Dipole-dipole bound Rydberg molecules

and electronic structure of highly excited optical lattices

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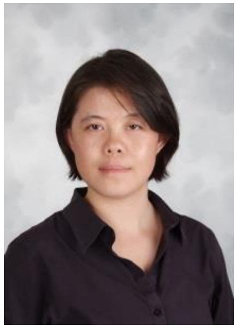


Wenhui Li

Mingxia Huo

Martin Kiffner

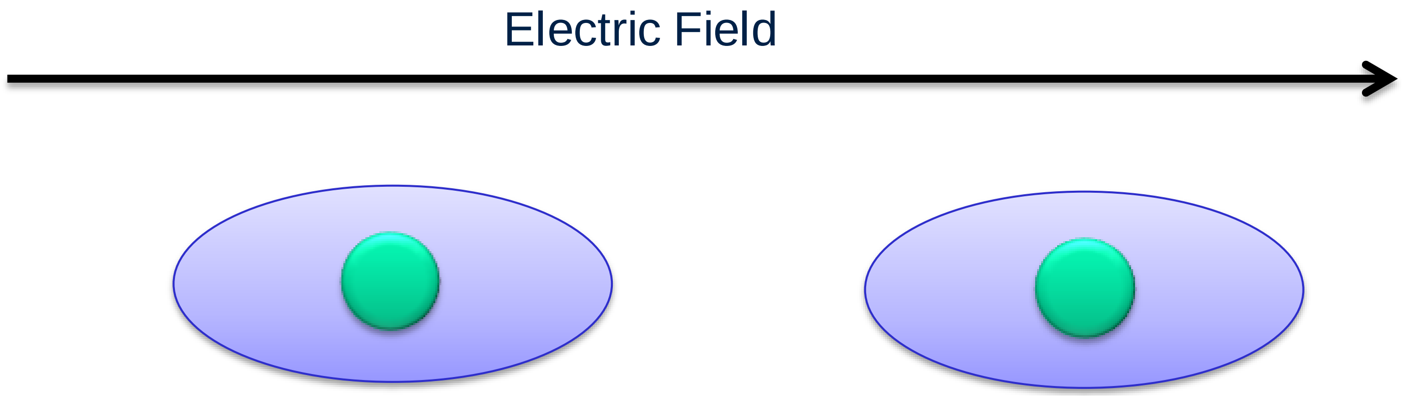
Samantha Massey

	Atoms	**Rydberg**	**CMP**	**CMP cooled**	**Bio**
Experiment Time	s – ms	μs – ns	ps – fs	ps – fs	ps - fs
Energy E/h	Hz - kHz	MHz	THz	THz	THz
Temperature T	nK	nK	300K	mK	300K
Ratio $E/k_B T$	$1 - 10$	$10^4 - 10^6$	$1 - 10$	$10^4 - 10^6$	1 – 10
Coherence γ, κ	Hz	kHz	THz	GHz	THz
Driving frequency Ω	kHz	MHz	THz	THz	THz

