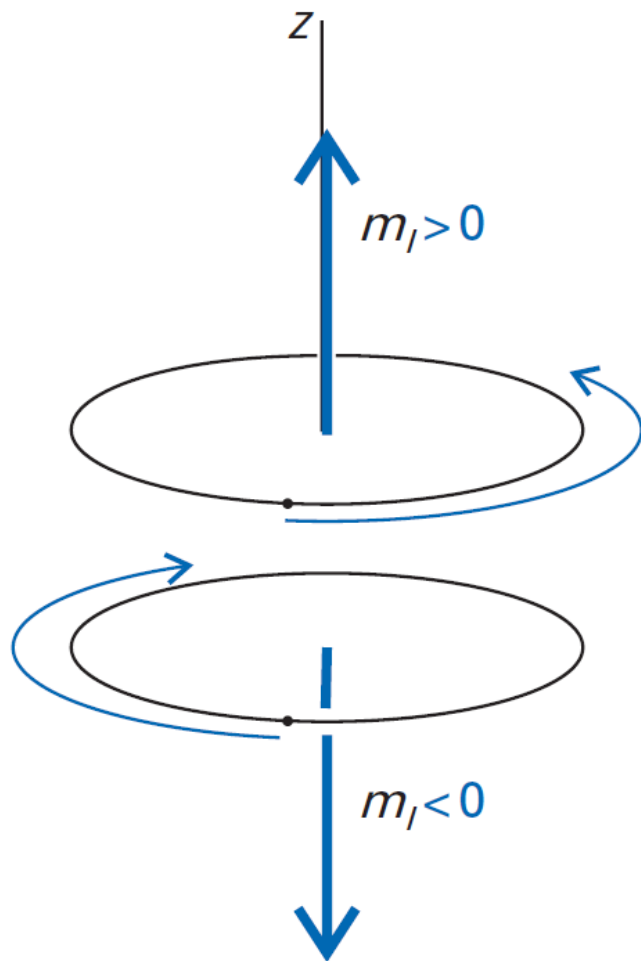
Recursion relation: $H_{\nu+1} = 2zH_\nu - 2\nu H_{\nu-1}$

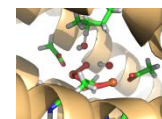
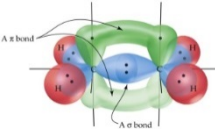
Orthogonality: $\int_{-\infty}^{\infty} H_\nu(z)H_{\nu'}(z)e^{-z^2} dz = 0$ for $\nu \neq \nu'$

Normalization: $\int_{-\infty}^{\infty} H_\nu(z)^2 e^{-z^2} dz = \pi^{1/2} 2^\nu \nu!$

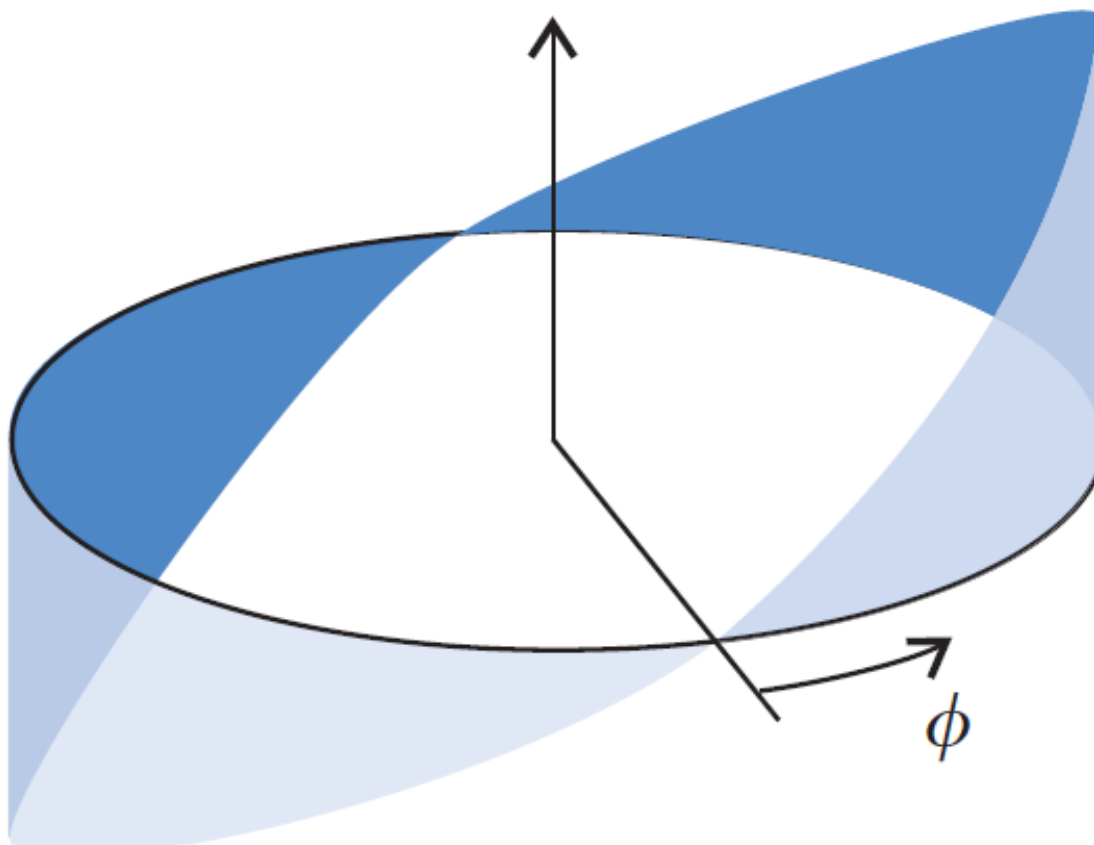


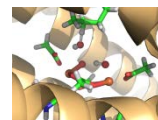
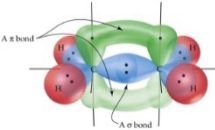
Moment hybnosti částice na kruhu



