Rydberg Atoms

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Outline

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- 2 Definition and characteristics
 - Definition of a Rydberg atom
 - Characteristics
- Interactions
 - External electric field
 - Interaction with radiation
 - Dipole and van der Waals interaction
 - Pair states
 - Collectivity
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Motivation Definition and characteristics Interactions

Experimental realisation Universal scaling theory Rydberg Phase Gate

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- **5** Universal scaling theory
- 6 Rydberg Phase Gate

Several applications of Rydberg atoms

- Quantum computation: 1- and 2-Qubit operations
- Photon detection due to high sensitivity to extern fields
- Quantum simulations
- Biological issues: Foerster-resonance



Definition of a Rydberg atom Characteristics

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Definition of a Rydberg atom Characteristics

Definition

- Rydberg atom has at least 1 electron far away from its core (compared to ground state electrons)
- High principle quantum number n, typically n ≥ 20
- Correspondence principle applicable, which leads to Bohr model (H-atom-like)
- Rydberg atoms show exaggerated properties



Definition of a Rydberg atom Characteristics

Estimated Properties - Scaling with n

Size Energy Level spacing Geom. cross section Dipole moment Polarizability vdW parameter Radiative lifetime

$$r = a_0 \cdot n^2 \sim n^2$$

$$E = \frac{-E_R}{n^2} \sim n^{-2}$$

$$\Delta E \sim n^{-3}$$

$$\sigma = \pi r^2 \sim n^4$$

$$d = e \cdot r \sim n^2$$

$$\alpha = \frac{d^2}{\Delta E} \sim n^7$$

$$C_6 = \frac{-(d_1 \cdot d_2)^2}{\Delta E} \sim n^{311}$$

Definition of a Rydberg atom Characteristics

Quantum defect

Approximation valid, if

• High-n-electron sees attractive Coulomb-potential with 1 elemental charge

• Inner shell electrons screen core High distances (high n), high angular momenta \rightarrow low spatial overlap between electron wavefunctions \rightarrow Alkali atoms



Definition of a Rydberg atom Characteristics

Quantum defect



Definition of a Rydberg atom Characteristics

Quantum defect

Effects of low angular momenta and high spatial overlap respectively:

- Penetration of inner shells leads to higher charges and greater forces
- Passing electron polarizes ion-core: Induced dipole-charge-interaction
- I-degeneracy is lifted

Empirical energy equation:

	w=5	n-5
<u>n=5</u>		
n=4	<u>n=4</u>	<u></u>
	n-3	<i>n</i> =3
<i>n</i> =3		
	n-2	

$$E_B = -\frac{E_{R,2}}{(n-\delta_{n,l})^2}$$

(1)

External electric field Interaction with radiation Dipole and van der Waals interaction Pair states Collectivity

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Stark effect and ionisation

Application of a static, external electric field shows

- Linear Stark effect for degenerate states (high I) $\Delta E = d \cdot E$
- Quadratic Stark effect for non-degenerate states (low I) $\Delta E = -\frac{1}{2} |\alpha| E^2$
- Ionisation at high electric fields



External electric field Interaction with radiation Dipole and van der Waals interaction Pair states Collectivity

Ionisation



(2)

External electric field Interaction with radiation Dipole and van der Waals interaction Pair states Collectivity

Atom-Light Interaction

Assuming a 2-level atom with dipole approximation:

$$\hat{H} = \hat{H}_{atom} + \hat{H}_{light} + \hat{H}_{interaction}$$
(3)

$$\hat{H}_{a} = \frac{\hat{p}^{2}}{2m} + \hbar \omega_{0} \left| e \right\rangle \left\langle e \right| \tag{4}$$

$$\hat{H}_L = \hbar \omega_L (\hat{a}^{\dagger} \hat{a} + \frac{1}{2})$$
(5)

$$\hat{H}_i = -d \cdot E(r, t) \tag{6}$$

- Ultracold, frozen atom \rightarrow neglect kinetic energy
- \bullet Semiclassical picture \rightarrow neglect quantisation of light field

External electric field Interaction with radiation Dipole and van der Waals interaction Pair states Collectivity

Atom-Light Interaction

Atom-light interaction of a single atom:

$$\hat{H} = -\frac{\hbar\Delta}{2}(1-\sigma_z) + \hbar\Omega\sigma_x \tag{7}$$

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Dipole-dipole interaction

Consider two H-atoms in Born-Oppenheimer approximation



- Strong, long range interaction due to $d \sim n^2$
- Permanent dipoles for $l \ge 4$, for lower I only in external fields

External electric field Interaction with radiation Dipole and van der Waals interaction Pair states Collectivity

van der Waals interaction

Perturbation theory with dipole Hamiltonian:

$$E_{1} = \left\langle \psi_{0} \middle| \hat{H}_{int} \middle| \psi_{0} \right\rangle = 0 \tag{10}$$