$$200\text{Hz} \Leftrightarrow 10\text{nK} \Leftrightarrow 1\text{peV}$$

Dipole-dipole interactions

- Excite atoms to high lying states with large electron orbit

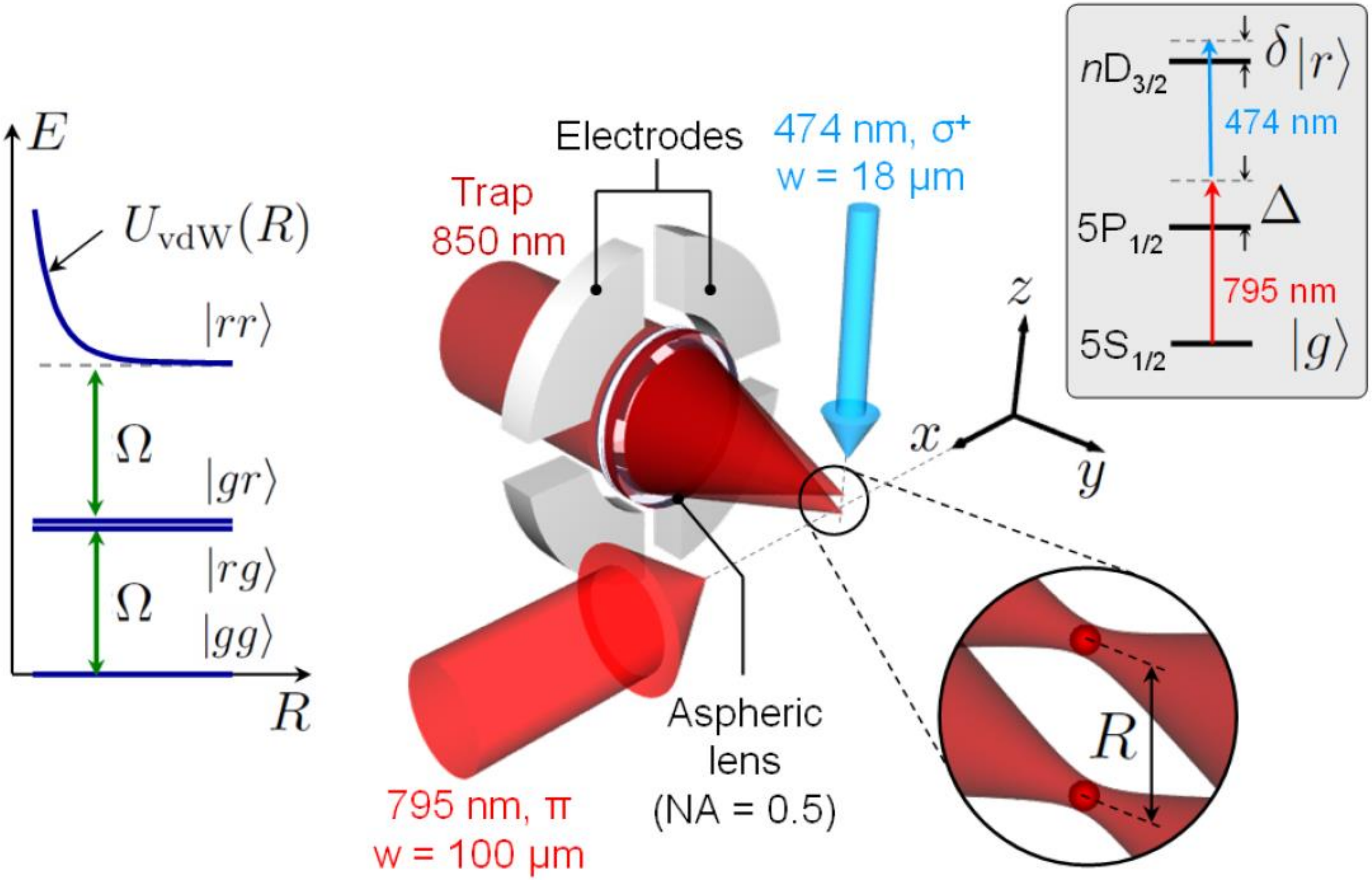


- Apply electric field to induce large dipoles
- Dipole-dipole interaction potential (atomic units)

$$\hat{V}_{\mathrm{dd}} = \frac{1}{R^3}[\hat{\boldsymbol{d}}^{(1)} \cdot \hat{\boldsymbol{d}}^{(2)} - 3(\hat{\boldsymbol{d}}^{(1)} \cdot \vec{\boldsymbol{R}})(\hat{\boldsymbol{d}}^{(2)} \cdot \vec{\boldsymbol{R}})]$$

- Large molecules bound by this interaction can be formed for large n

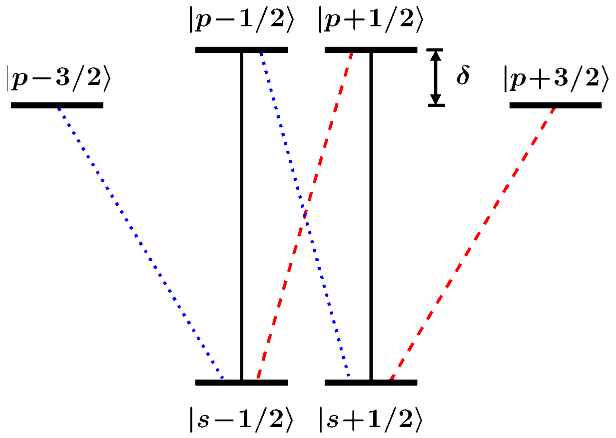
Measuring the Diople-Dipole Interaction

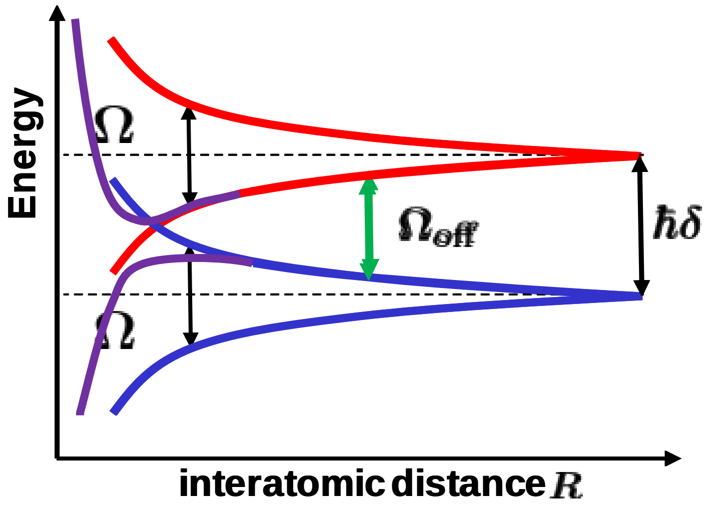


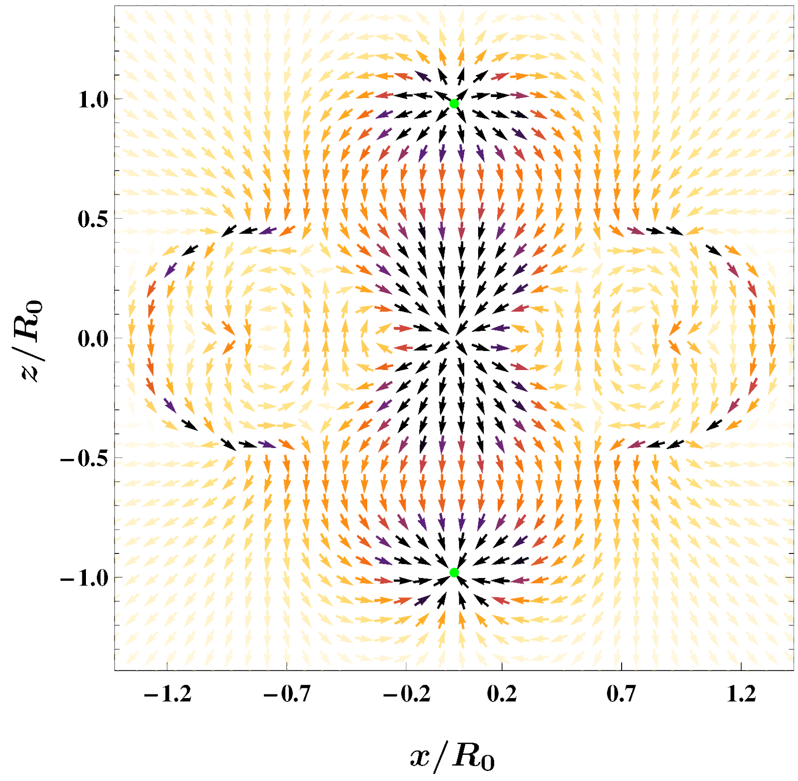
Lucas Béguin, Aline Vernier, Radu Chicireanu, Thierry Lahaye, Antoine Browaeys , Phys. Rev. Lett. **110**, 263201 (2013)