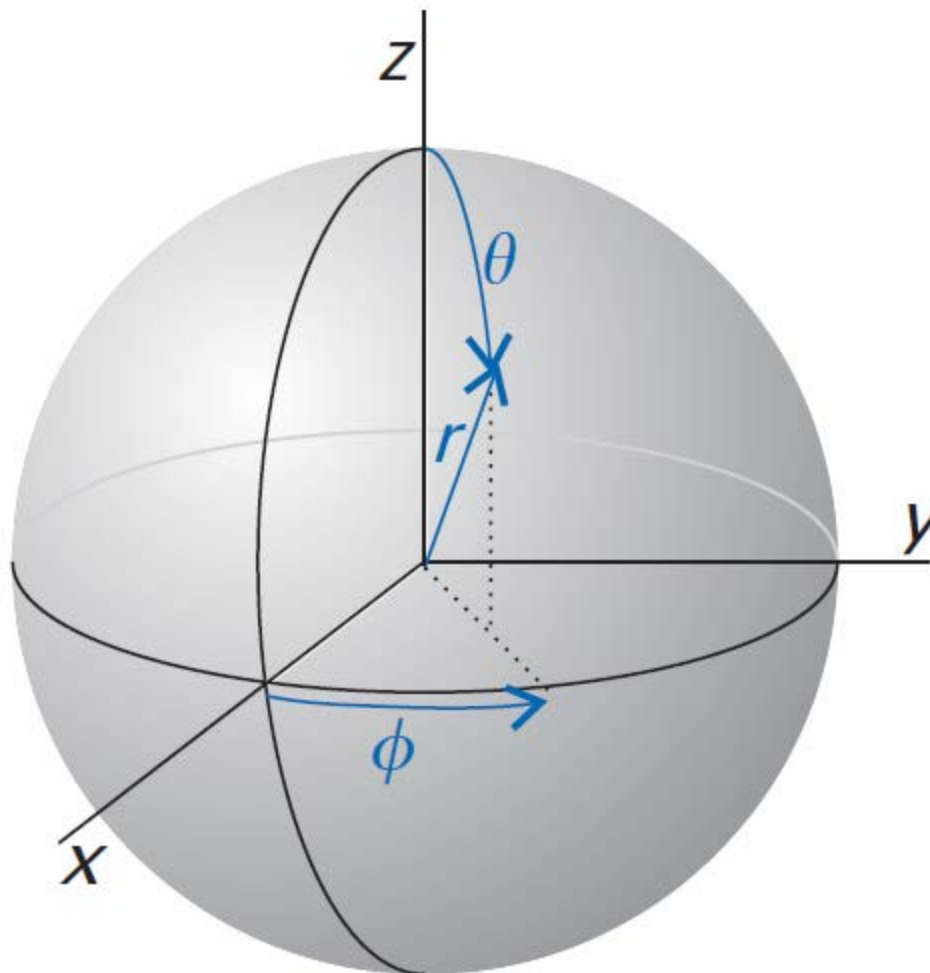


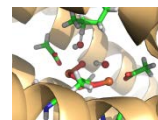
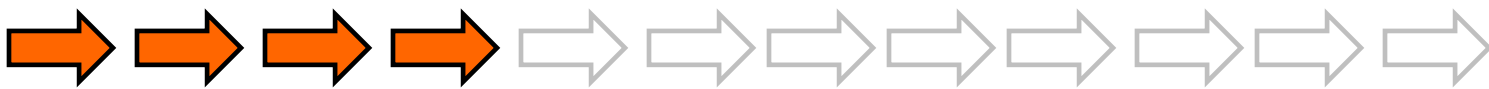
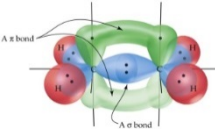
Reálná část vlnové funkce pro $m_l = \pm 1$





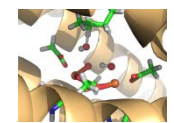
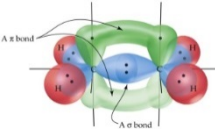
Sférické polární souřadnice



