

## Libri di testo consigliati

### **In Italiano:**

J.E. Huheey, E.A. Keiter, R.L. Keiter

Chimica Inorganica

Piccin Editore

G. L. Miessler, D. A. Tarr

Chimica Inorganica

Piccin Editore

D.F. Shriver & P.W. Atkins

Chimica Inorganica

(II edizione, dalla V edizione Inglese)

Zanichelli

### **In Inglese:**

C.E. Housecroft, A.G. Sharpe

Inorganic Chemistry (3rd edition)

Pearson

D.F. Shriver & P.W. Atkins

Inorganic Chemistry (4th or 5th edition)

Oxford

In the last 5 years, the average American (and likely European) has relied on **80** elements for quality of life.

General Electric uses **72** of the first **82** elements in its product line.



### Pharmaceuticals

Pd, Rh, Os, Ir



### Household Items

Rh, Pt



### Refining

La, Pt



### Hybrid/Electric Cars

Nd, Tb, Dy, Pr



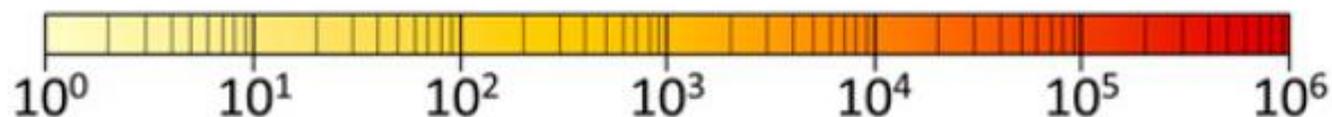
### Alternative Energy

Ru, Nd, Tb, Dy, Pr

# Concentrazione (in ppm) dei 44 elementi che si trovano in un comune circuito elettronico stampato

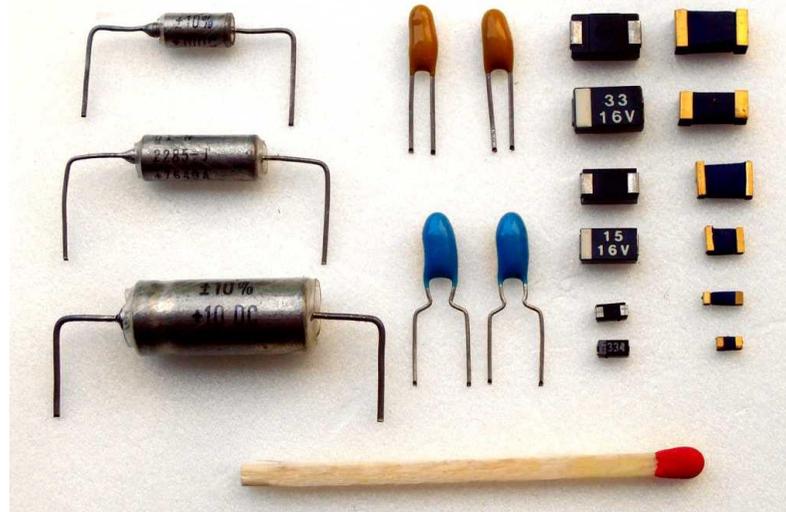
H																	He
Li	Be											B	C	N	O	F	Ne
Na	Mg											Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba	*	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra	**	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	Uu	Fl	Uu	Lv	Uus	Uuo

* Lanthanides	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
** Actinides	Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr



**OSRAM**  = **OS**mio + Wolf**RAM**io

Columbite – Tantalite = **Coltan**  
 $(\text{Fe, Mn})(\text{Nb}_n, \text{Ta}_m)_2\text{O}_6$



	Proton	Electron	Neutron
Charge / C	$+1.602 \times 10^{-19}$	$-1.602 \times 10^{-19}$	0
Charge number (relative charge)	1	-1	0
Rest mass / kg	$1.673 \times 10^{-27}$	$9.109 \times 10^{-31}$	$1.675 \times 10^{-27}$
Relative mass	1837	1	1839

$h$  = costante di Planck =  $6.626 \times 10^{-34}$  J·s

$\hbar = h/2\pi = 1.052 \times 10^{-34}$  J·s

$a_0$  = raggio di Bohr =  $5.293 \times 10^{-11}$  m = 52.93 pm = 0.529 Å

(1 pm =  $10^{-12}$  m; 1 Å =  $10^{-10}$  m, cioè 1 Å = 100 pm;

1 nm = 1000 pm, 1 nm = 10 Å)

Raggio del protone: ca. 1 fm (1 fm =  $10^{-15}$  m)

Raggio di un nucleo atomico: ca. 10 fm

Nell'atomo di H, rapporto raggio atomo/raggio nucleo = ca. 50.000

*...se il protone dell'atomo di idrogeno avesse raggio 1m e fosse posto in Piazza Unità, l'elettrone starebbe – mediamente – a più di 50 km di distanza, cioè quasi a Palmanova del Friuli..*

# equazione di Schrödinger

(caso monodimensionale)