Rydberg Dimers – Artificial Gauge Fields

- Consider relative motion of two Rydberg excited atoms



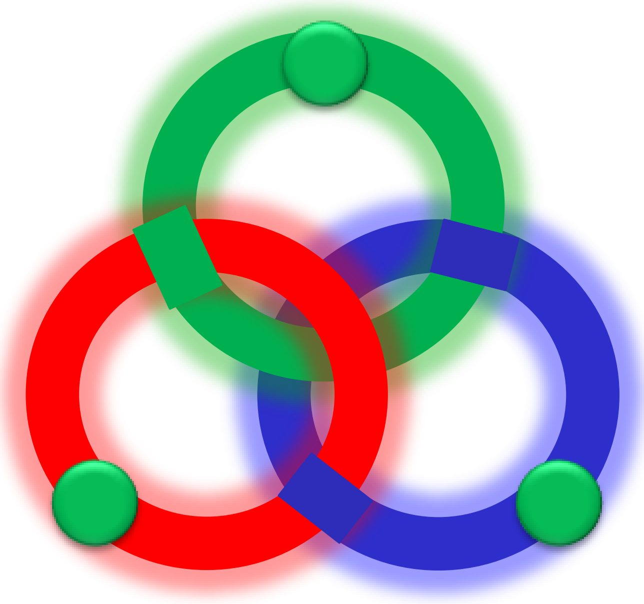


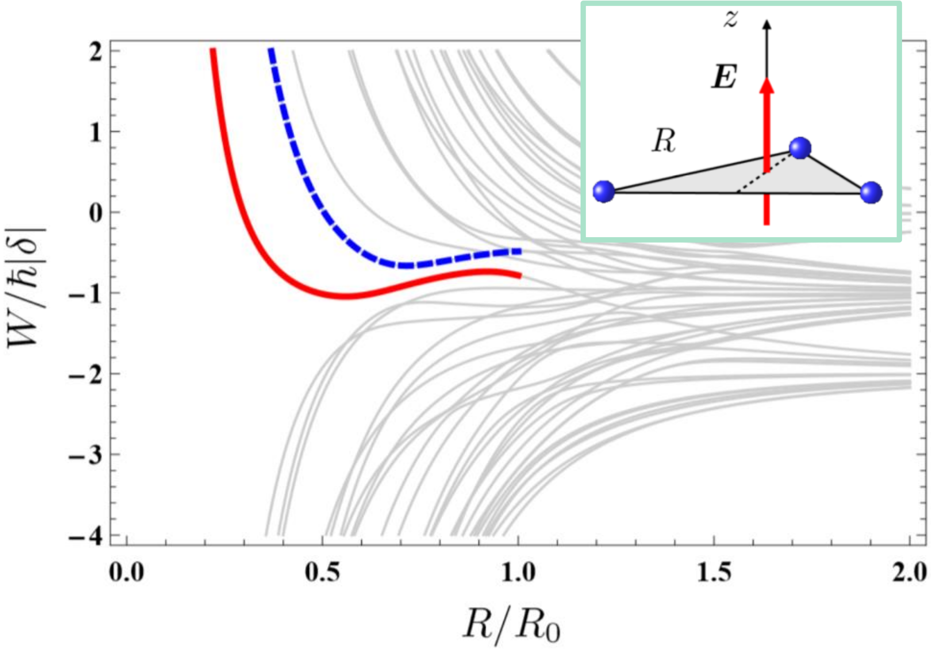


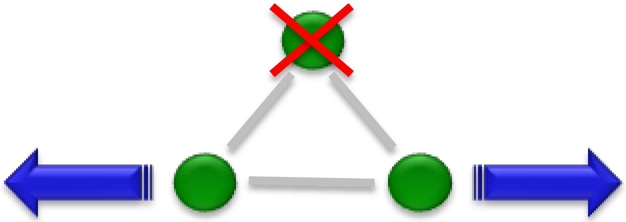
$$\boxed{R_0 = \left[\frac{|\mathcal{D}|^2}{4\pi\epsilon_0\hbar|\delta|}\right]^{1/3}}$$

M Kiffner, H Park, W Li, TF Gallagher, Phys. Rev. A **86**, 031401(R) (2012).
M Kiffner, W Li, and DJ, PRL **110** 170402 (2013)