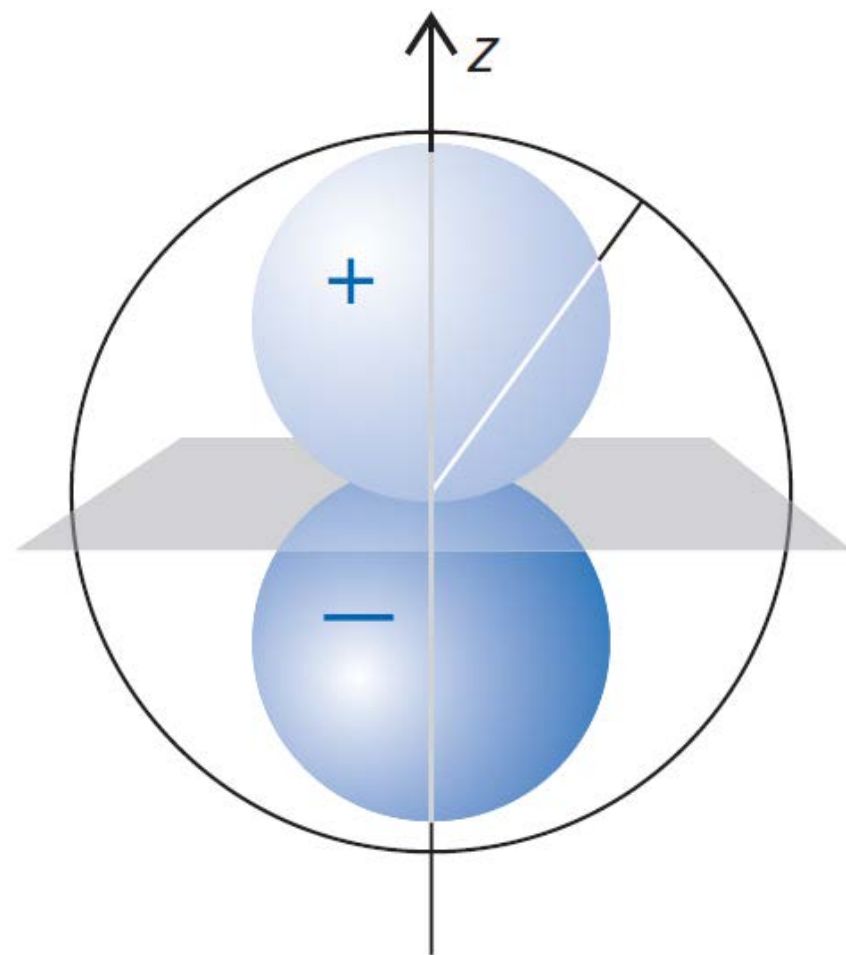
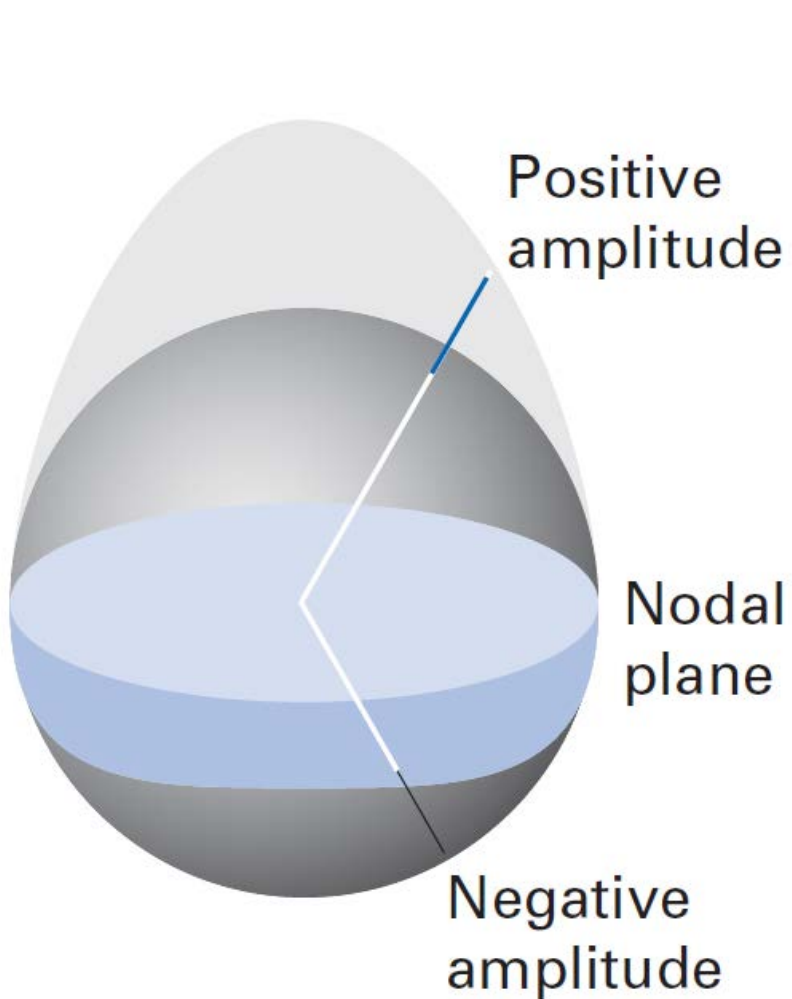


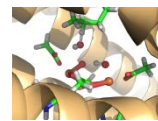
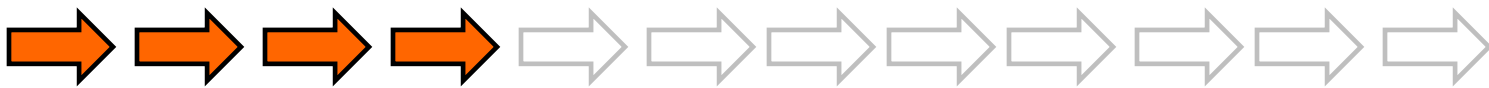
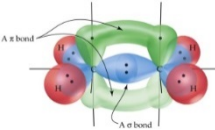
Sférické harmonické funkce

l	m_l	$Y_{lm_l}(\theta, \phi)$
0	0	$1/2\pi^{1/2}$
1	0	$\frac{1}{2}(3/\pi)^{1/2} \cos \theta$
	± 1	$\mp(3/2\pi)^{1/2} \sin \theta e^{\pm i\phi}$
2	0	$\frac{1}{4}(5/\pi)^{1/2} (3 \cos^2 \theta - 1)$
	± 1	$\mp\frac{1}{2}(15/2\pi)^{1/2} \cos \theta \sin \theta e^{\pm i\phi}$
	± 2	$\frac{1}{4}(15/2\pi)^{1/2} \sin^2 \theta e^{\pm 2i\phi}$
3	0	$\frac{1}{4}(7/\pi)^{1/2} (2 - 5 \sin^2 \theta) \cos \theta$
	± 1	$\mp\frac{1}{8}(21/\pi)^{1/2} (5 \cos^2 \theta - 1) \sin \theta e^{\pm i\phi}$
	± 2	$\frac{1}{4}(105/2\pi)^{1/2} \cos \theta \sin^2 \theta e^{\pm 2i\phi}$
	± 3	$\mp\frac{1}{8}(35/\pi)^{1/2} \sin^3 \theta e^{\pm 3i\phi}$

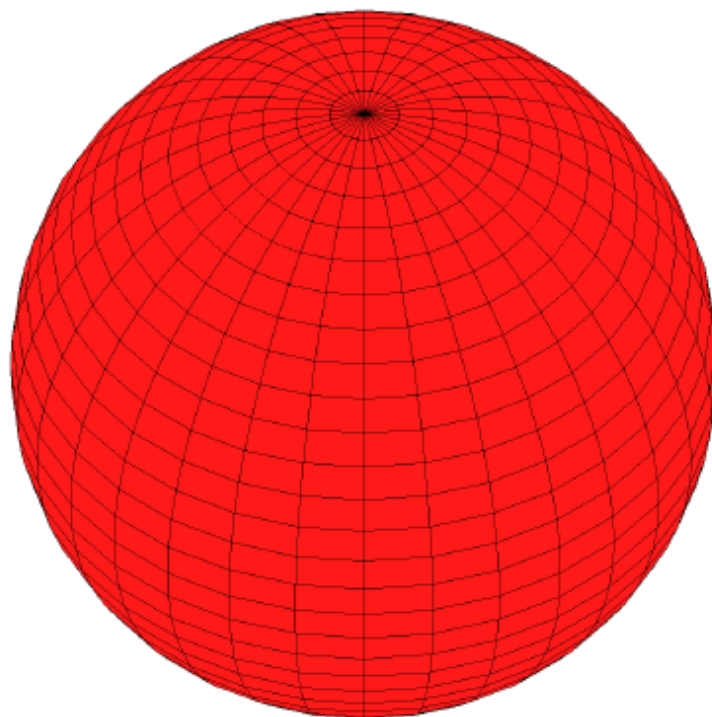


Zobrazení řešení částice na kouli

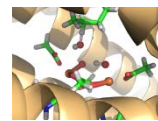
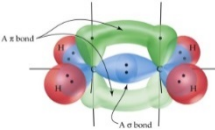