Assuming a two level atom with $\langle e | d_i | g \rangle = \frac{d}{\sqrt{3}}$

$$E_2 = \frac{\left(\left|\left\langle g \left| \hat{H}_{int} \left| e \right\rangle \right|\right)^2}{E_g - E_e} = \frac{4d^4}{9} \frac{1}{E_g - E_e} \frac{1}{R^6} = -\frac{C_6}{r^6} \qquad (11)$$

External electric field Interaction with radiation Dipole and van der Waals interaction **Pair states** Collectivity

Pair states

Consider two Rydberg atoms in state $|s\rangle$, energy difference gives system $|ss\rangle$, $|p'p\rangle$ with $\Delta = (E_s - E_p) - (E_{p'} - E_s)$. Then $\hat{H} = \begin{pmatrix} 0 & U(r) \\ U(r) & \Delta \end{pmatrix}$ with $U(r) = \frac{\vec{d}_1 \cdot \vec{d}_2}{r^3}$ gives the new

with $U(r) = \frac{d_1 d_2}{r^3}$ gives the r eigenenergies

$$E_{\pm} = \frac{\Delta}{2} \pm \sqrt{(\frac{\Delta}{2})^2 + U(r)^2}$$
 (12)



External electric field Interaction with radiation Dipole and van der Waals interaction **Pair states** Collectivity

Pair states

$$E_{\pm} = \frac{\Delta}{2} \pm \sqrt{\left(\frac{\Delta}{2}\right)^2 + U(r)^2}$$
(13)

Case 1: $U(r) \gg \Delta$ Dipole interaction: $E_{\pm} = \frac{C_3}{r^3}$ $\Delta = 0 \rightarrow Förster-resonance$ **Case 2**: $\Delta \gg U(r)$ Taylor expansion leads to: $E_{\pm} = \Delta \pm \frac{U(r)^2}{\Delta}$ van der Waals interaction $\rightarrow Rydberg \ blockade$ **Case 3**: $U(r) \approx \Delta \rightarrow Crossover$

External electric field Interaction with radiation Dipole and van der Waals interaction **Pair states** Collectivity

Förster resonance



Crossover

Since there's a transition from van der Waals to dipole-dipole dominated region at $U(r) \approx \Delta$, one can define a crossover distance



(14)

External electric field Interaction with radiation Dipole and van der Waals interaction **Pair states** Collectivity

Rydberg blockade

- spatial dependant energy shift
- compare to line (saturation) broadening
- no other Rydberg atom in blockade sphere \rightarrow sort of lattice order
- strong interaction $r_B \gg r_{particle}$, typically $\frac{10^3 particles}{sphere}$

$$Z\frac{C_6}{r_B^6} = ZC_6 n_r^2 = \sqrt{N}\hbar\Omega_R \qquad (15)$$





External electric field Interaction with radiation Dipole and van der Waals interaction Pair states Collectivity

Collectivity

Laser acts on bunch of atoms:

$$\begin{split} |0\rangle &= |g_1, g_2, ..., g_N\rangle \\ \text{Superatom:} \\ |1\rangle &= \frac{1}{\sqrt{N}} \sum_{i=1}^{N} |g_1, g_2, ..., r, ..., g_N\rangle \\ \text{One atom excitation:} \\ \hbar\Omega_0 &= \left\langle g \left| \hat{H}_{Laser} \right| r \right\rangle \end{split}$$



$$\begin{split} &\hbar\Omega_{C} = \left\langle 0 \left| \hat{H}_{Laser} \right| 1 \right\rangle = \hbar \sqrt{N} \Omega_{0} \\ &\text{Using } N(r) = \frac{n_{g}(r)}{n_{R}(r)} \text{ and blockade radius:} \end{split}$$

$$n_{R}(r) = \left(\frac{2\hbar}{ZC_{6}}\right)^{\frac{2}{5}} (n_{g}(r)\Omega_{0}^{2})^{\frac{1}{5}}$$
$$\Omega_{N}(r) = \left(\frac{ZC_{6}}{2\hbar}\right)^{\frac{1}{5}} (n_{g}(r)\Omega_{0}^{2})^{\frac{2}{5}}$$

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Method

Requirements

- Sufficiently intense and narrow laser for coherent evolution within natural lifetime. Intensity to overcome low dipole matrix elements and coherence for full Rabi oscillations
- \bullet Detection via field ionisation \rightarrow fast ion detection (most common)
- Low temperatures to fulfill frozen gas approximation, low black body radiation, no collisions, low Doppler shift (counterpropagating lasers)
- Excitation from ultracold gas or BEC