$$-\hbar^2/2m \times d^2\Psi/dx^2 + V\Psi = E\Psi$$



*cinetica*

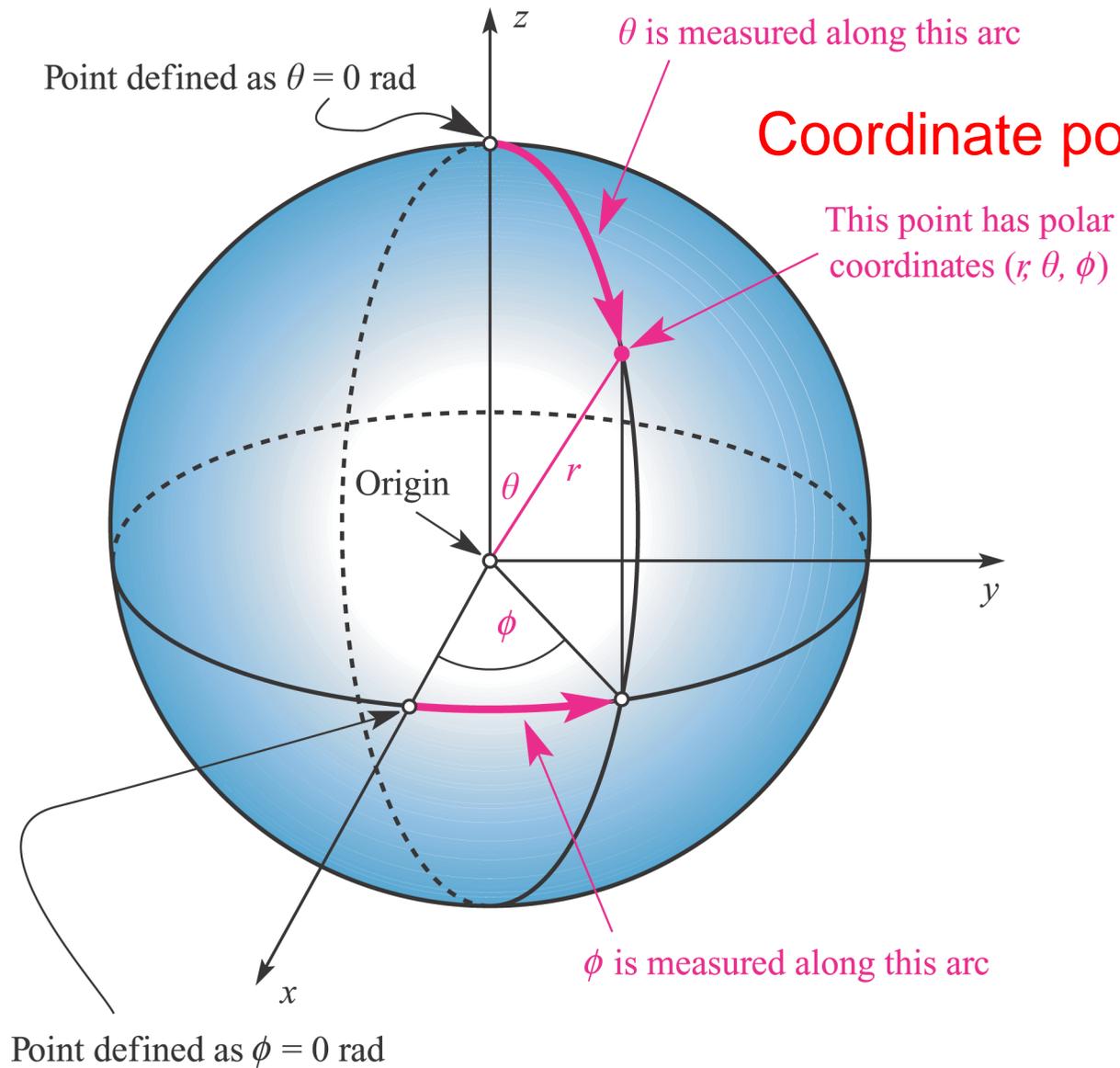


*potenziale*

$\Psi$  = funzione d'onda

$$d^2\Psi/dx^2 + 8\pi^2m/h^2 \cdot (E - V) \Psi = 0$$

Alle funzioni d'onda  $\Psi$  sono associati valori quantizzati di energia



## Coordinate polari sferiche

$$\Psi(x, y, z) = R_{n,l}(r) \cdot A_{l,m}(\theta, \phi)$$

Ogni **orbitale atomico**, descritto da una  $\Psi$ , è definito univocamente da un set di 3 numeri interi, i numeri quantici,  $n$ ,  $l$  ed  $m_l$

$n =$  **numero quantico principale** ( $n \geq 1$ ): energia, grandezza

$l =$  **numero quantico (del momento angolare) orbitale**: forma

$l = 0, 1, 2, 3, 4, \dots, n-1$  (in totale  $n$  valori interi)

La grandezza del momento angolare orbitale è data da  $\frac{h}{2\pi} \times \sqrt{l(l+1)}$

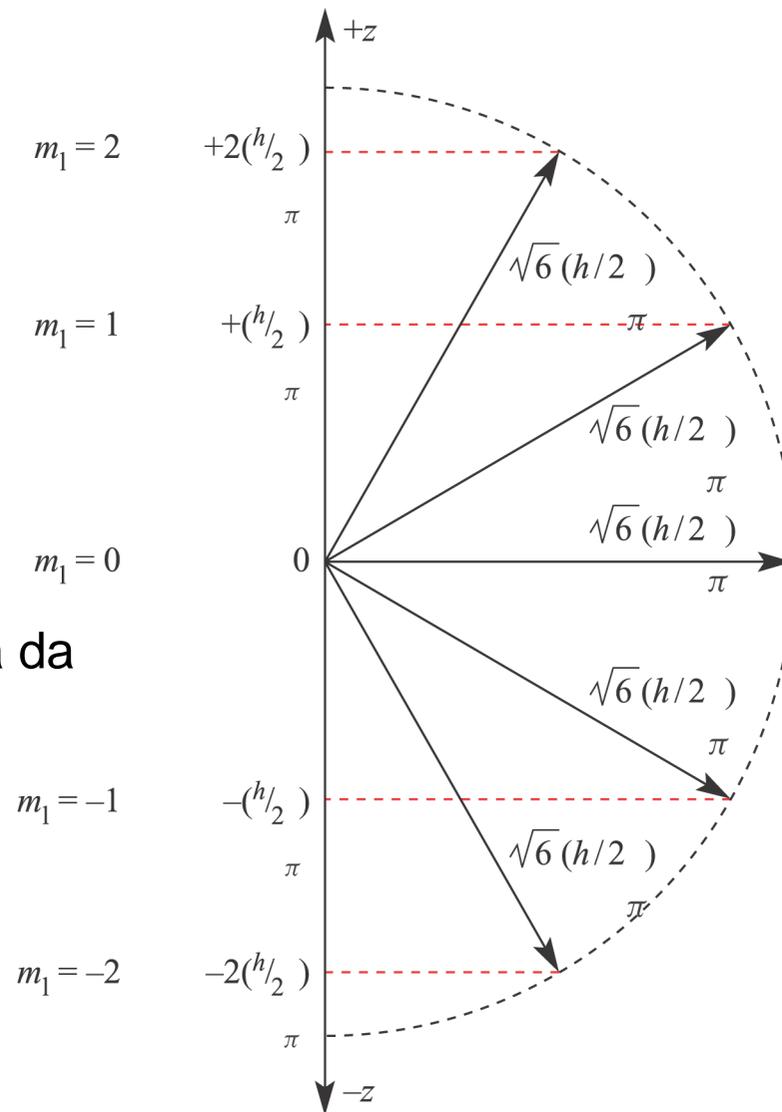
$m_l =$  **numero quantico magnetico**: orientazione

$m_l = -l, -l+1, \dots, 0, \dots, l-1, l$  (in totale  $2l+1$  valori interi)

Il numero quantico  $m_l$  specifica la componente (proiezione) del momento angolare orbitale lungo un asse arbitrario (tipicamente  $z$ ) che passa per il nucleo

# Momento angolare associato a un elettrone in un orbitale d ( $l = 2$ ) e sue componenti sull'asse z

La grandezza del momento angolare orbitale è data da  $\frac{h}{2\pi} \times \sqrt{l(l+1)}$

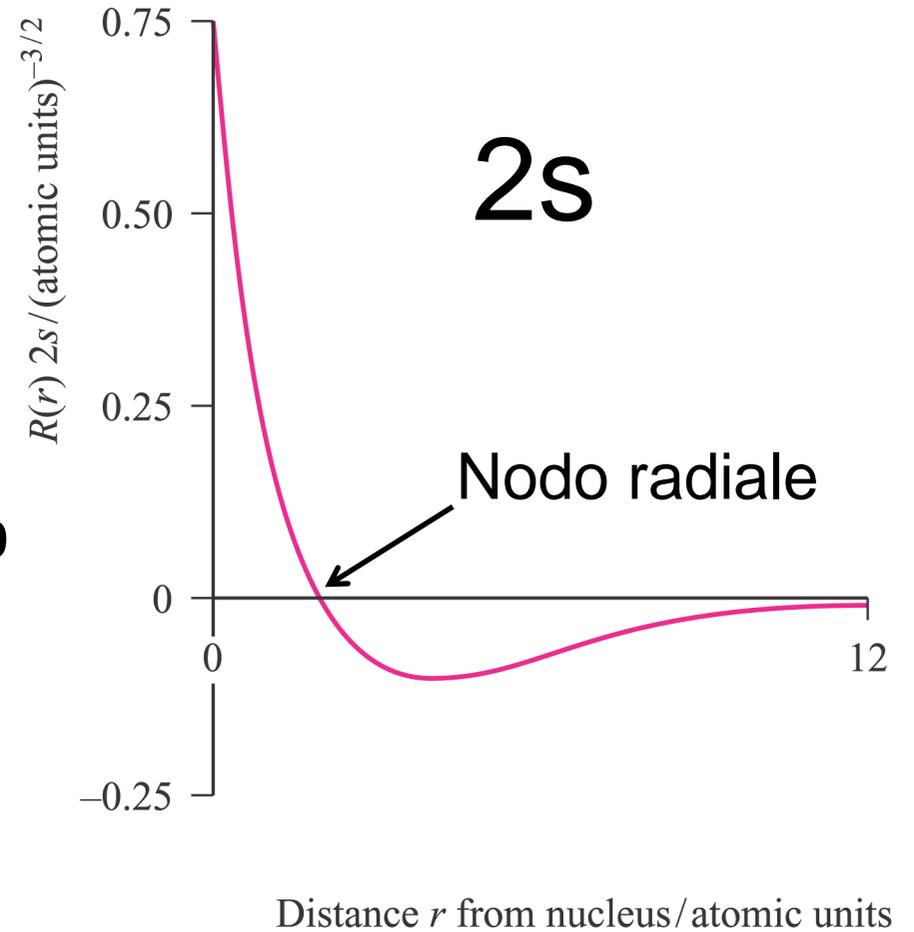
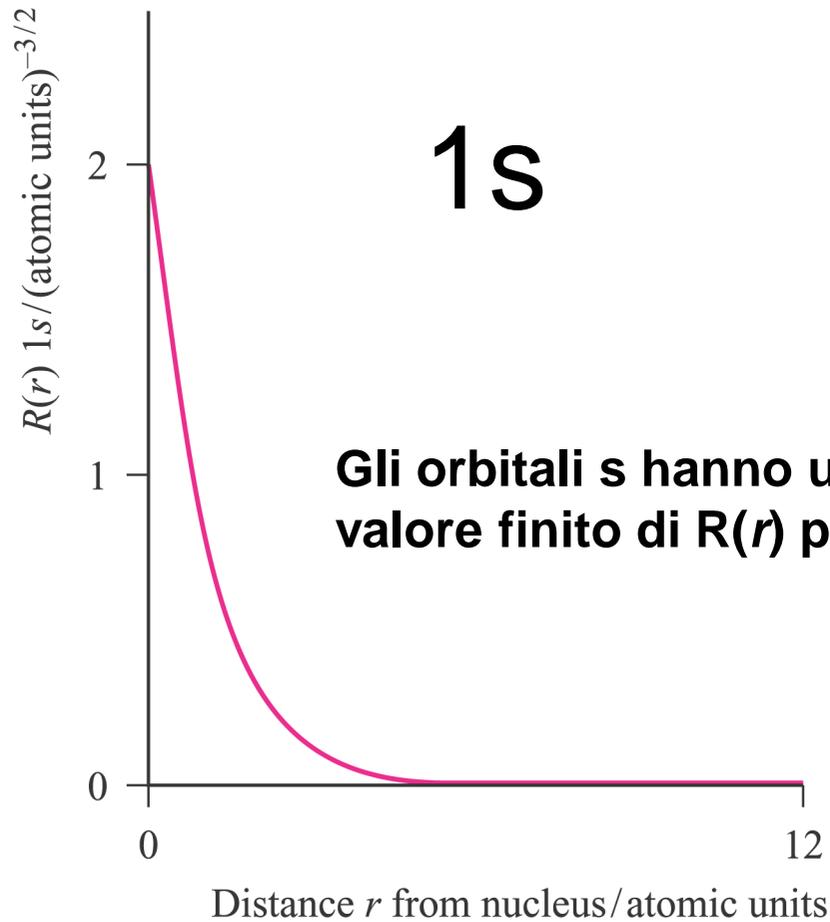