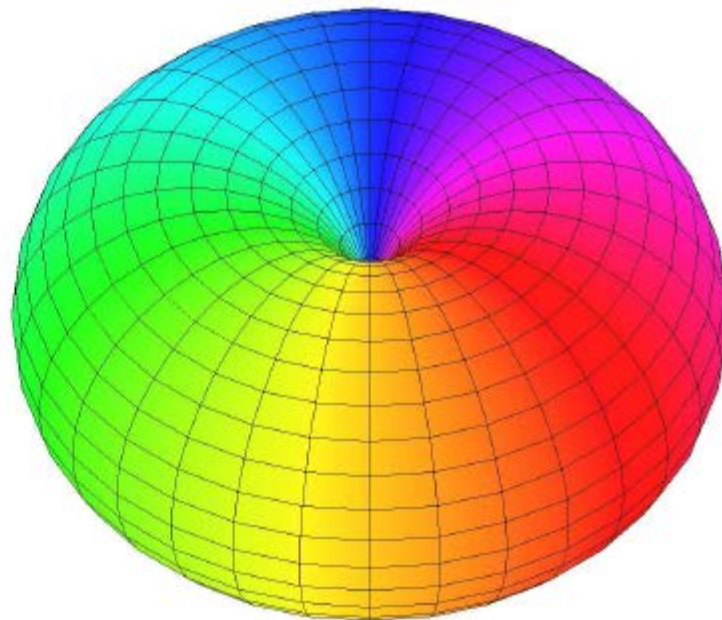
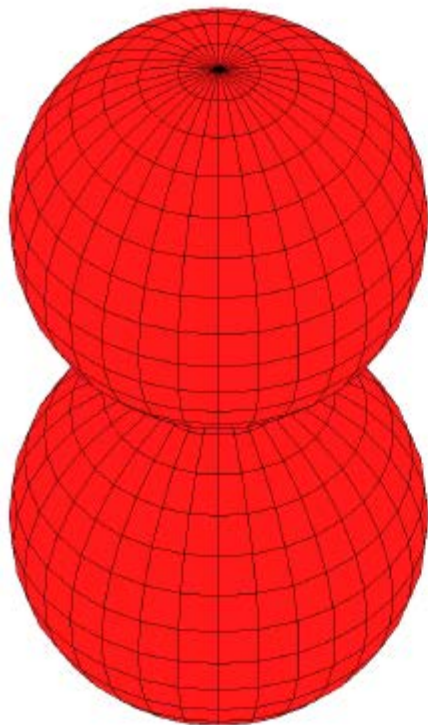
sférická harmonika $Y_0^0(\theta, \phi)$



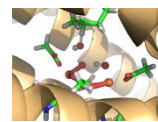
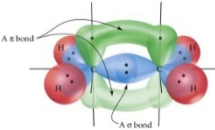
fáze (argument) kódovaný barvou na povrchu $|Y|$



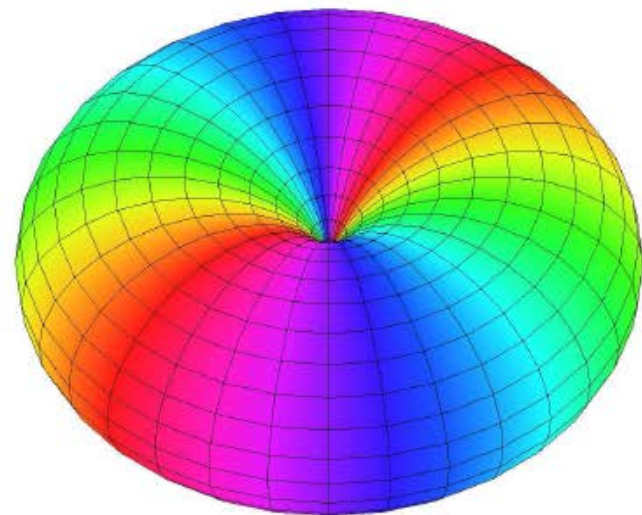
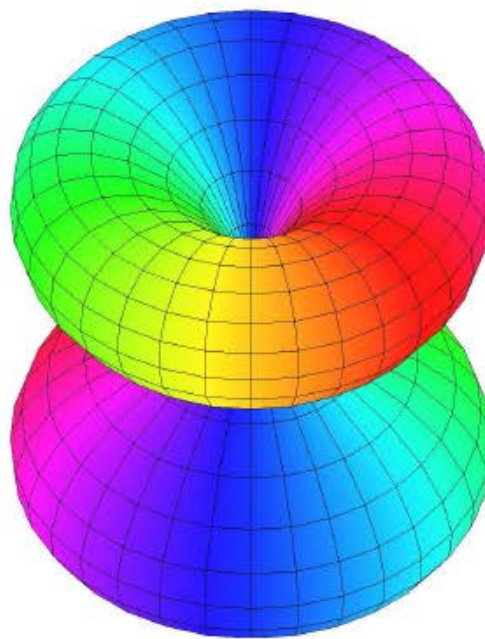
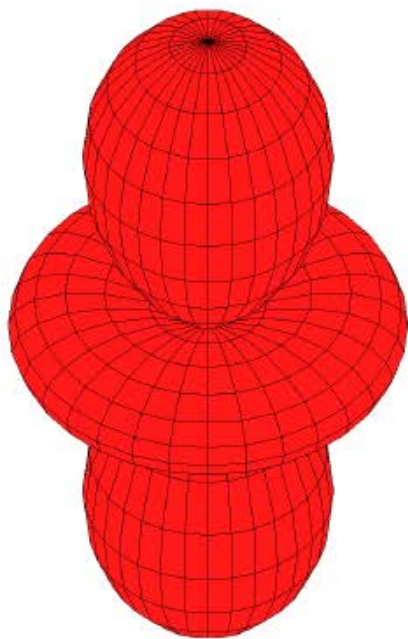
sférické harmoniky $Y_1^0(\theta, \phi)$ a $Y_1^{-1}(\theta, \phi)$