Experiment

- Selection rules: Conservation of angular momentum
- Effective 2-level system due to large detuning δ; 5p not populated

•
$$\Omega_R = \sqrt{\frac{\Omega_r^2 \Omega_b^2}{4\delta^2} + \Delta^2}$$



Universality Rydberg atoms

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Universality Rydberg atoms

Universality

- tool to describe system without knowing microscopic details
- macroscopic behaviour is dominated by long-range physics
- critical phenomenom, f.e. near critical point of 2nd order phase transition
- ullet only one characteristic length scale ξ
- critical exponents are universal

Universality Rydberg atoms

Example: Ferromagnet

- T > T_C demagnetized, rotational symmetry
- $T_C > T$ symmetry lose, order parameter \vec{M}
- conjugate field *H*, reduced temperature $t = \frac{T}{T_C} - 1$, diverging length scale $\xi \sim \frac{1}{t^{v}}$

•
$$H=0$$
: $M\sim t^{eta}$; $t=0$: $M\sim H^{rac{1}{\delta}}$

• powers of *H*, *t*: universal critical exponents



Universality Rydberg atoms

Rydberg atoms

$$\hat{H} = -\frac{\hbar\Delta}{2} \sum_{i} (1 - \sigma_z^{(i)}) + \frac{\hbar\Omega}{2} \sum_{i} \sigma_x^{(i)} + C_6 \sum_{j < i} \frac{P_{rr}^{(i)} P_{rr}^{(j)}}{|r_i - r_j|^6}$$
(16)
with $P_{rr}^{(i)} = |r_i\rangle \langle r_i| = \frac{1 - \sigma_z^{(i)}}{2}$

- order parameter: Rydberg fraction $f = \left\langle P_{rr}^{(i)} \right\rangle = \frac{N_R}{N_g}$
- diverging length scale

$$\xi = rac{a_R}{a_g} = rac{1}{a_g} \sqrt{rac{C_6}{\hbar\Omega_N}}$$

• 'conjugate field' $\alpha = \frac{\hbar\Omega_0}{C_6 n_g^2} = \frac{couplingstrength}{interaction}$

•
$$t = \Delta' = \frac{\hbar \Delta}{C_6 n_g^2}$$



Universality Rydberg atoms

Rydberg atoms

Second order phase transition for $1\gg\alpha$ between pure ground state (paramagnetic) and arranged Rydberg atoms in crystal (ferromagnetic)

- ξ diverges for lpha
 ightarrow 0
- Δ' = 0: system independant of microscopic details
- $\alpha = 0$: $f \sim \Delta'^{\kappa}$; $\Delta' = 0$: $f \sim \alpha^{\nu}$
- κ, ν universal scaling exponents in critical region, i.e. $1 \gg \alpha, 1 \gg \Delta'$



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Quantum Computation and Rydberg atoms

- quantum computation requires coherent manipulation of large number of coupled quantum systems
- storage of information in collective excitations of many-atom ensembles
- single atom absorption cross-section generally low
- \rightarrow make use of
 - collective behaviour of Rydberg excitations
 - Rydberg blockade control and strong interaction
 - well developped techniques (cooling, trapping, ...)

Rydberg storage and switch



Two-level dynamics



$$\begin{pmatrix} |g(t)\rangle \\ |r(t)\rangle \end{pmatrix} = \begin{pmatrix} \cos(\theta(t)) & -i \cdot \sin(\theta(t)) \\ i \cdot \sin(\theta(t)) & \cos(\theta(t)) \end{pmatrix} \begin{pmatrix} |g(0)\rangle \\ |r(0)\rangle \end{pmatrix}$$

with $\theta(t) = \sqrt{N} \int_0^t \frac{\Omega(\tau)}{2} d\tau$

• Population transfer via π -pulse: $\pi = \int \Omega_f(\tau) d\tau$

Arbitrary manipulation from known state to final state possible

Phase Gate



Realisation of a phase gate (total phase shift of π):

- $|g,e\rangle \rightarrow^{\pi} |r,e\rangle \rightarrow^{\Delta t = \frac{\phi}{U(r)}} |r,e\rangle \rightarrow^{\pi} |e,g\rangle$ • or $|g,g\rangle \rightarrow^{\pi} |r,g\rangle \rightarrow^{2\pi} (-1) \cdot |r,g\rangle \rightarrow^{\pi} |g,g\rangle$
- Error sources: Dephasing, double excitation

Conclusion

- Rydberg atom H-like behaviour (Bohr atom, quantum defect) and extraordinary properties
- Interactions in picture of two level atom
- Experiment
- Quantum critical behaviour, universality and phase diagram
- Examples of quantum computation with Rydberg atoms