# Funzioni d'onda per l'atomo H

Atomic orbital	$n$	$l$	$m_l$	Radial part of the wavefunction, $R(r)^\dagger$	Angular part of wavefunction, $A(\theta, \phi)$
1s	1	0	0	$2e^{-r}$	$\frac{1}{2\sqrt{\pi}}$
2s	2	0	0	$\frac{1}{2\sqrt{2}}(2-r)e^{-r/2}$	$\frac{1}{2\sqrt{\pi}}$
$2p_x$	2	1	+1	$\frac{1}{2\sqrt{6}}r e^{-r/2}$	$\frac{\sqrt{3}(\sin \theta \cos \phi)}{2\sqrt{\pi}}$
$2p_z$	2	1	0	$\frac{1}{2\sqrt{6}}r e^{-r/2}$	$\frac{\sqrt{3}(\cos \theta)}{2\sqrt{\pi}}$
$2p_y$	2	1	-1	$\frac{1}{2\sqrt{6}}r e^{-r/2}$	$\frac{\sqrt{3}(\sin \theta \sin \phi)}{2\sqrt{\pi}}$

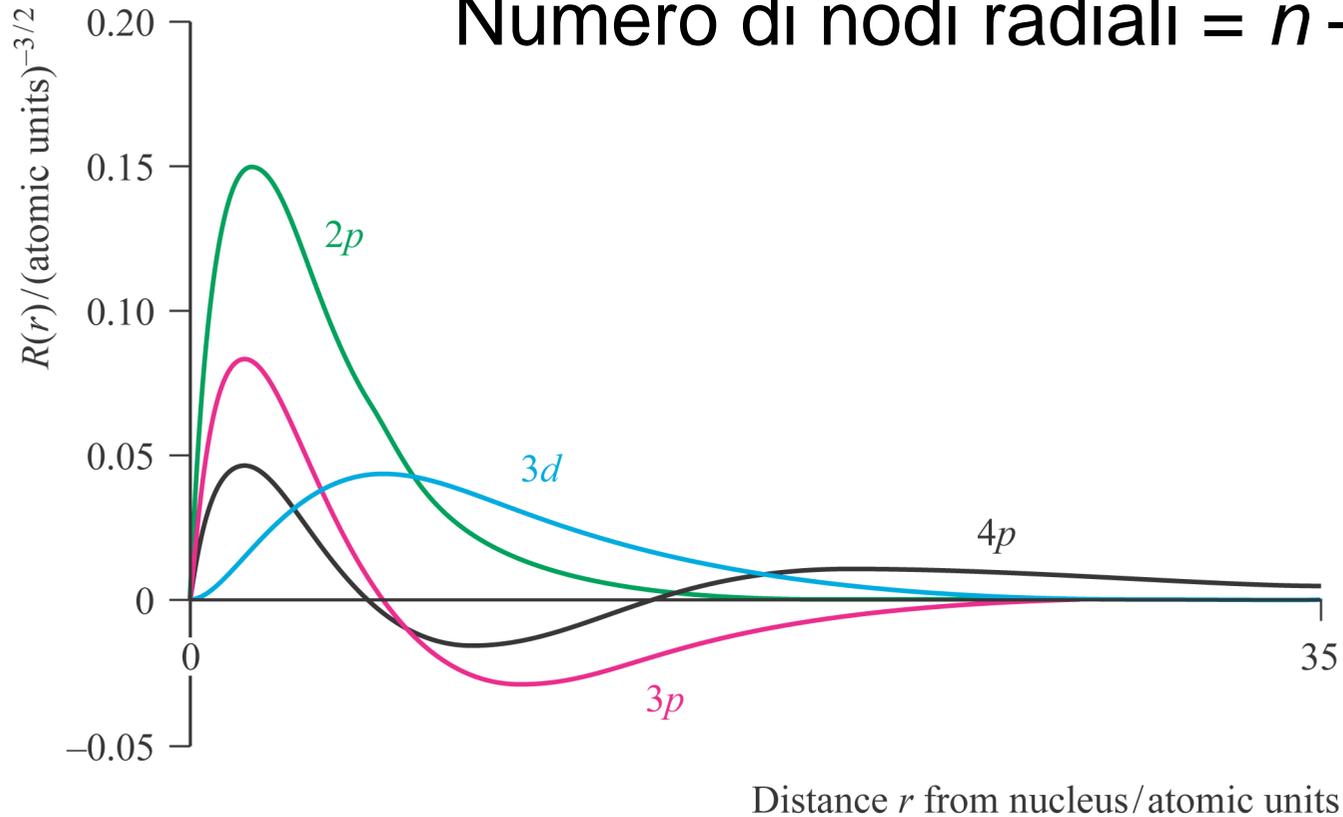
<sup>†</sup> For the 1s atomic orbital, the formula for  $R(r)$  is actually  $2\left(\frac{Z}{a_0}\right)^{3/2} e^{-Zr/a_0}$  but for the hydrogen atom,  $Z = 1$  and  $a_0 = 1$  atomic unit. Other functions are similarly simplified.

$$\Psi(x, y, z) = R_{n,l}(r) \cdot A_{l,m}(\theta, \phi)$$



Componente radiale della funzione d'onda

Numero di nodi radiali =  $n - l - 1$



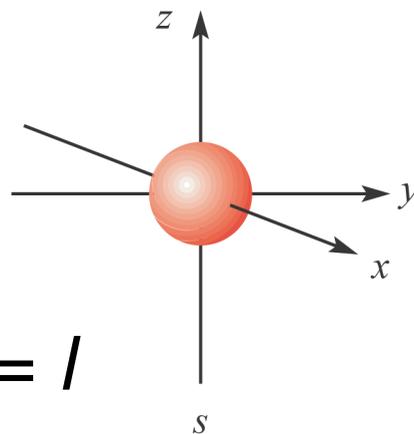
Componente radiale della funzione d'onda

