

Teoria quantistica

Sistemi semplici risolvibili

esattamente

Conclusione sui momenti angolari:

lo SPIN

ROTAZIONE in 3D

Chimica Fisica 2

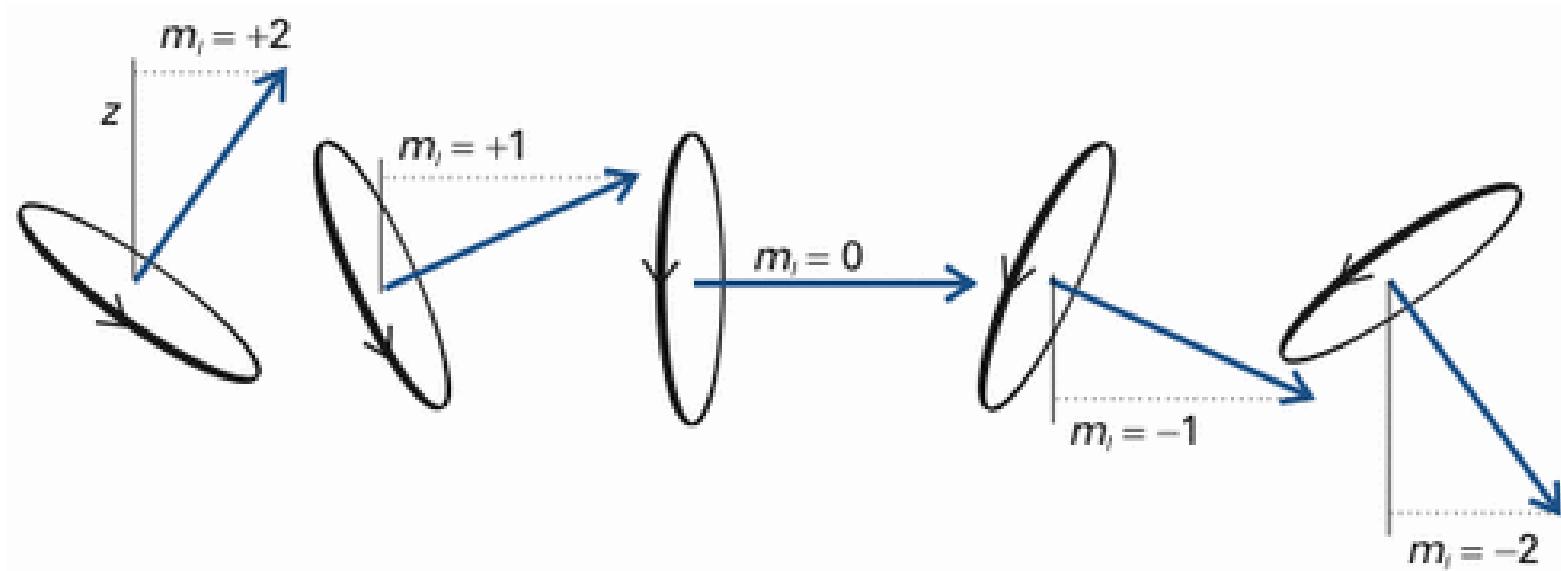
Laurea Tri. Chim. Industriale

2022-23

Prof. Antonio Toffoletti

Rotational motion

3 dimensions



The permitted orientations of angular momentum when $l = 2$. We shall see soon that this representation is too specific because the azimuthal orientation of the vector (its angle around z) is indeterminate.

QUANTIZZAZIONE SPAZIALE della **ROTAZIONE** di un corpo
microscopico

Rotational motion

3 dimensions

$$\hat{l}_x = \frac{\hbar}{i} \left(y \frac{\partial}{\partial z} - z \frac{\partial}{\partial y} \right) \quad \hat{l}_y = \frac{\hbar}{i} \left(z \frac{\partial}{\partial x} - x \frac{\partial}{\partial z} \right) \quad \hat{l}_z = \frac{\hbar}{i} \left(x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right)$$