Rydberg Trimers – Borromean States







$$\omega_{vib} = \sqrt{\frac{\hbar|\delta|}{\mu R_0}}$$

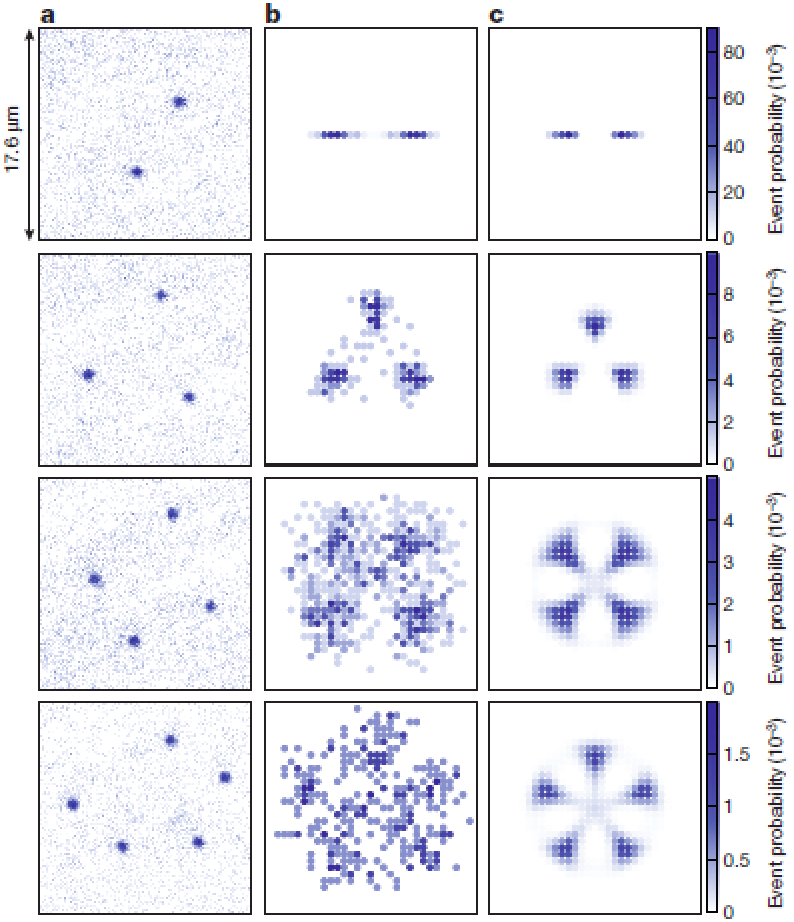
… on the order of MHz

M. Kiffner, W. Li, and DJ, Phys. Rev. Lett. **111**, 233003 (2013)
M. Kiffner, M. Huo, W. Li, and DJ, Phys. Rev. A **89**, 052717 (2014).

Recent Rydberg Atom Experiments

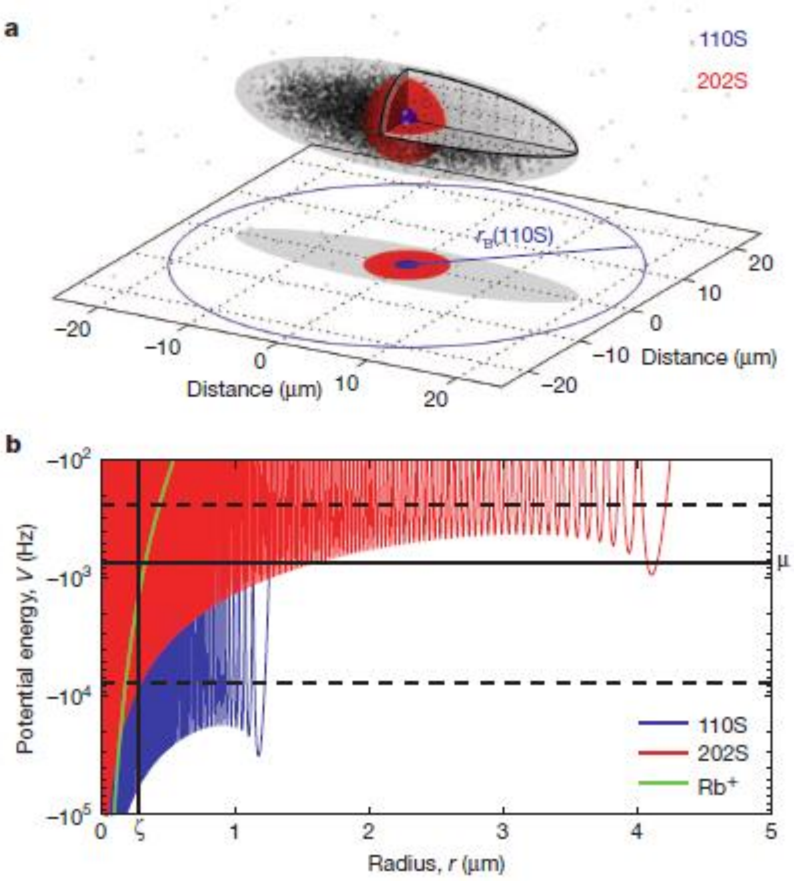
- Rydberg excitations in optical lattice

P. Schauß et al., Nature **491**, 87 (2012).



- Electron interacting with a BEC

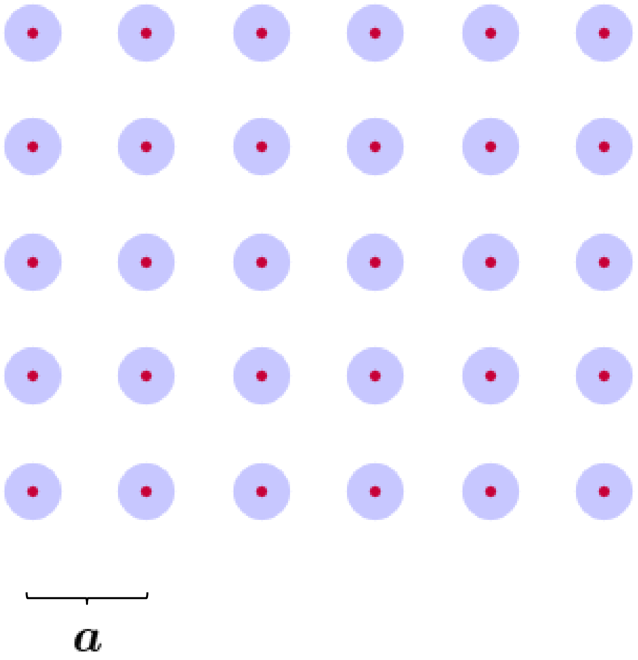
J. B. Balewski et al., Nature **502**, 664 (2013).