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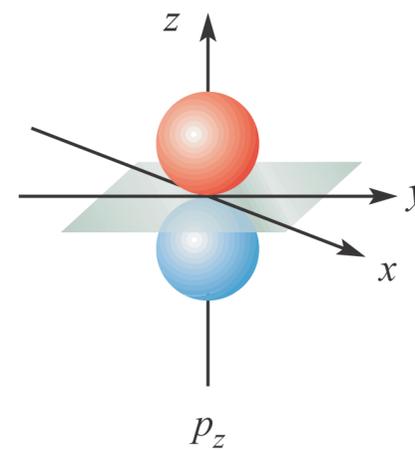
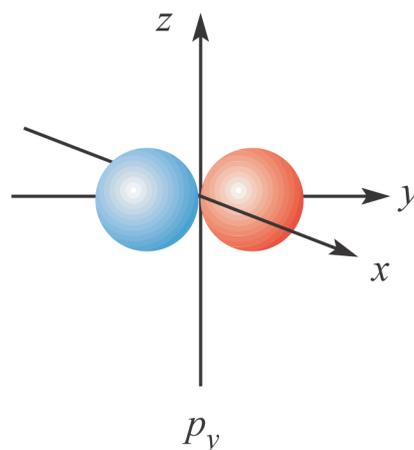
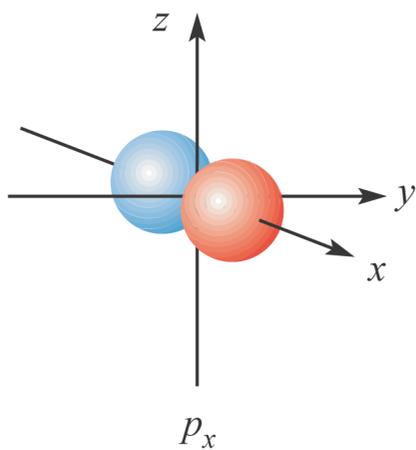
Atomic orbital	$n$	$l$	$m_l$	Radial part of the wavefunction, $R(r)^\dagger$	Angular part of wavefunction, $A(\theta, \phi)$
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2s	2	0	0	$\frac{1}{2\sqrt{2}}(2-r)e^{-r/2}$	$\frac{1}{2\sqrt{\pi}}$
2p <sub>x</sub>	2	1	+1	$\frac{1}{2\sqrt{6}}re^{-r/2}$	$\frac{\sqrt{3}(\sin\theta\cos\phi)}{2\sqrt{\pi}}$
2p <sub>z</sub>	2	1	0	$\frac{1}{2\sqrt{6}}re^{-r/2}$	$\frac{\sqrt{3}(\cos\theta)}{2\sqrt{\pi}}$
2p <sub>y</sub>	2	1	-1	$\frac{1}{2\sqrt{6}}re^{-r/2}$	$\frac{\sqrt{3}(\sin\theta\sin\phi)}{2\sqrt{\pi}}$

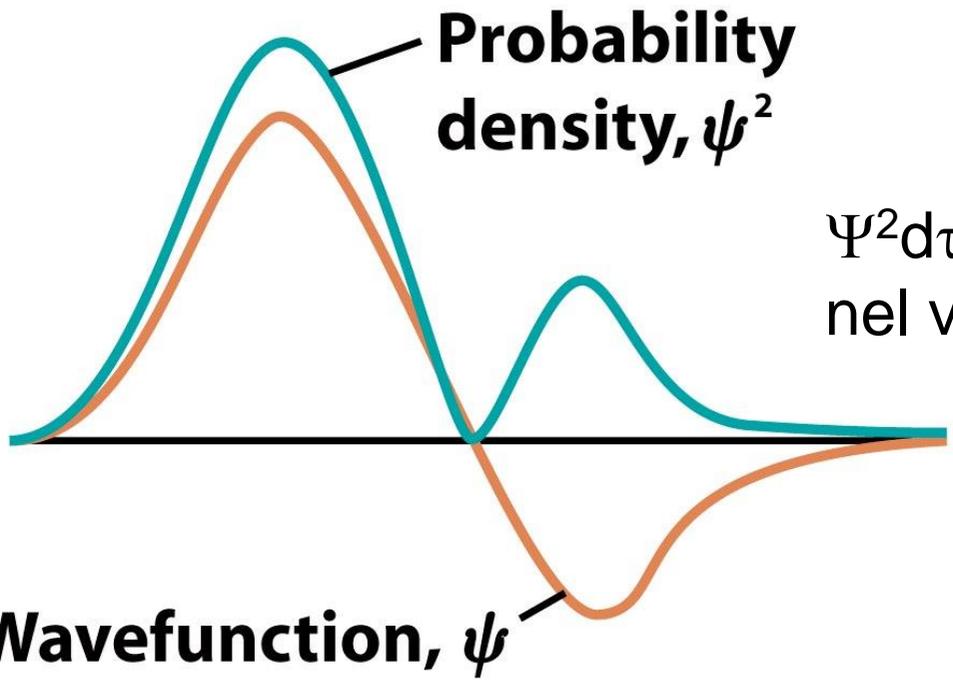
<sup>†</sup> For the 1s atomic orbital, the formula for  $R(r)$  is actually  $2\left(\frac{Z}{a_0}\right)^{3/2} e^{-Zr/a_0}$  but for the hydrogen atom,  $Z = 1$  and  $a_0 = 1$  atomic unit. Other functions are similarly simplified.

# Superfici di confine senza significato fisico, $A(\theta, \phi)$



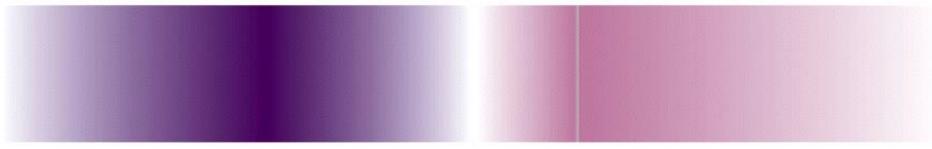
Numero di piani nodali =  $l$





$\Psi^2 d\tau =$  probabilità di trovare l'elettrone nel volume infinitesimo  $d\tau$