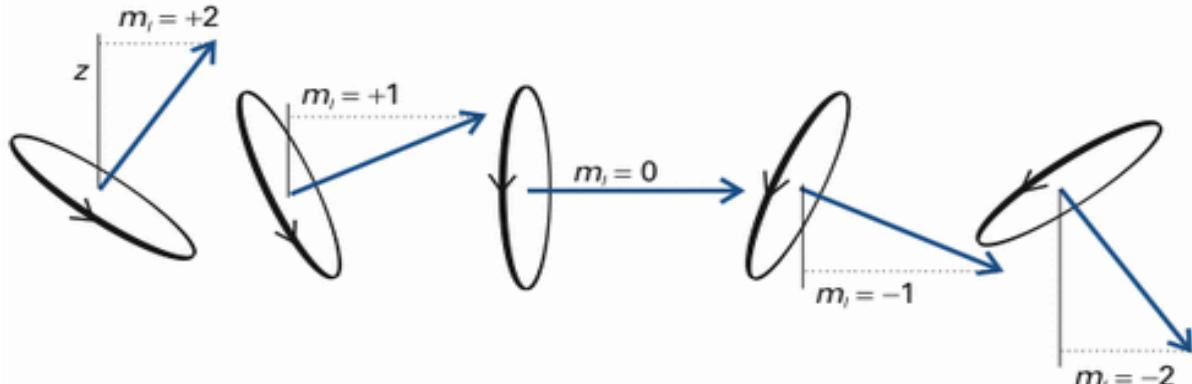
$$[\hat{l}_x, \hat{l}_y] = i\hbar \hat{l}_z \quad [\hat{l}_y, \hat{l}_z] = i\hbar \hat{l}_x \quad [\hat{l}_z, \hat{l}_x] = i\hbar \hat{l}_y$$

$$\hat{l}^2 = \hat{l}_x^2 + \hat{l}_y^2 + \hat{l}_z^2 = \hbar^2 \Lambda^2$$

$$[\hat{l}^2, \hat{l}_q] = 0 \quad q = x, y, \text{ and } z$$

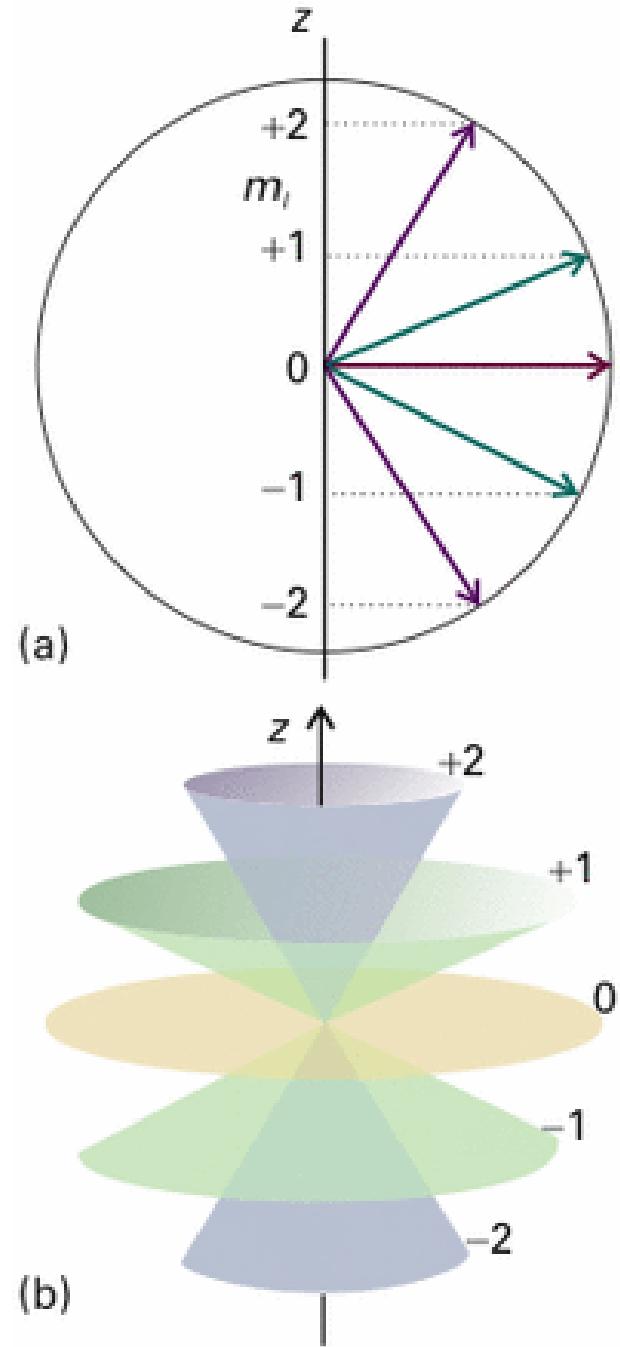
Rotational motion

3 dimensions



The permitted orientations of angular momentum when $l = 2$. We shall see soon that this representation is too specific because the azimuthal orientation of the vector (its angle around z) is indeterminate.

(a) A summary of the preceding figure.
Because the azimuthal angle of the vector around the z-axis is indeterminate, a better representation is shown in (b), where each vector lies at an unspecified azimuthal angle on its cone.



