State dependent interaction of Rydberg atoms in tight magnetic quadrupole traps via permanent electric dipole momenta

Igor Lesanovsky[1], Peter Schmelcher[1,2], and Jörg Schmiedmayer[1]
[1] *Physikalisches Institut, Universität Heidelberg, 69120 Heidelberg, Germany*
[2] *Physikalisch-Chemisches Institut, Universität Heidelberg, 69120 Heidelberg, Germany*

In the description of the motion of neutral atoms in an external magnetic field, the atom is usually treated as a point-like particle which couples through its magnetic moment to the field. This description holds only for fields that are homogeneous over the size of the atom. If the spatial extent of the atom becomes comparable with the characteristic variation length of the magnetic field, the above approach fails and the atomic structure becomes important. Even though the atom as a whole is neutral, the charge of the nucleus and the electrons are 'visible' to the field. This leads to further interaction terms in the Hamiltonian as both magnetic momenta and charges couple to the field. In our work we have investigated the dynamics of excited electronic states (Rydberg states) in tightly confining magnetic quadrupole traps. The corresponding high magnetic field gradients can be produced in the (sub)micron vicinity of surface mounted structures as are currently being used in many laboratories investigating micropotentials on atom chips [1]. The solutions of the system's stationary Schrödinger equation show unique features like the occurrence of a state dependent permanent electric dipole moment induced by the external magnetic field. Here, we present properties of the electronic eigenstates obtained as a result of a numerical approach we have developed and outline a path towards applications in the direction of inter-atom entanglement via the electric dipole-dipole interaction. To the best of our knowledge, this is the first treatment of the quantum dynamics of the internal electronic structure of trapped atoms [2].

The rotationally symmetric quadrupole field depends only on a single parameter: the magnetic field gradient $\mathcal{B}$. Since the common atomic species used in cold atom physics are alkalies, excited states can be described in a good approximation by the hydrogen Hamiltonian. Together with the assumption of the proton being located in the trap center, the following Hamiltonian describes the electron dynamics:

$$\begin{aligned}\hat{H} \;=\; & -\frac{\hbar^2}{2m_e}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)-\frac{1}{4\pi\epsilon_0}\frac{e^2}{\sqrt{x^2+y^2+z^2}} \\ & +\frac{\hbar e}{i m_e}\mathcal{B}\,z\left(y\frac{\partial}{\partial x}-x\frac{\partial}{\partial y}\right)+\frac{e^2}{2m_e}\mathcal{B}^2\,z^2\left(x^2+y^2\right) \\ & +\mu_B\mathcal{B}\left(\sigma_x x+\sigma_y y-2\sigma_z z\right)\end{aligned} \tag{1}$$

Here σ_x, σ_y and σ_z represent the Pauli spin matrices. Due to the coupling of spin and spatial variables, the motion in position and in spin space cannot be factorized but is intimately coupled. The investigation of the above Hamiltonian reveals a rotational symmetry and a generalized time reversal invariance which leads to a twofold degeneracy of each energy level *in the presence of the field*.

The numerical calculation of the eigenstates has been done by a linear variational approach where the Schrödinger equation was transformed into a generalized algebraic eigenvalue problem. This was done by developing a basis set particularly suited to investigate the electronic structure in the field. The solutions of this algebraic eigenvalue equation were obtained by applying a Krylov-space method (Arnoldi-algorithm) together with a spectral transformation approach. With this powerful method it became possible to compute eigenstates and -energies up to energy-levels which correspond to a hydrogen principle quantum number of $n \approx 60$. Due to the unique coupling between spatial and spin degrees of freedom, the resulting eigenstates show intricate spin polarization patterns. The external magnetic field leads to a deformation of the electronic states such that a *permanent electric dipole moment* arises.

The modulus of the dipole moment increases with increasing energy of the excited states; thus it should be possible to tune the dipole-dipole interaction between two separately trapped atoms. By addressing specific states via laser radiation, the electric dipole moment of the atom can be either switched on or off or even be varied in strength. Here, we present the status of our investigations concerning the feasibility of an implementation of QIP based on magnetic field induced permanent electric dipole momenta.

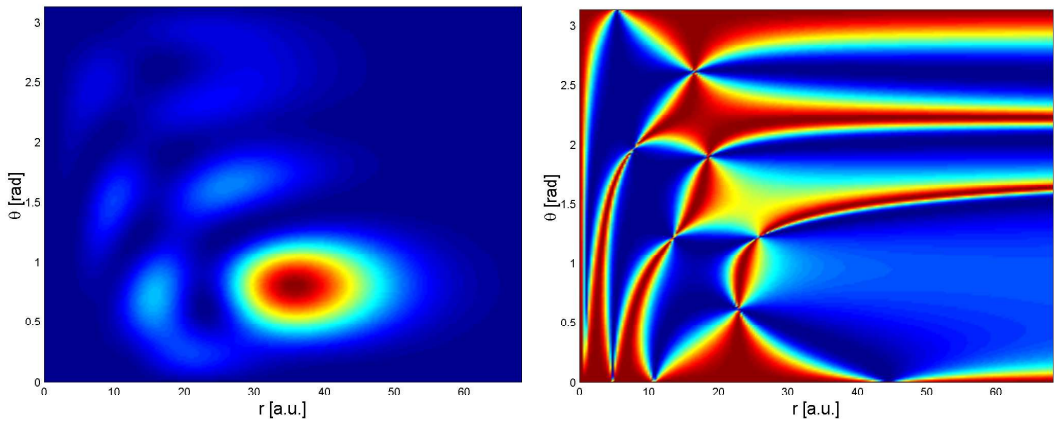

FIG. 1: Examples of an eigenstate and its corresponding spatial spin polarization pattern (in spherical coordinates). The quantities plotted are rotationally symmetric about the z-axis and are therefore independent on the azimuthal angle ϕ. **left**: Probability density of the 21st excited state. **right**: Spin polarization pattern of the same state. In red regions the spin points upwards, while blue denotes regions where the spin is pointing downwards. In this case the gradient of the quadrupole trap is $\mathcal{B} = 4.4 \cdot 10^5 \frac{T}{m}$

[1] R. Folman, P. Krüger, J. Schmiedmayer, J. Denschlag, C. Henkel, *Microscopic Atom Optics from Wires to an Atom Chip*, Adv. At. Mol. Opt. Phys. **48**, 263 (2002)
[2] I. Lesanovsky, P. Schmelcher and J. Schmiedmayer, submitted to Phys. Rev. Lett.