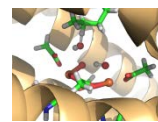
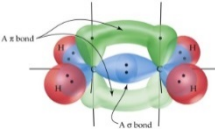
fáze (argument) kódovaný barvou na povrchu $|Y|$



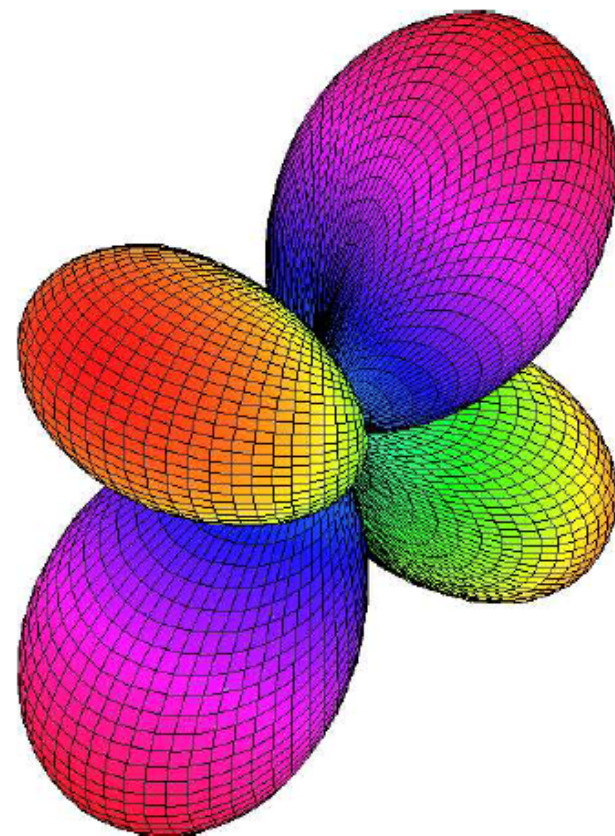
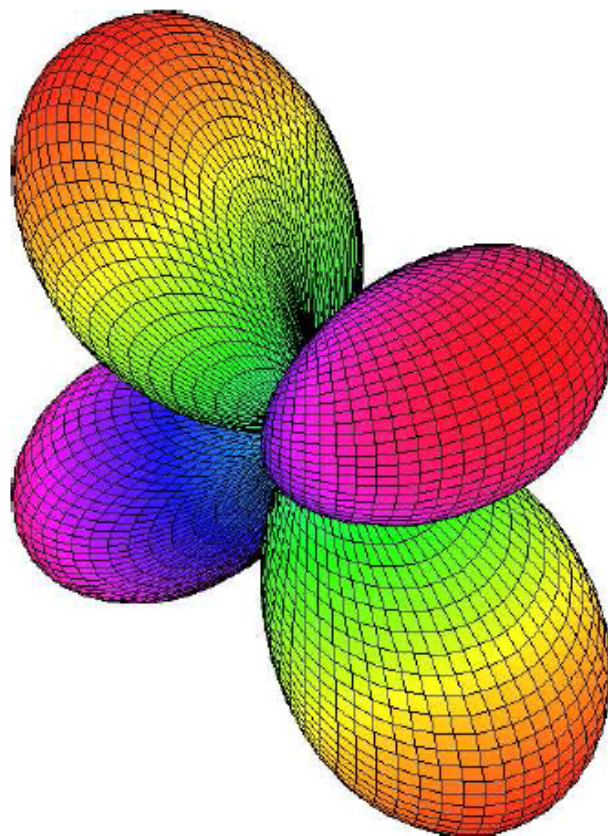
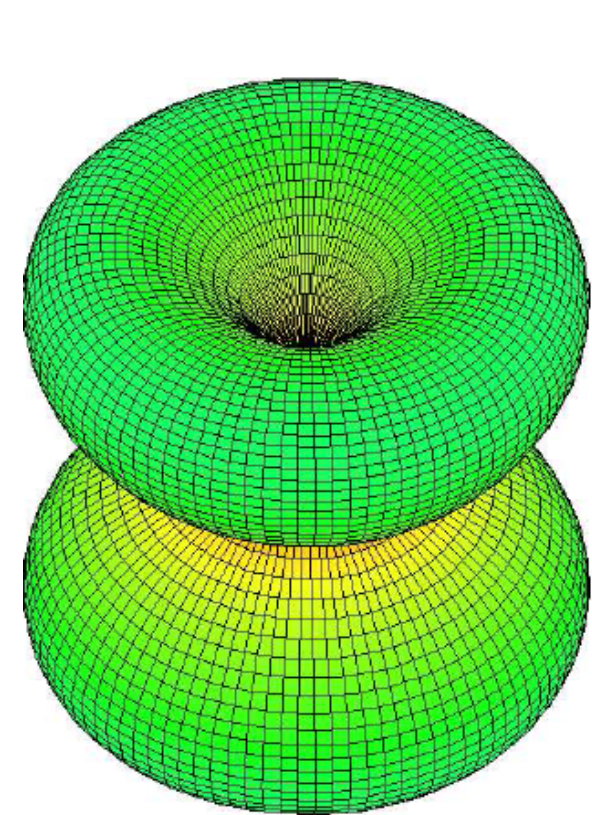
sférické harmoniky $Y_2^0(\theta, \phi)$, $Y_2^{-1}(\theta, \phi)$ a $Y_2^{-2}(\theta, \phi)$