$$\int \Psi^2 d\tau = 1$$



**Probability density**

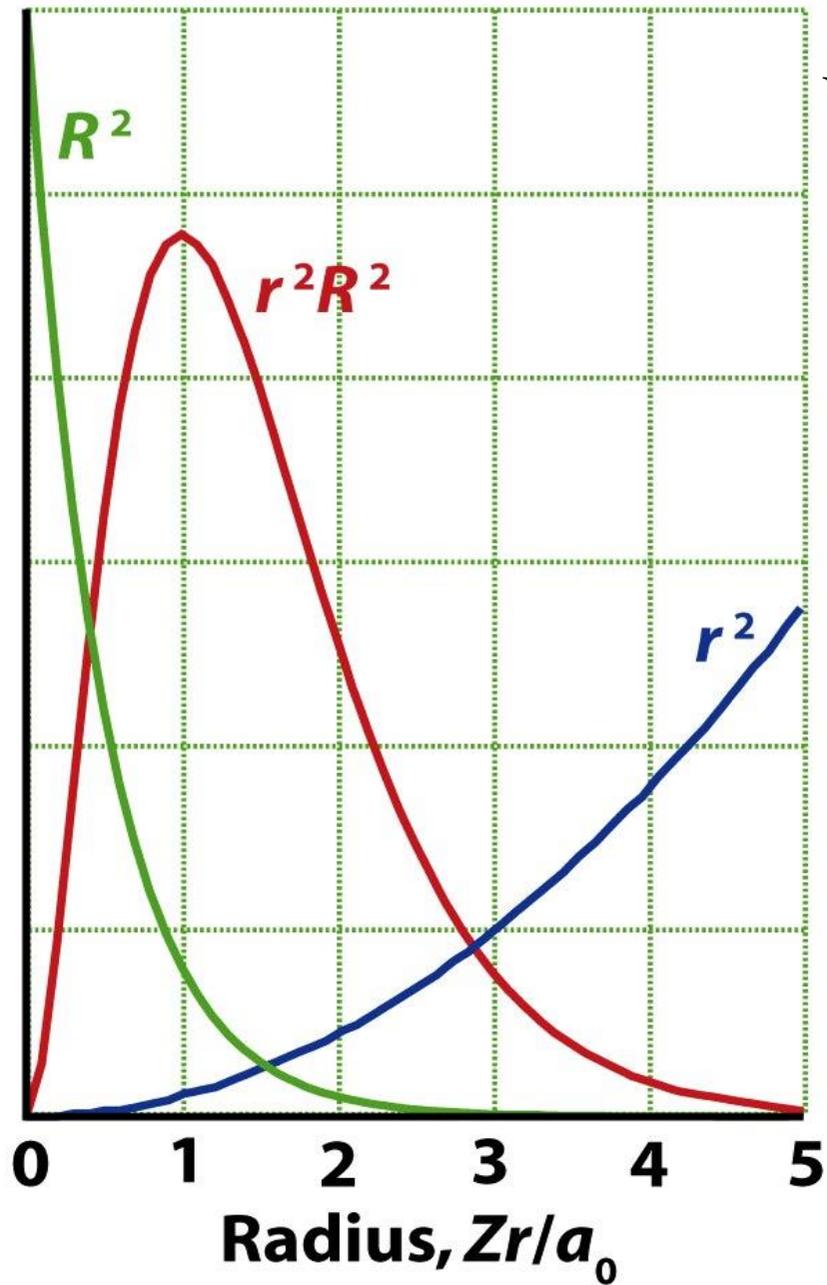
$$\Psi^2(x, y, z) = R_{n,l}(r)^2 \cdot A_{l,m}(\theta, \phi)^2$$

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**funzione di  
distribuzione radiale**

$$P(r) = 4\pi r^2 R(r)^2$$

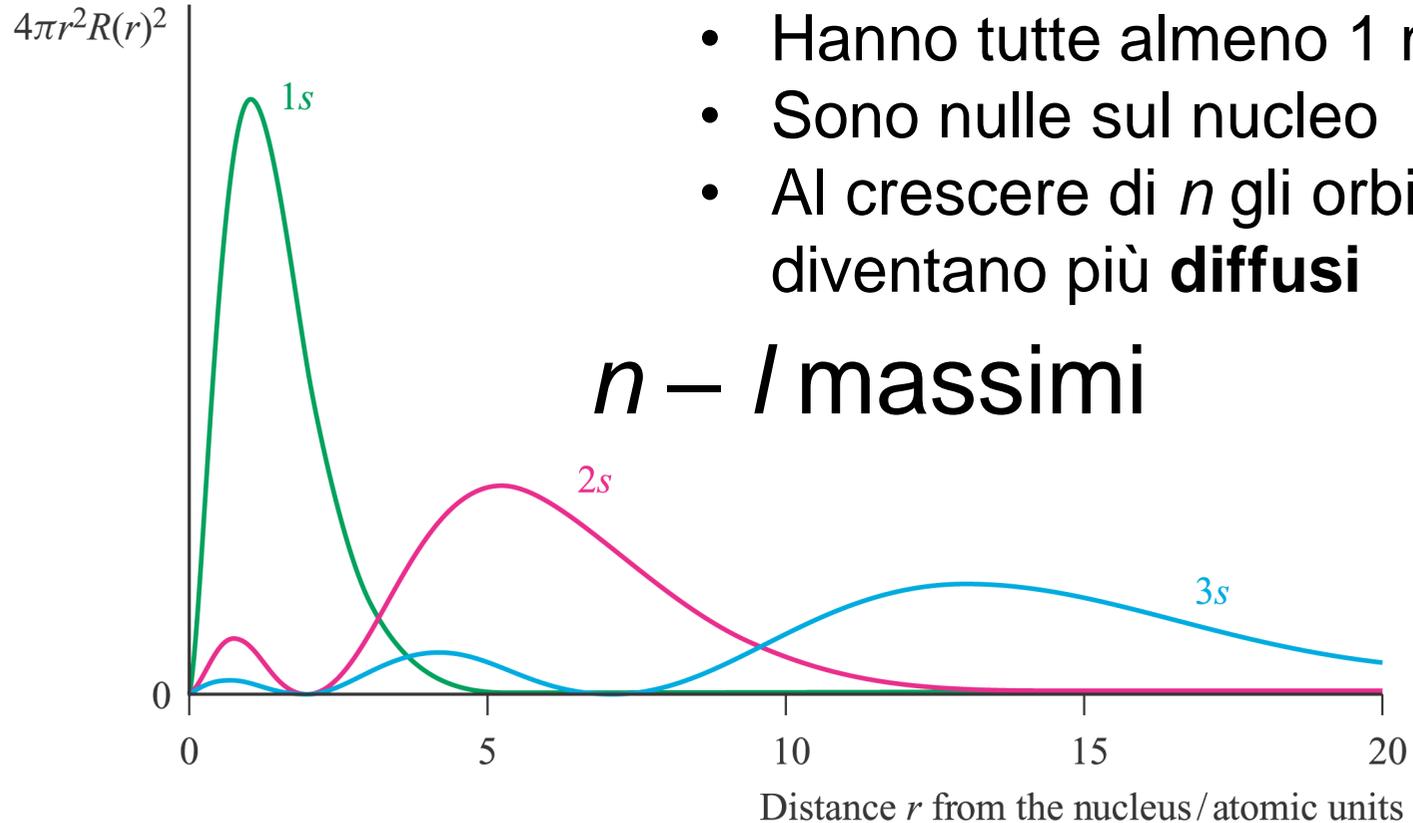
probabilità di trovare l'elettrone a una distanza  $r$  dal nucleo (in un guscio sferico di superficie  $4\pi r^2$  e di spessore  $dr$ ), indipendentemente dalla direzione. È l'integrale di  $\Psi^2 dr$  esteso su tutti gli angoli



