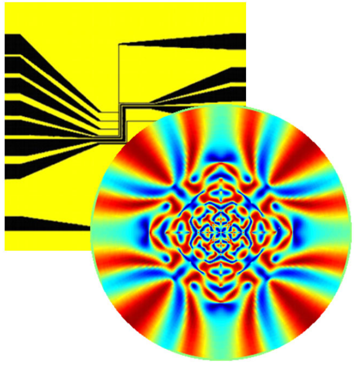


Rydberg Atoms in Magnetic Quadrupole Traps

I. Lesanovsky[1], J. Schmiedmayer[1], and P. Schmelcher[1,2]

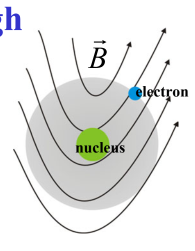
[1]*Physikalisches Institut, Universität Heidelberg, Philosophenweg 12, 69120 Heidelberg, Germany*

[2]*Physikalisch-Chemisches Institut, INF 229, 69120 Heidelberg, Germany*

E-mail: igor.lesanovsky@physi.uni-heidelberg.de

References: EPL **65**, 478 (2004) – PRA **69**, 53405 (2004) – PRA **70** (2004)

Electronically excited atoms in a high gradient magnetic field



- for highly excited states, e.g. Rydberg states, in strongly inhomogeneous fields the adiabatic approximation does not hold
- atom size is comparable to the length scale of the field variation → both nucleus and electrons are separately 'visible' to the field
- electrons and nucleus couple through their charge and magnetic moment to the field
- spin-orbit and nuclear spin-total spin coupling can be neglected ($V_{FS} \sim r^{-3}$)

Alkali atoms

- alkali atoms are used in almost all experimental applications
- atoms in highly excited states (Rydberg states) can in good approximation be treated as hydrogenic systems

The general Hamiltonian

$$\hat H_g = \frac{1}{2m_e}\left(\vec p_e + e\vec A(\vec r_e)\right)^2 + \frac{1}{2m_n}\left(\vec p_n - e\vec A(\vec r_n)\right)^2 - \frac{1}{4\pi\varepsilon_0}\frac{e^2}{|\vec r_e - \vec r_n|} - \vec\mu_e \vec B(\vec r_e) - \vec\mu_n \vec B(\vec r_n)$$

kinetic energy of the electron – kinetic energy of the nucleus – Coulomb-Interaction – coupling of the magnetic moment of the electron to the field – coupling of the magnetic moment of the nucleus to the field

Symmetries

J_z	total angular momentum (z-component)
P_i	x_i-parity
σ_i	Pauli spin matrices
T	conventional time reversal
I_{xy}	coordinate exchange (x↔y)
S_1	$\sigma_x\to-\sigma_y$, $\sigma_y\to-\sigma_x$, $\sigma_z\to-\sigma_z$
S_2	$\sigma_x\to-\sigma_y$, $\sigma_y\to\sigma_x$, $\sigma_z\to\sigma_z$

Quadrupole Field

J_z	$T\sigma_xP_z$
TP_y	$P_y\sigma_xP_z$

- dynamics takes place in separated 2-dimensional subspaces characterized by the J_z-quantum number m_J

Magnetic Guide

$\Sigma_x=\sigma_xP_yP_z$	$\Sigma_y=P_x\sigma_yP_z$	$\Sigma_z=P_xP_y\sigma_z$
$T\sigma_xP_z$	$TP_xP_yP_z\sigma_y$	$TP_z\sigma_z$
TP_y	$I_{xy}S_1$	$P_yP_zI_{xy}$
$P_xP_yI_{xy}S_1^*$	$TP_xP_yP_zI_{xy}S_2^*$	$TP_zI_{xy}S_2$
$P_xP_zI_{xy}S_2^*$	$TP_xI_{xy}S_1^*$	$P_yP_zI_{xy}S_2$

- non-Abelian symmetry group
- no continuous symmetry → system requires full 3-dimensional treatment

commuting set of operators

four separate $P_yP_zI_{xy}S_2$–sub spaces

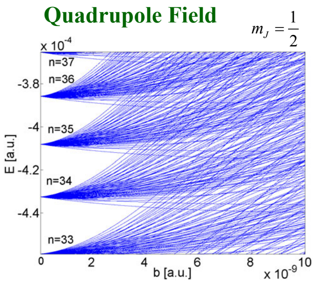
$$P_yP_zI_{xy}S_2|E,\kappa\rangle = \kappa|E,\kappa\rangle$$

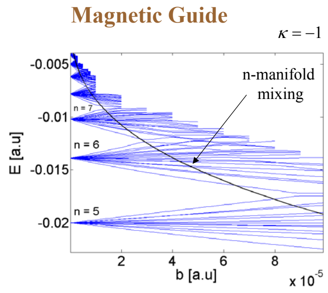
quantum numbers: $\kappa = \pm1, \pm i$

In both fields the interplay of the symmetries leads to a two-fold degeneracy of any energy level.