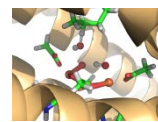
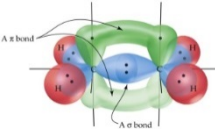


fáze (argument) kódovaný barvou na povrchu $|Y|$

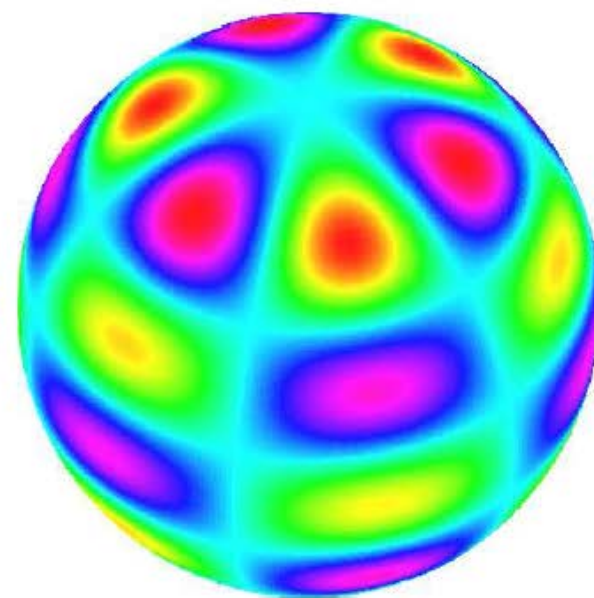
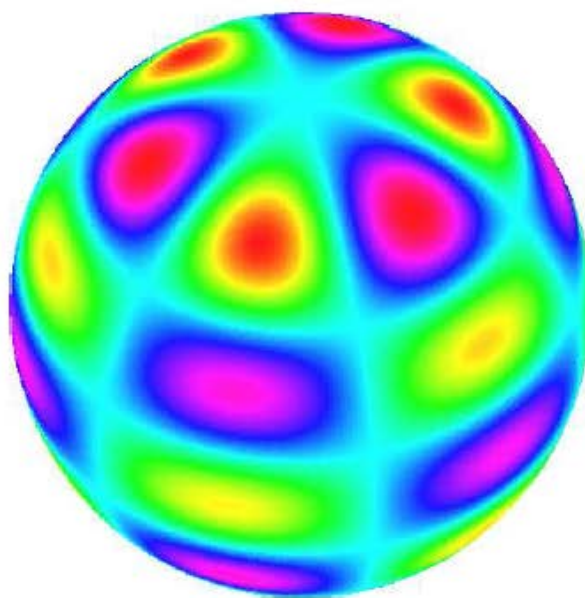
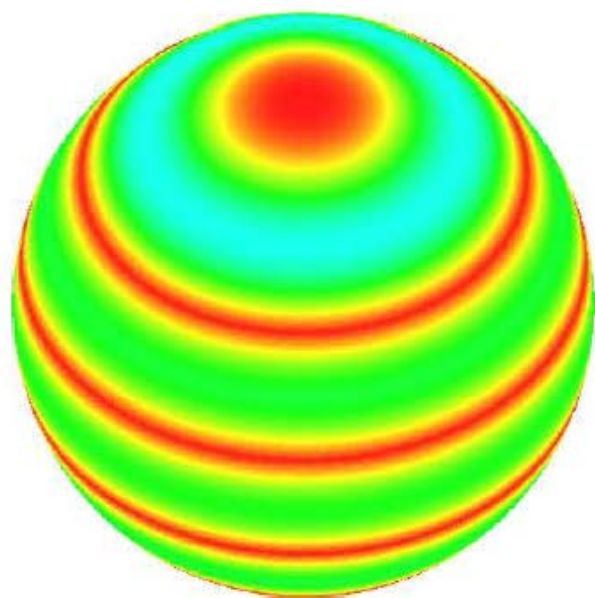


sférická harmonika $Y_2^1(\theta, \phi)$: $|Y_2^1|$, $\text{Re}(Y_2^1)$, $\text{Im}(Y_2^1)$

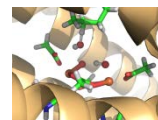
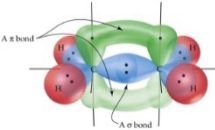




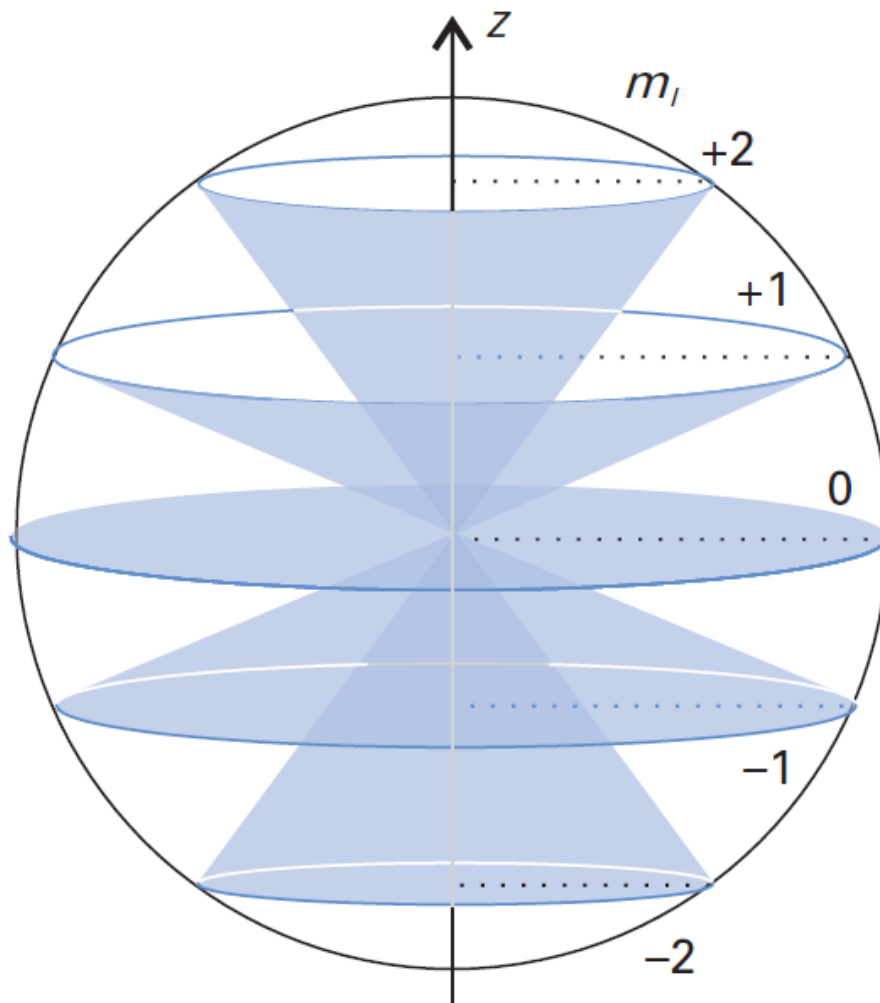
sférická harmonika $Y_7^3(\theta, \phi)$: $|Y_7^3|$, $\text{Re}(Y_7^3)$, $\text{Im}(Y_7^3)$



hodnoty kódované barvou na povrchu jednotkové koule



Kvantování směru/projekce momentu hybnosti ($l = 2$)