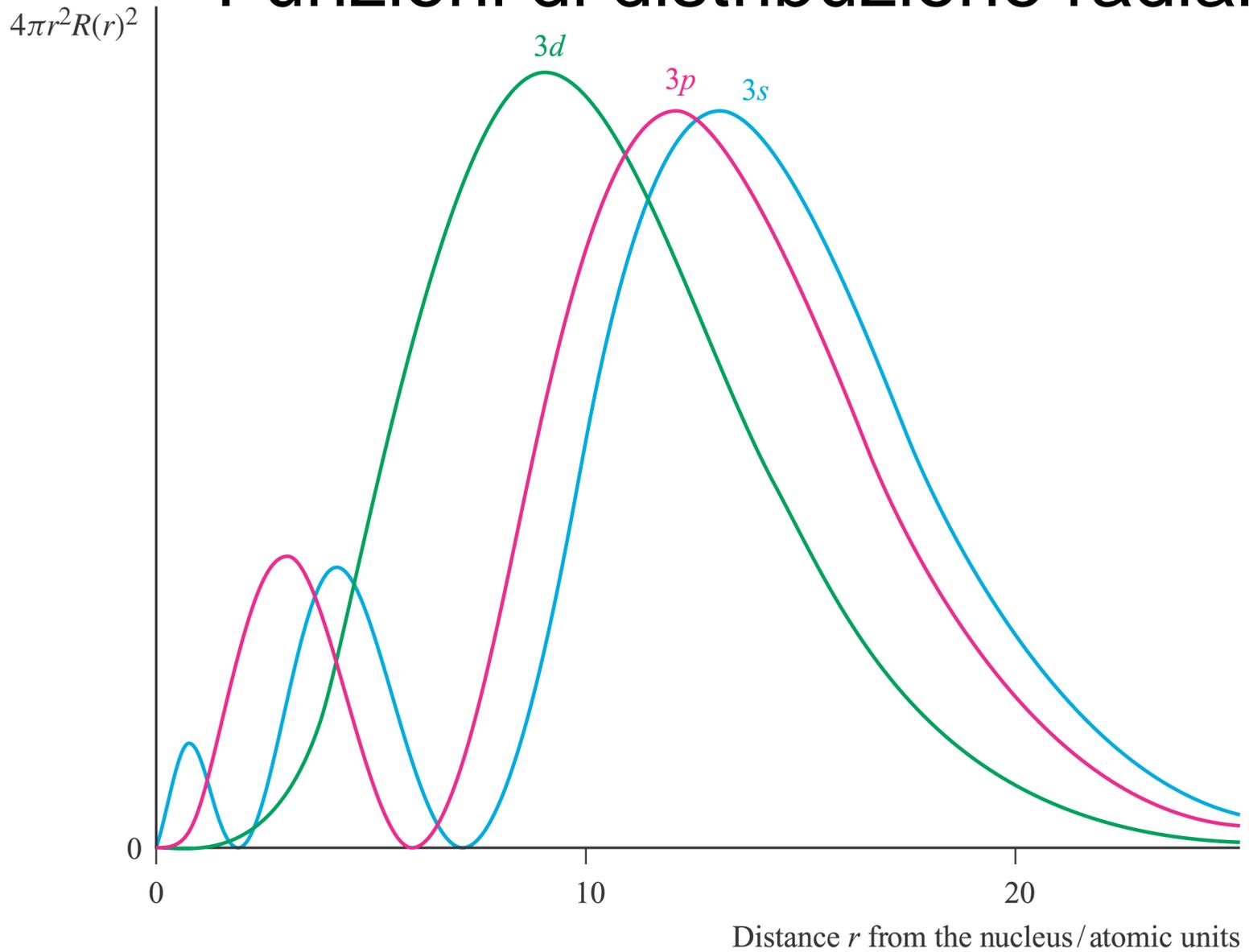
**Orbitale 1s**

$$P(r) = 4\pi r^2 \Psi^2$$

# Funzioni di distribuzione radiale

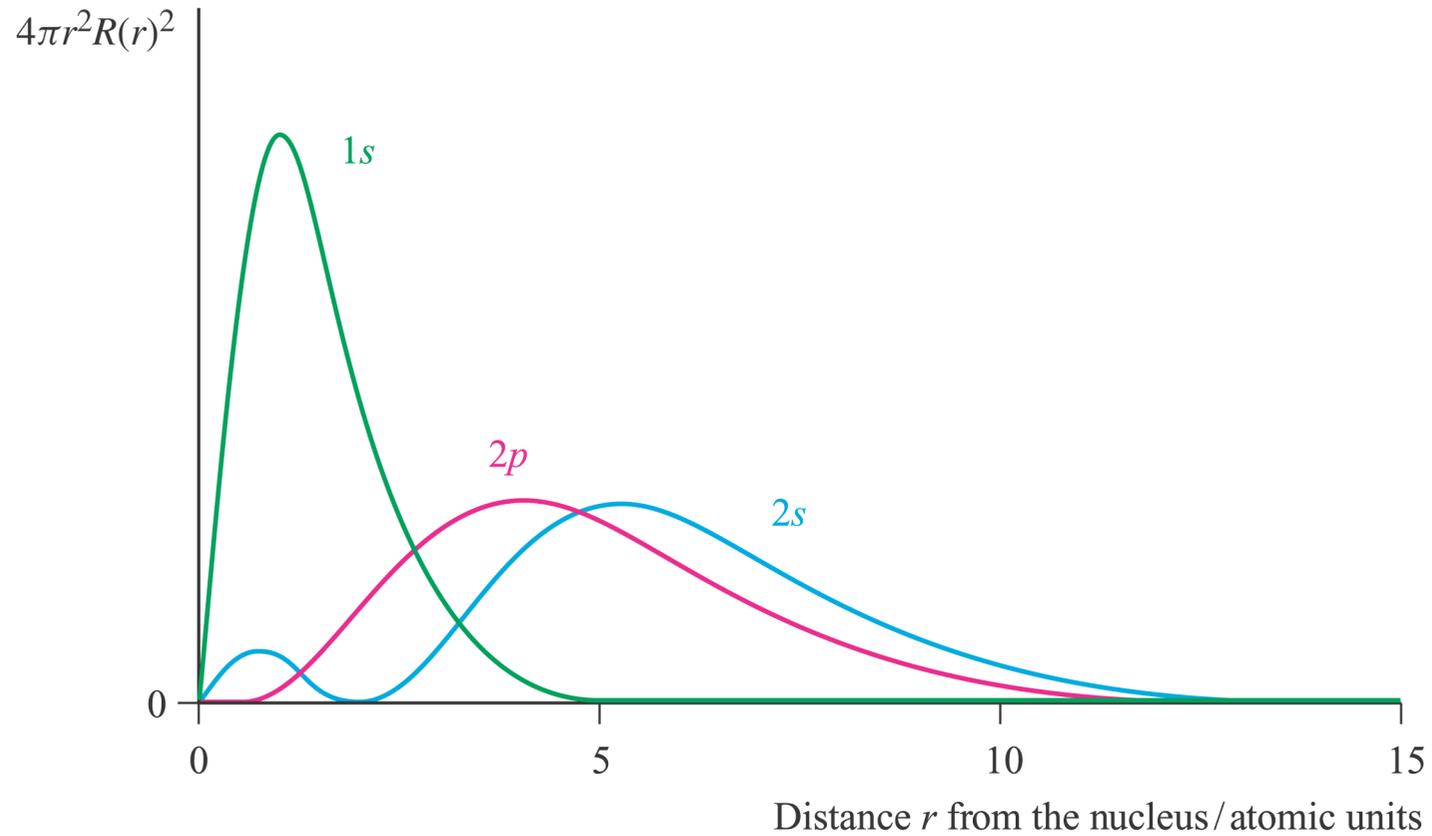


# Funzioni di distribuzione radiale



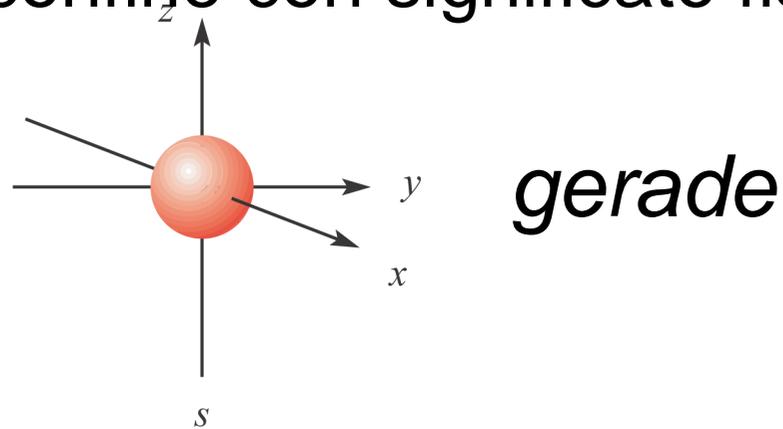
A parità di  $n$ , orbitali con  $l$  più piccolo sono più **penetranti**