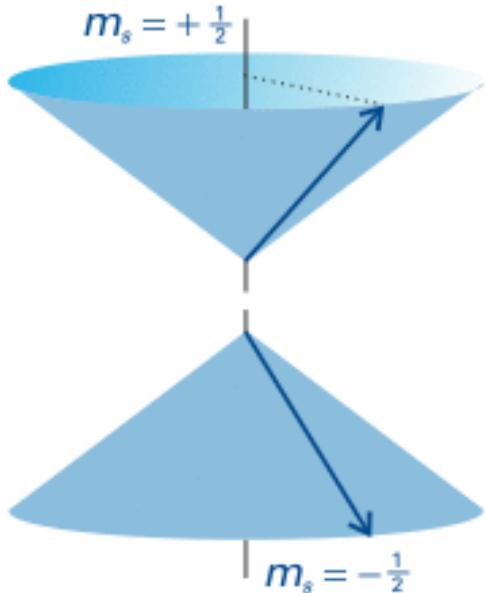
Angular momentum to spin

The spin of an electron about its own axis does not have to satisfy the same boundary conditions as those for a particle circulating around a central point, so the quantum number for spin angular momentum is subject to different restrictions. To distinguish this spin angular momentum from orbital angular momentum we use the **spin quantum number** s (in place of l ; like l , s is a non-negative number) and m_s , the **spin magnetic quantum number**, for the projection on the z -axis. The magnitude of the spin angular momentum is $\{s(s + 1)\}^{1/2}\hbar$ and the component $m_s\hbar$ is restricted to the $2s + 1$ values

$$m_s = s, s - 1, \dots, -s$$

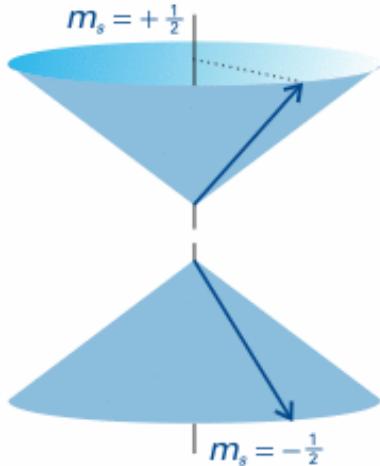
Angular momentum lo spin

For an electron it turns out that only one value of s is allowed, namely $s = \frac{1}{2}$, corresponding to an angular momentum of magnitude $(\frac{3}{4})^{1/2}\hbar = 0.866\hbar$. This spin angular momentum is an intrinsic property of the electron, like its rest mass and its charge, and every electron has exactly the same value: the magnitude of the spin angular momentum of an electron cannot be changed. The spin may lie in $2s + 1 = 2$ different orientations



An electron spin ($s = 1/2$) can take only two orientations with respect to a specified axis. An α electron (top) is an electron with $m_s = +1/2$; a β electron (bottom) is an electron with $m_s = -1/2$. The vector representing the magnitude of the spin angular momentum lies at an angle of 55° to the z-axis (more precisely the half-angle of the cones is $\arccos(1/3^{1/2})$).

Angular momentum lo spin



Particelle dotate di spin

	numero quantico	modulo del momento angolare di spin
elettrone	$\frac{1}{2}$	$(\frac{3}{4})^{1/2}\hbar = 0.866\hbar$
protone	$\frac{1}{2}$	$(\frac{3}{4})^{1/2}\hbar = 0.866\hbar$
neutrone	$\frac{1}{2}$	$(\frac{3}{4})^{1/2}\hbar = 0.866\hbar$
fotone	1	$(2)^{1/2}\hbar = 1.414 \hbar$

Angular momentum to spin

Properties of angular momentum

Quantum number	Symbol	Values*	Specifies
Orbital angular momentum	l	0, 1, 2, ...	Magnitude, $\{l(l+1)\}^{1/2}\hbar$
Magnetic	m_l	$l, l-1, \dots, -l$	Component on z -axis, $m_l\hbar$
Spin	s	$\frac{1}{2}$	Magnitude, $\{s(s+1)\}^{1/2}\hbar$
Spin magnetic	m_s	$\pm\frac{1}{2}$	Component on z -axis, $m_s\hbar$
Total	j	$l+s, l+s-1, \dots, l-s $	Magnitude, $\{j(j+1)\}^{1/2}\hbar$
Total magnetic	m_j	$j, j-1, \dots, -j$	Component on z -axis, $m_j\hbar$

To combine two angular momenta, use the Clebsch–Gordan series:

$$j=j_1+j_2, j_1+j_2-1, \dots, |j_1-j_2|$$

For many-electron systems, the quantum numbers are designated by uppercase letters (L, M_L, S, M_S etc.).

*Note that the quantum numbers for magnitude (l, s, j , etc.) are never negative.

Riassunto dei sistemi con soluzione esatta dell'eqn di Schroedinger

- Particella libera
- Particella nella scatola
 - 1 dimensione
 - 2 dimensioni
 - 3 dimensioni *traslazione delle molecole gassose*
- Oscillatore armonico (1 dimensione) *vibrazione delle molecole biatomiche*
- Particella in rotazione
 - 2 dimensioni (su una circonferenza)
 - 3 dimensioni (su una superficie sferica)
rotazione delle molecole biatomiche