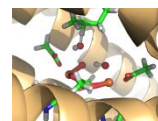
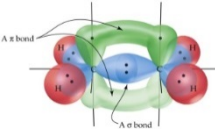


Table 3.2 Hydrogenic radial wavefunctions

n	l	Orbital	$R_{nl}(r)$
1	0	1s	$(Z/a)^{3/2} 2e^{-\rho/2}$
2	0	2s	$(Z/a)^{3/2} (1/8)^{1/2} (2 - \rho)e^{-\rho/2}$
	1	2p	$(Z/a)^{3/2} (1/24)^{1/2} \rho e^{-\rho/2}$
3	0	3s	$(Z/a)^{3/2} (1/243)^{1/2} (6 - 6\rho + \rho^2)e^{-\rho/2}$
	1	3p	$(Z/a)^{3/2} (1/486)^{1/2} (4 - \rho)\rho e^{-\rho/2}$
	2	3d	$(Z/a)^{3/2} (1/2430)^{1/2} \rho^2 e^{-\rho/2}$

$\rho = (2Z/na)r$ with $a = 4\pi\epsilon_0\hbar^2/\mu e^2$. For an infinitely heavy nucleus, $\mu = m_e$ and $a = a_0$, the Bohr radius.

Relation to associated Laguerre functions:

$$R_{nl}(r) = -\left\{ \left(\frac{2Z}{na}\right)^3 \frac{(n-l-1)!}{2n[(n+l)!]^3} \right\} \rho^l L_{n+l}^{2l+1}(\rho) e^{-\rho/2}$$