# Funzioni di distribuzione radiale

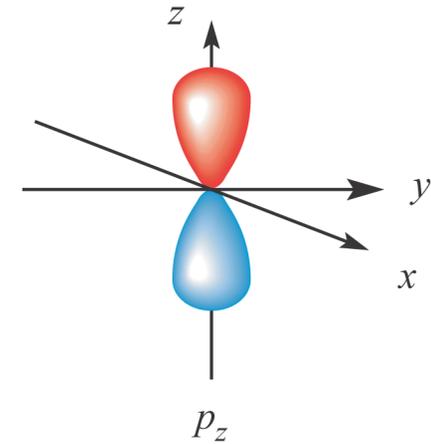
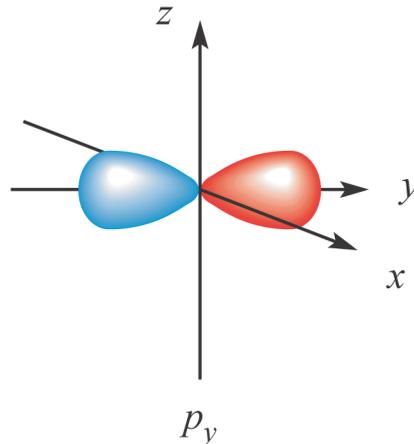
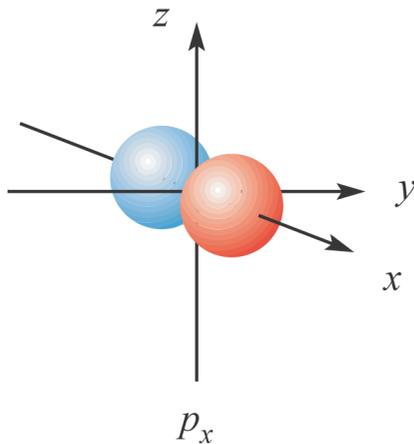


# Funzione di distribuzione angolare $A(\theta, \phi)^2$

## Superfici di confine con significato fisico

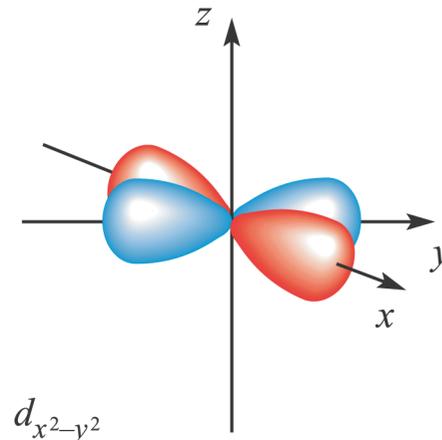
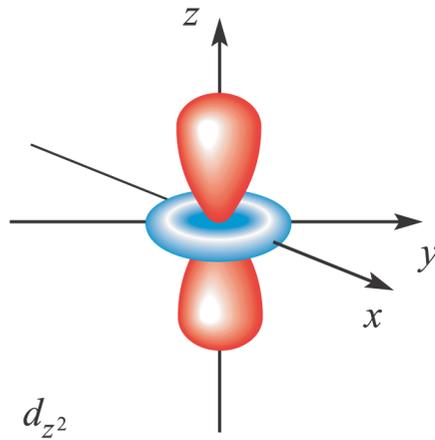
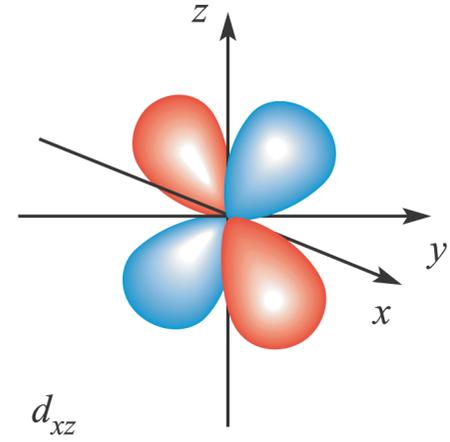
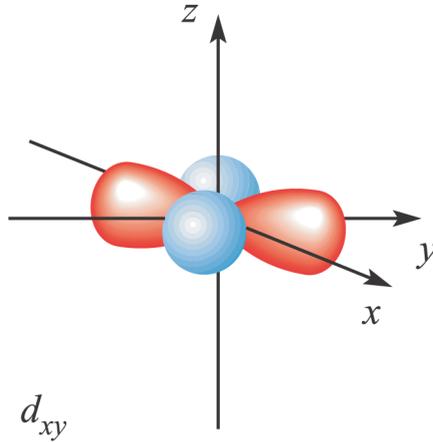
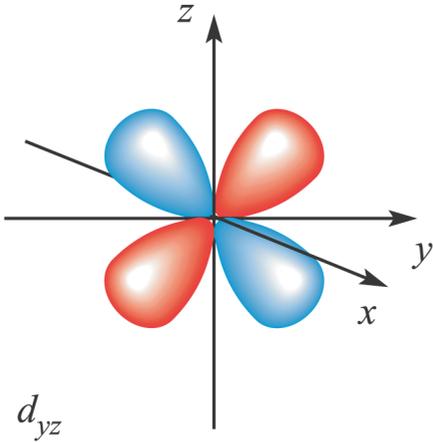


*ungerade*



$A(\theta, \phi)^2$  rappresenta la probabilità di trovare un elettrone in funzione dei due angoli  $\theta$  e  $\phi$

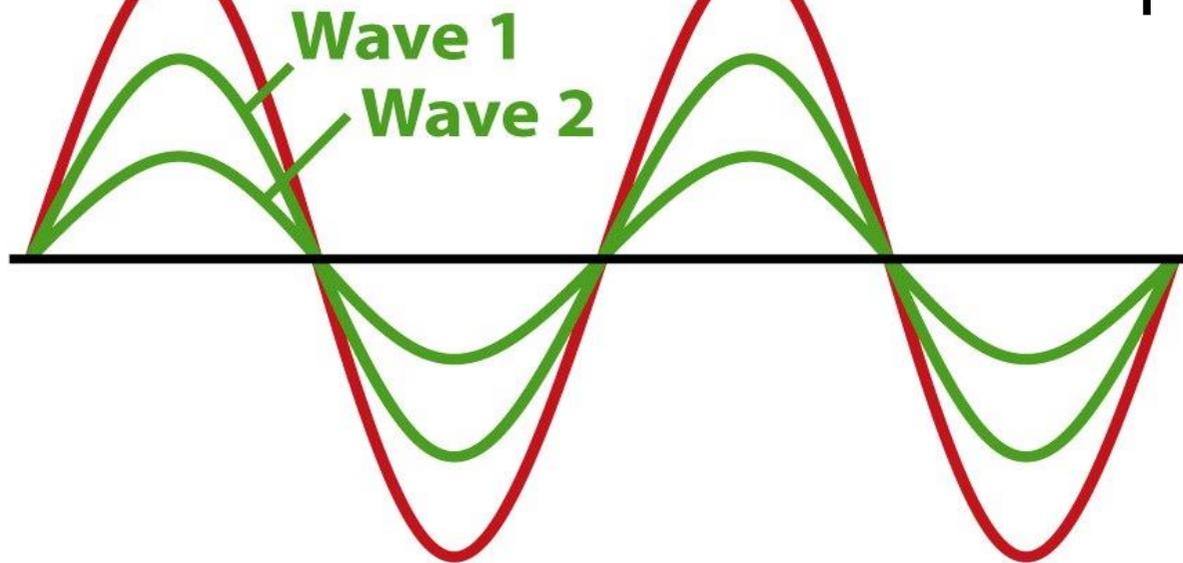
# Superfici di confine con significato fisico, $A(\theta, \phi)^2$