Electronic Structure in optical lattices

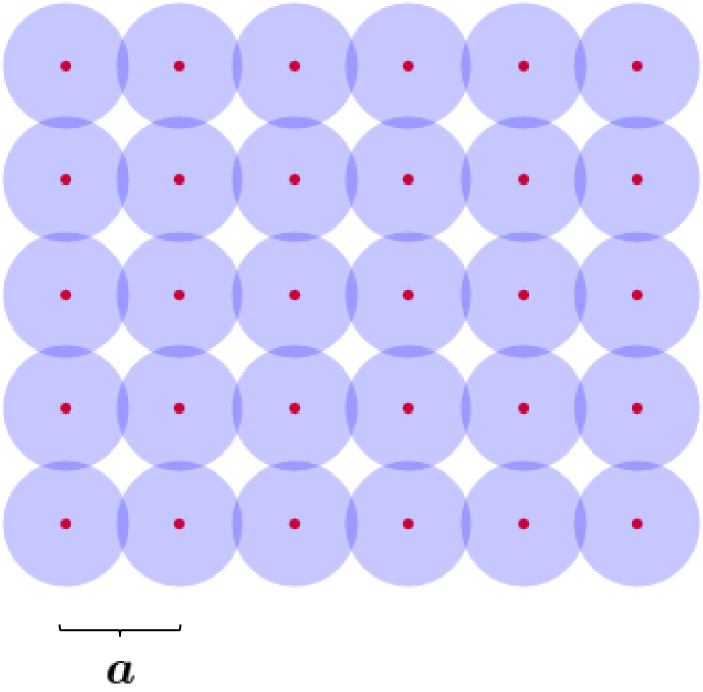
Towards strongly correlated electron systems

- Rydberg atoms in optical lattice



Towards strongly correlated electron systems

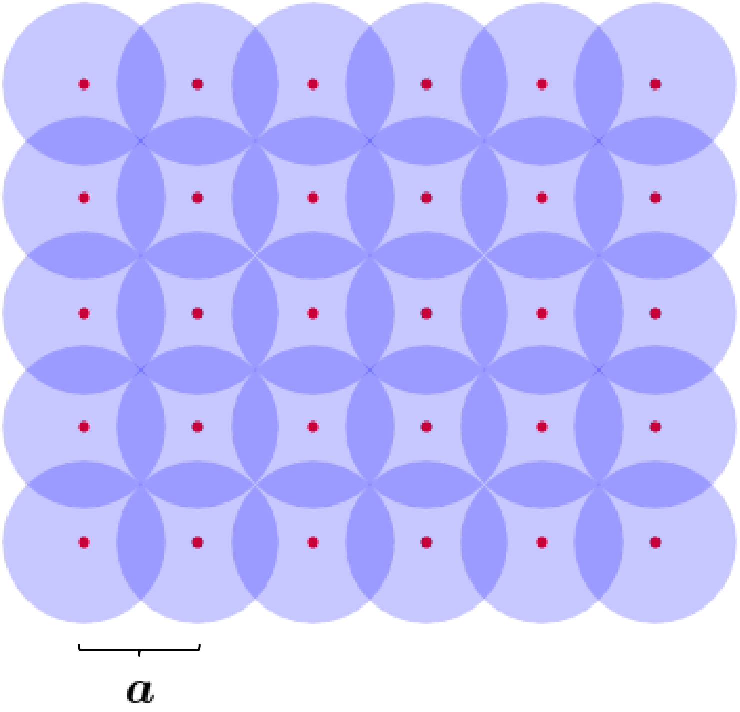
- Overlapping electron clouds



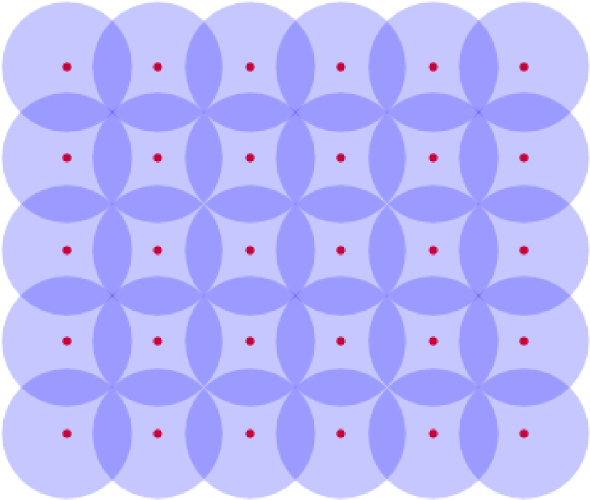
Valence electron clouds start overlap when $4n^2 a_0 \geq a$