Energy spectrum

Quadrupole Field $m_J = \frac{1}{2}$ — **Magnetic Guide** $\kappa = -1$





- overlap of adjacent n-manifolds scales as $b \propto n^{-11/2}$

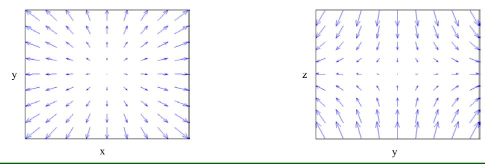
Quadrupole Field

Magnetic field: $\vec B = b\begin{pmatrix} x \\ y \\ -2z\end{pmatrix} = \nabla\times\vec A$

Vector potential: $\vec A = b\begin{pmatrix} yz \\ -xz \\ 0\end{pmatrix} = \frac{1}{3}\left[\vec B\times\vec r\right]$

- rotation invariance around z-axis

Vectorial Plot of the Magnetic Field



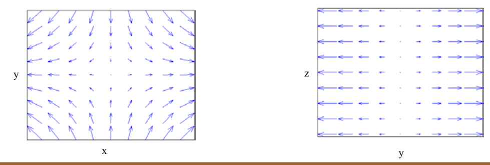
Magnetic Guide

Magnetic field: $\vec B = b\begin{pmatrix} x \\ -y \\ 0\end{pmatrix} = \nabla\times\vec A$

Vector potential: $\vec A = b\begin{pmatrix} 0 \\ 0 \\ xy\end{pmatrix}$

- translation invariance along z-axis

Vectorial Plot of the Magnetic Field



The Hamiltonian

- the two-body problem cannot be separated due to the presence of the external magnetic field

→ Application of the following approximations:

- coupling of the nuclear spin to the field is neglected
- motion of electron and nucleus is assumed to be decoupled (mass ratio: $\frac{m_e}{m_n}\to 0$)
- nucleus position is fixed in the center of the trap (coordinate origin)

non-trivial coupling of the electronic spin to spatial degrees of freedom

no separation of spin space and real space dynamics possible

Electronic Hamiltonian in spherical coordinates (r,θ,φ)

Quadrupole Field

$$H = -\frac{1}{2}\Delta - \frac{1}{r} + ibr\cos\theta\frac{\partial}{\partial\phi} + \frac{1}{2}b^2r^4\sin^2\theta\cos^2\theta + \frac{1}{2}br\left[\sin\theta\{\sigma_x\cos\phi + \sigma_y\sin\phi\} - 2\cos\theta\sigma_z\right]$$

Magnetic Guide

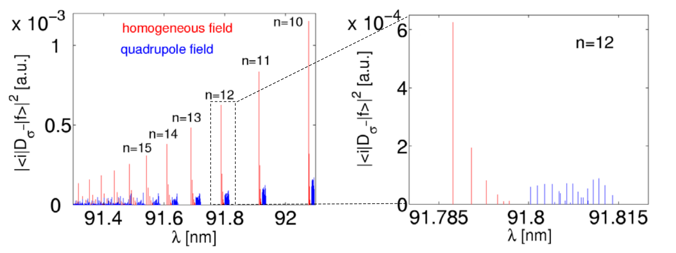
$$H = -\frac{1}{2}\Delta - \frac{1}{r} + ibr\sin\phi\cos\phi\left[\sin^2\theta\cos\theta\, r\frac{\partial}{\partial r} - \sin^3\theta\frac{\partial}{\partial\theta}\right] + \frac{1}{2}b^2r^4\sin^4\theta\sin^2\phi\cos^2\phi + \frac{1}{2}br\sin\theta\left[\sigma_x\cos\phi - \sigma_y\sin\phi\right]$$