*gerade*

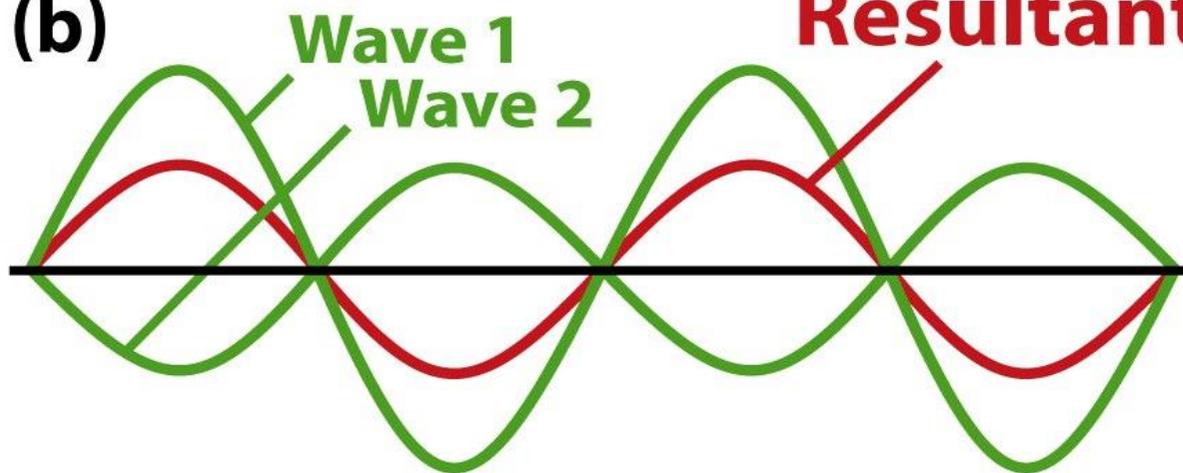
**(a) Resultant**

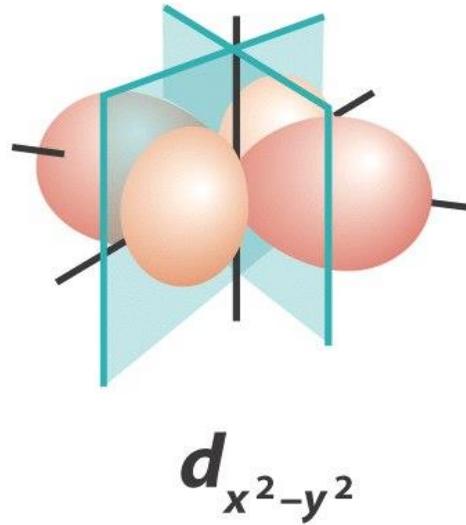
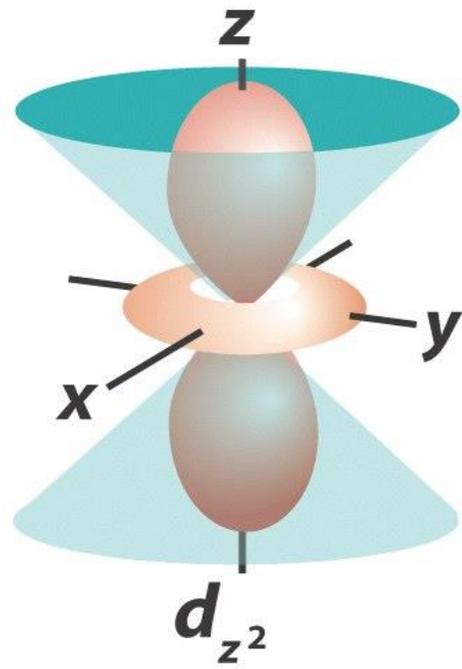
Importanza della fase



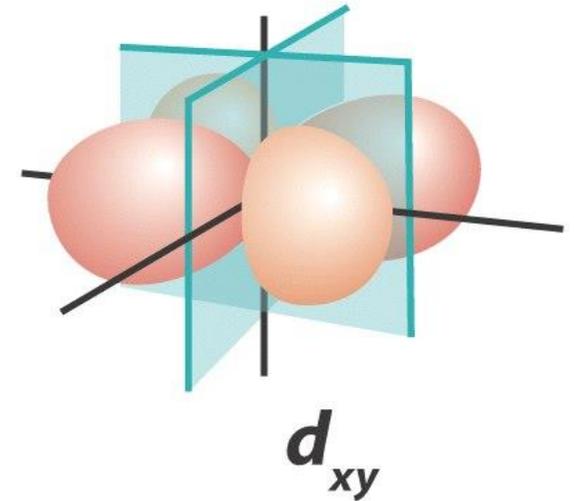
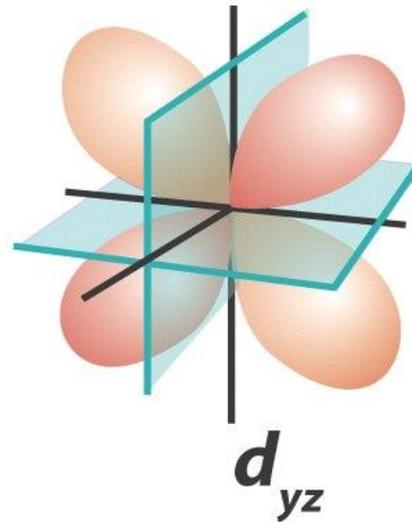
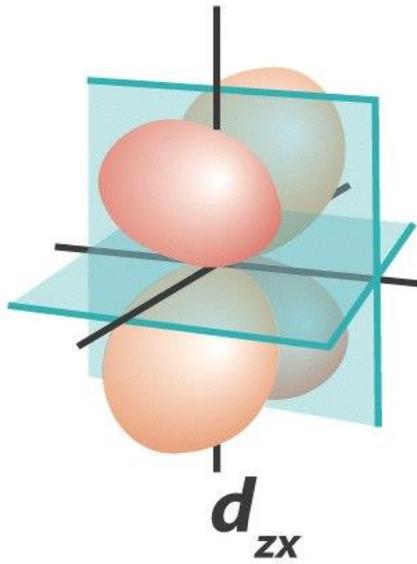
**(b)**

**Resultant**



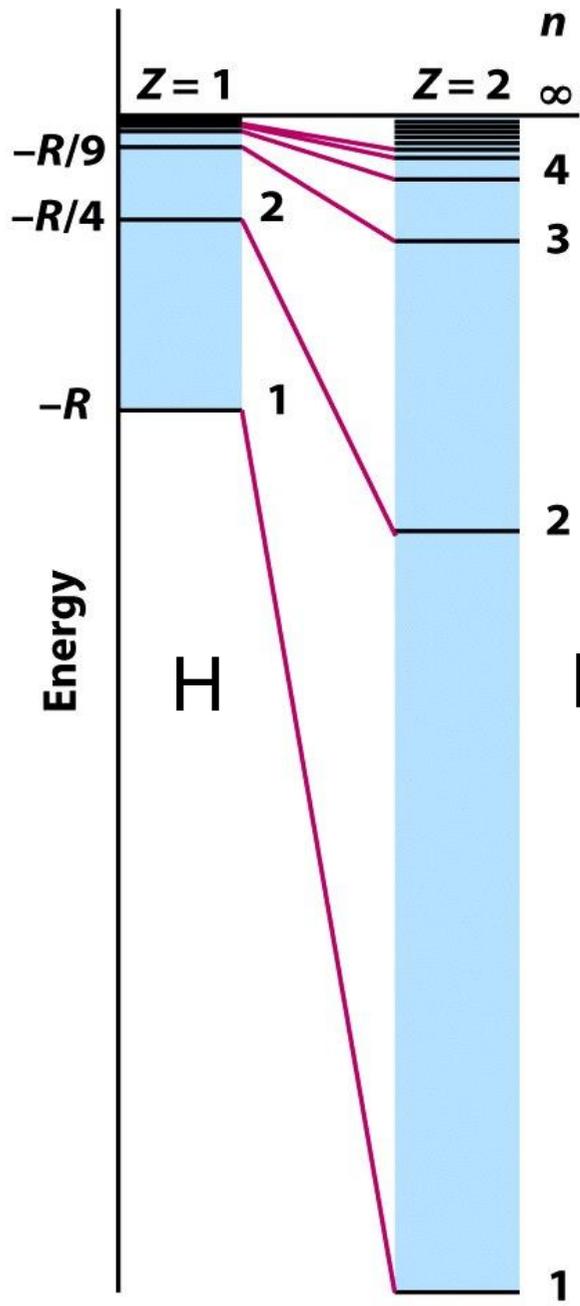


Le funzioni di distribuzione angolare hanno / piani nodali



eccellenti rappresentazioni degli orbitali si  
possono trovare sul sito:

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



$$E = -kZ^2/n^2$$

$$k = 1.312 \times 10^3 \text{ kJ mol}^{-1}$$

H

He<sup>+</sup>

# Subshells