Towards strongly correlated electron systems

- Overlapping electron clouds



Towards strongly correlated electron systems

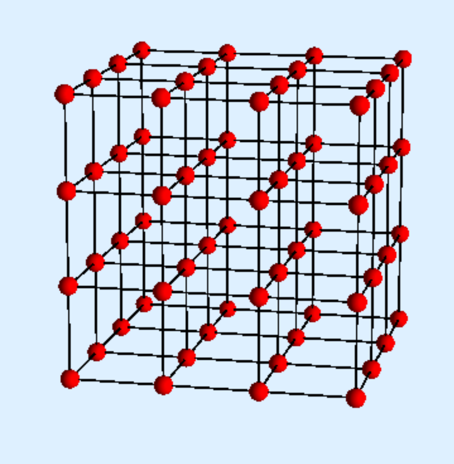


- **Electronic structure**
  - temporal and spatial resolution of electron dynamics (e.g., photoelectric effect)
  - solid state quantum simulator
  - potentially very low electron temperatures

- **Questions, issues, and other problems**
  - radiative decay, black body radiation
  - collision induced decay
  - preparation
  - lifetime

Rydberg matter – Energy

- Ion cores + electron gas



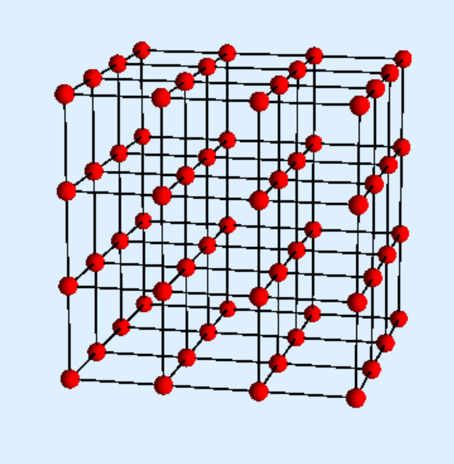
- Energy **per unit cell**:

$$E[n] = E_{\text{kin}}(\text{many-body}) + E_{\text{electron-electron}} + E_{\text{ion-ion}} + E_{\text{electron-ion}}$$

Density Functional Theory ↓ Kohn-Sham Ansatz

$$E[n] = E_{\text{kin}} + E_{\text{Hartree}} + E_{\text{ion-ion}} + E_{\text{electron-ion}} + E_{\text{exchange-correlation}}$$

Rydberg matter – Energy



- Ion cores + electron gas

- Energy **per unit cell**:

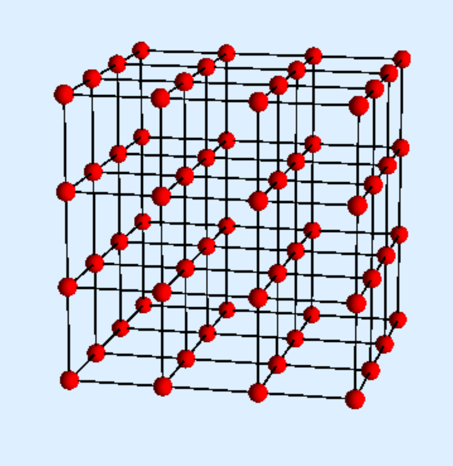
$$E = E_{\text{kin}} + E_{\text{Hartree}} + E_{\text{ion-ion}} + E_{\text{electron-ion}} + E_{\text{exchange-correlation}}$$

$E_{\text{electron-ion}}$: Coulomb potential for Hydrogen

Here: modified Coulomb potential due to

- core electrons (quantum defect theory)
- high excitation level

Rydberg matter – Energy scaling



- Ion cores + electron gas
- lattice constant a
- Parameter $\epsilon = \frac{a_0}{a}$
- Energy **per unit cell**

$$E = E_{\text{kin}} + E_{\text{Hartree}} + E_{\text{ion-ion}} + E_{\text{electron-ion}} + E_{\text{exchange-correlation}}$$

$$E_{\text{kin}} \propto \epsilon^2$$

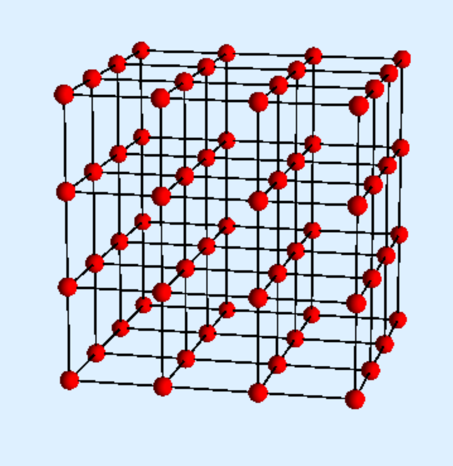
$$E_{\text{Hartree}} + E_{\text{ion-ion}} \propto \epsilon$$

$E_{\text{electron-ion}}$ depends on Rydberg level, Coulomb part $\propto \epsilon$

$$E_{\text{exchange}} \propto \epsilon$$

$$E_{\text{correlation}} ?$$

Rydberg matter – simple model



- simple cubic lattice
- lattice constant a
- ion cores + electron gas

- Energy **per unit cell (** $\alpha_i > 0$ **)**:

$$E = E_{\text{kin}} + E_{\text{Hartree}} + E_{\text{ion-ion}} + E_{\text{electron-ion}} + E_{\text{exchange}} + E_{\text{correlation}}$$

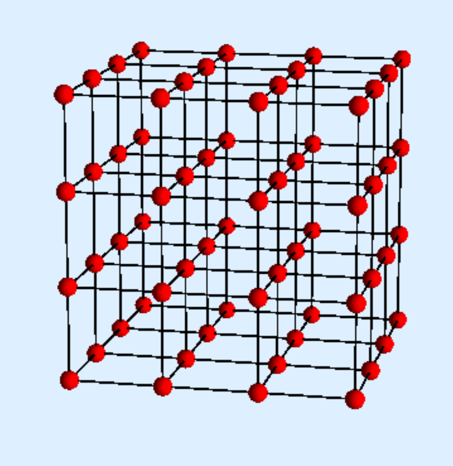
$E_{\text{kin}} = \alpha_1 \epsilon^2$ uniform electron gas