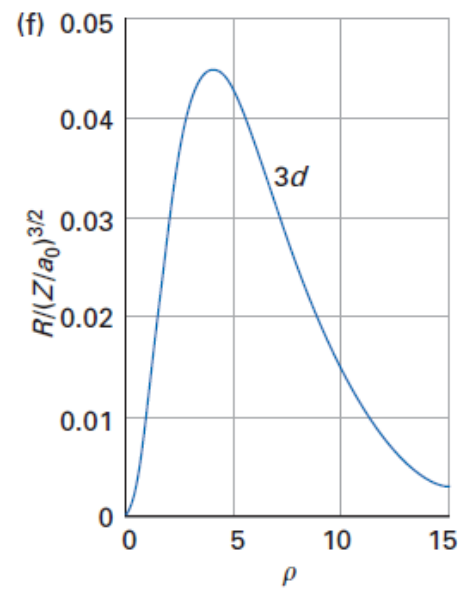
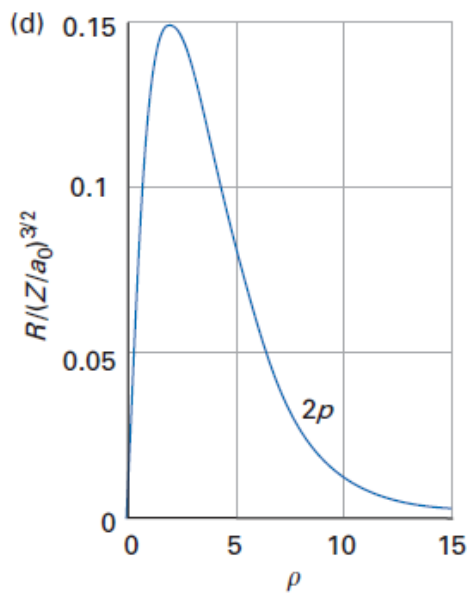
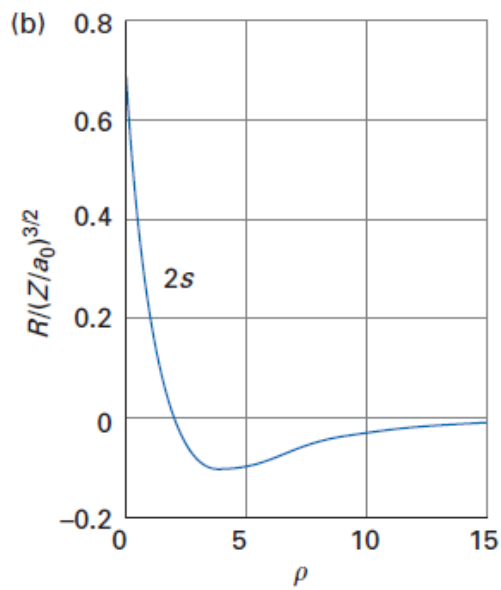
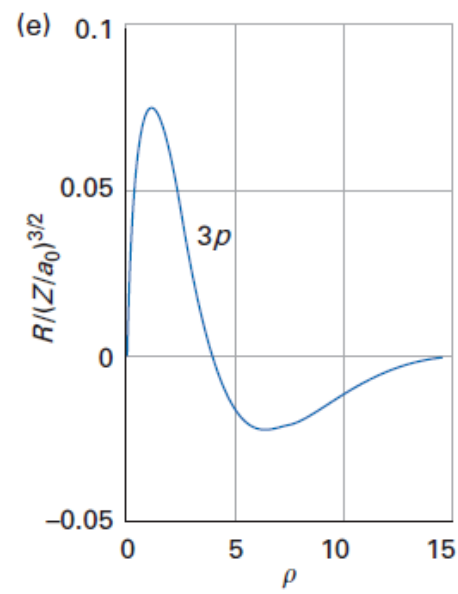
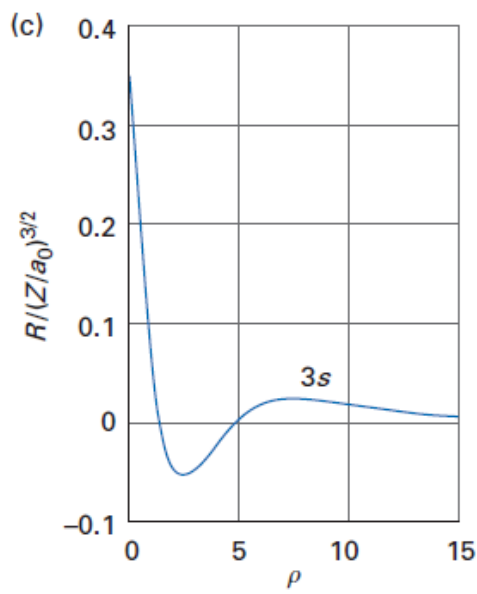
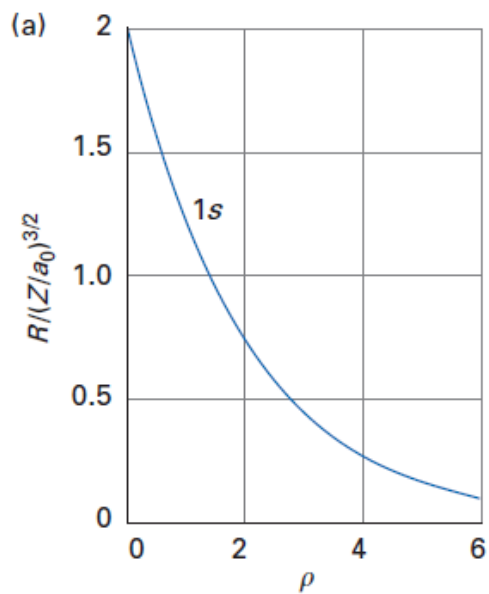
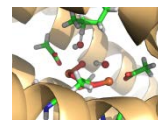
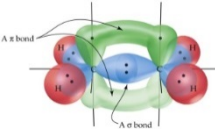
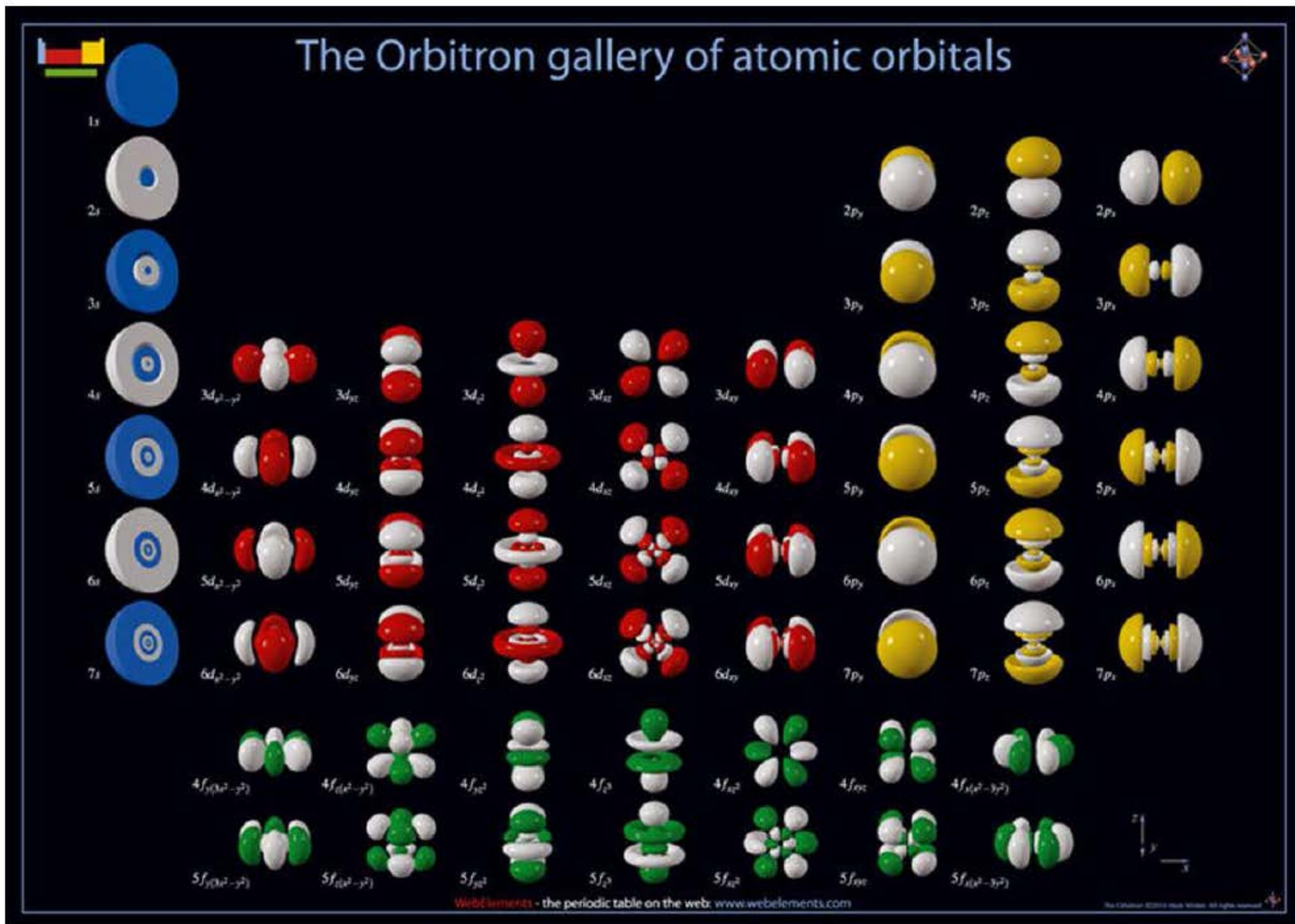
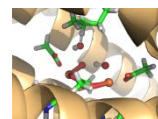
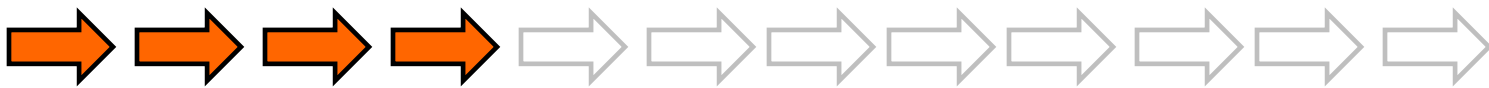
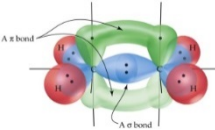


Fig. 3.18 Hydrogenic radial wavefunctions: (a) $1s$, (b) $2s$, (c) $3s$, (d) $2p$, (e) $3p$, (f) $3d$.



<http://winter.group.shef.ac.uk/orbitron>