Electric dipole transitions in the quadrupole field

Selection rules

	$\Delta m_J = m_J' - m_J$
π-transitions	0
σ+-transitions	1
σ−-transitions	-1

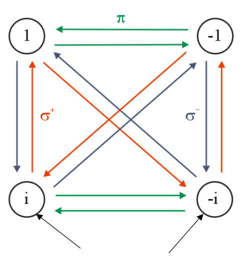
Transition amplitudes (σ− -transitions from the ground state)



- lines in the quadrupole field are systematically shifted towards higher wavelengths
- due to additional selection rules less sub-lines appear in the homogeneous field

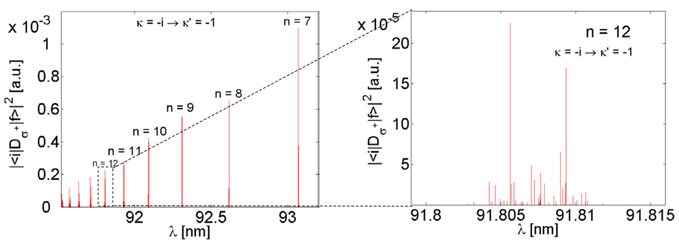
Electric dipole transitions in the magnetic guide

Selection rules



$P_yP_zI_{xy}S_2$–sub spaces

Transition amplitudes (σ+ -transitions from the ground state)

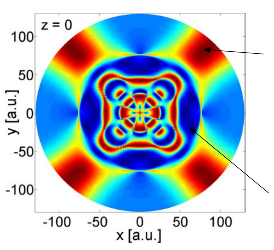


- much larger number of sub-lines than in the homogeneous and quadrupole field
- zoomed view reveals a dominant sub-line pair

Spin-orientation in the magnetic guide

- the inhomogeneous magnetic field prevents the factorization of spin and real space dynamics
- we investigate the expectation value of the cosine of the angle γ between the spin and the magnetic field

$$W_{\mu B}(\vec r) = \langle\cos\gamma\rangle = 2\frac{\langle\Psi|\vec r\rangle\left(S_x\cos\phi - S_y\sin\phi\right)\langle\vec r|\Psi\rangle}{|\langle\vec r|\Psi\rangle|^2}$$



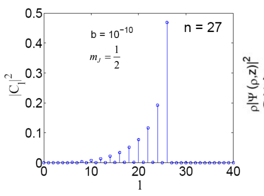
parallel spin-field alignment

anti-parallel spin-field alignment

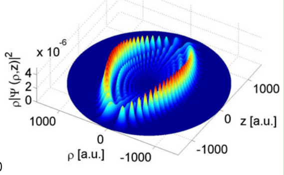
'Ellipsoidal States' in the quadrupole field

- exhibit large orbital angular momenta
- possess a unique angular momentum decomposition
- spatially compactness together with small radial uncertainty Δr → wavefunction is well localized outside the atomic core

Angular momentum decomposition



Probability density



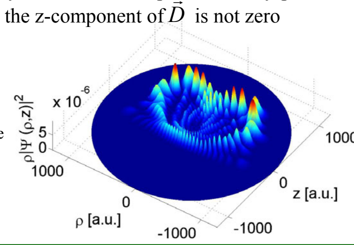
Magnetic field induced electric dipole moment

Field free atom (b = 0)

- operator of the electric dipole moment: $\vec D = e\vec r$
- due to the conservation of parity the expectation value of $\vec D$ vanishes

Atom in quadrupole field

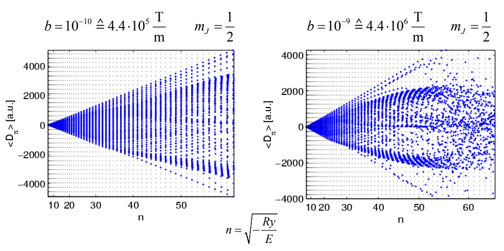
- the expectation value vanishes only for the x- and y-component of the dipole operator
- the charge distribution of the electronic states is in general not symmetric with respect to the x-y-plane → in general the z-component of $\vec D$ is not zero



non-symmetric charge distribution of an electronic state belonging to the n=22 multiplet

Electric dipole moment

- the states $|E, m_J\rangle$ exhibit a non-vanishing state dependent electric dipole moment which is induced by the external magnetic quadrupole field



$n = \sqrt{-\frac{Ry}{E}}$