$E_{\text{Hartree}} + E_{\text{ion-ion}} + E_{\text{electron-ion}} = -\alpha_2 \epsilon + \alpha_3 \epsilon^3$ Madelung energy + core correction

$E_{\text{exchange}} = -\alpha_4 \epsilon$ Hartree-Fock + uniform electron gas

$E_{\text{correlation}} = -\alpha_5 \epsilon + \alpha_6 \epsilon^{3/2}$ low density electron gas

Rydberg matter – simple model



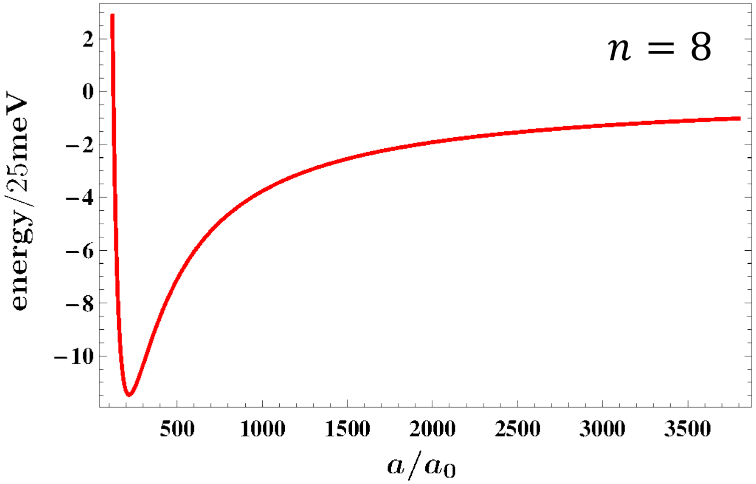
- simple cubic lattice
- lattice constant a
- ion cores + electron gas

- Energy **per unit cell (** $\alpha_i > 0$ **)**:

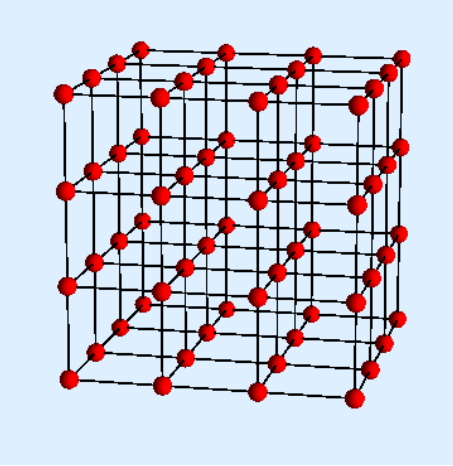
$$E(\epsilon) = \left[\alpha_1 \epsilon^2 - (\alpha_2 + \alpha_4 + \alpha_5)\epsilon + \alpha_3 \epsilon^3 + \alpha_6 \epsilon^{\frac{3}{2}}\right] E_I$$

$$\frac{dE(\epsilon)}{d\epsilon} = 0 \quad \Rightarrow \quad a_{\text{equilibrium}}$$

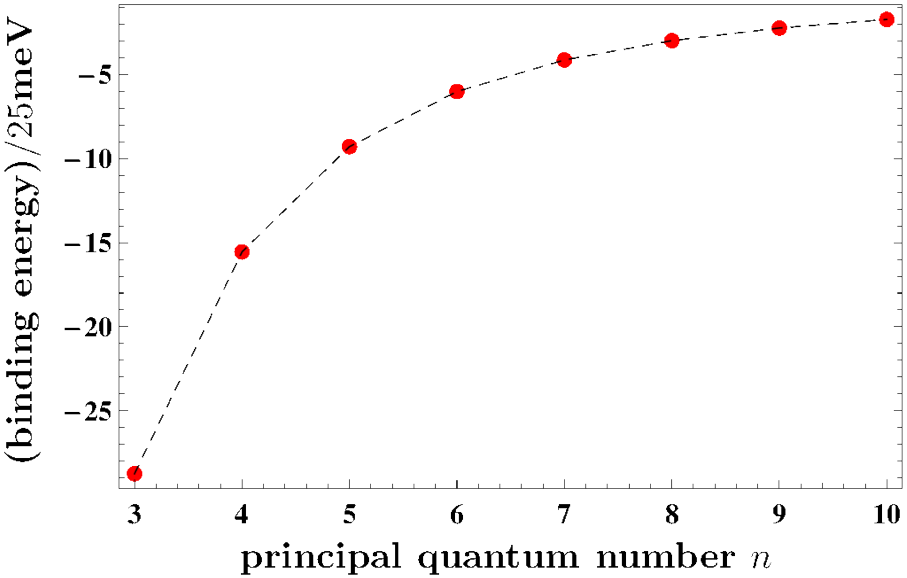
- Bulk modulus $B \approx 10^4 \text{Pa}$
- Density: $\rho \approx 90 \text{g}/\text{m}^3$
- Speed of sound: $c \approx 330 \text{m}/s$
- Ion trap: $f \approx 4.5 \text{GHz}$



Rydberg matter – simple model



- simple cubic lattice
- lattice constant a
- ion cores + electron gas
- Energy E **per unit cell**
- **Binding energy:** $E - E_{\text{ion}}(\text{independent atoms})$

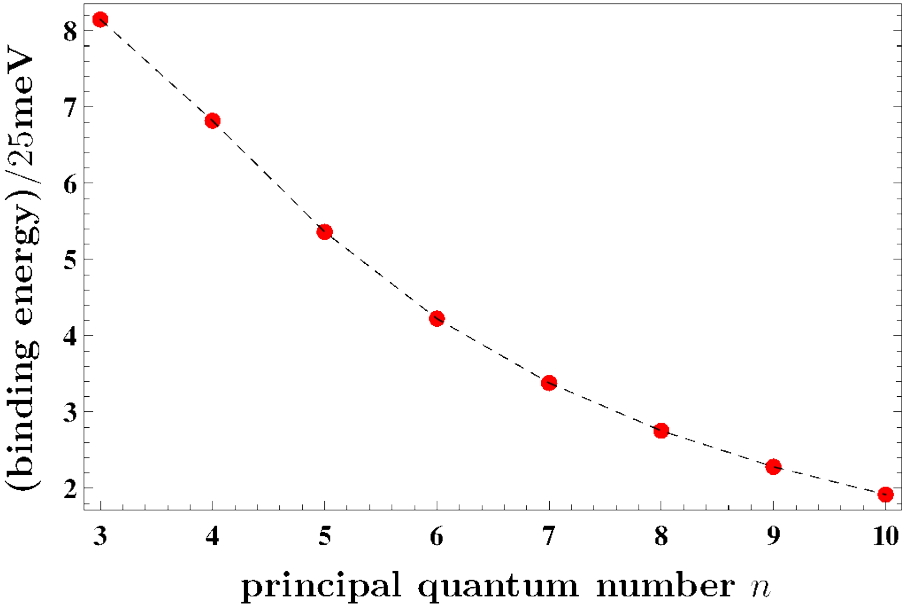


Rydberg matter – simple model

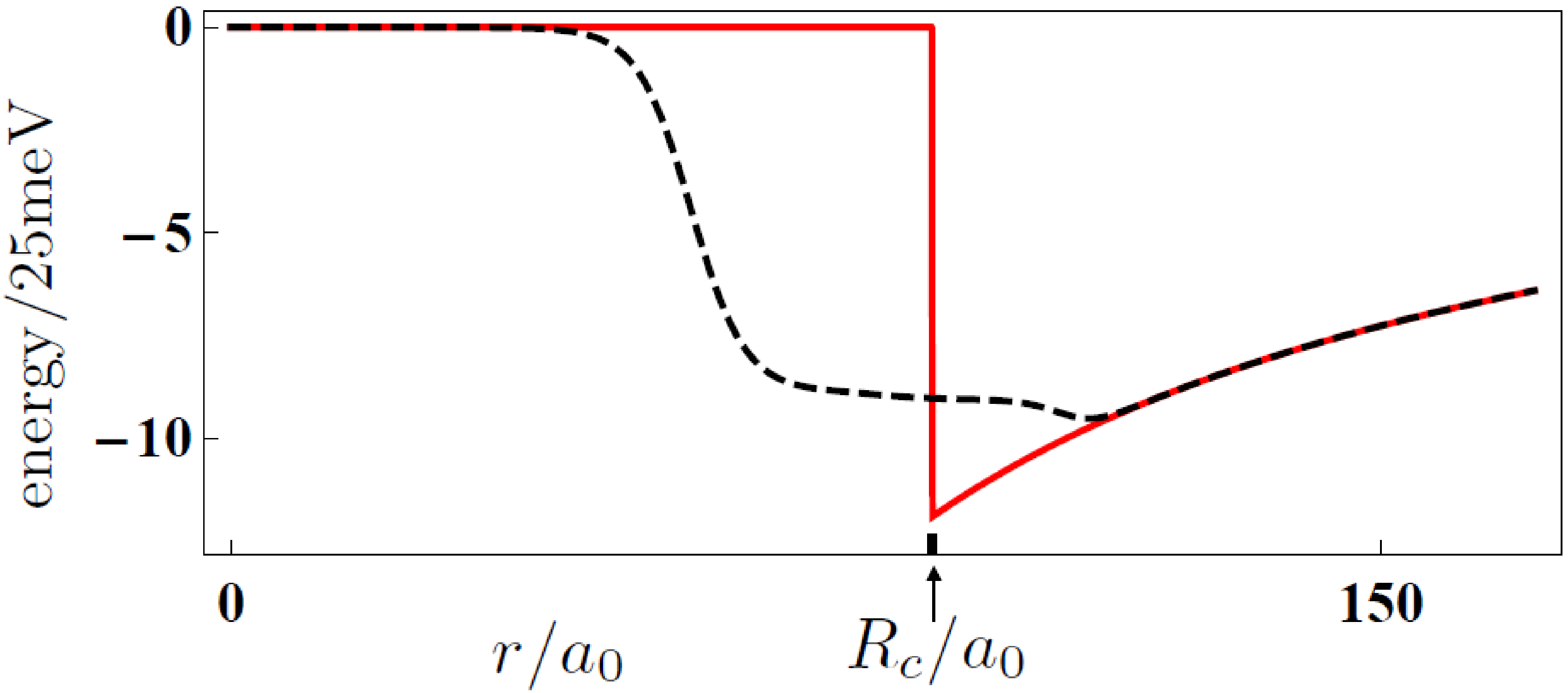
- Energy **per unit cell**:

$$E = E_{\text{kin}} + E_{\text{Hartree}} + E_{\text{ion-ion}} + E_{\text{electron-ion}} + E_{\text{exchange}} + \xcancel{E_{\text{correlation}}}$$

- **Binding energy:** $E - E_{\text{ion}}(\text{independent atoms})$

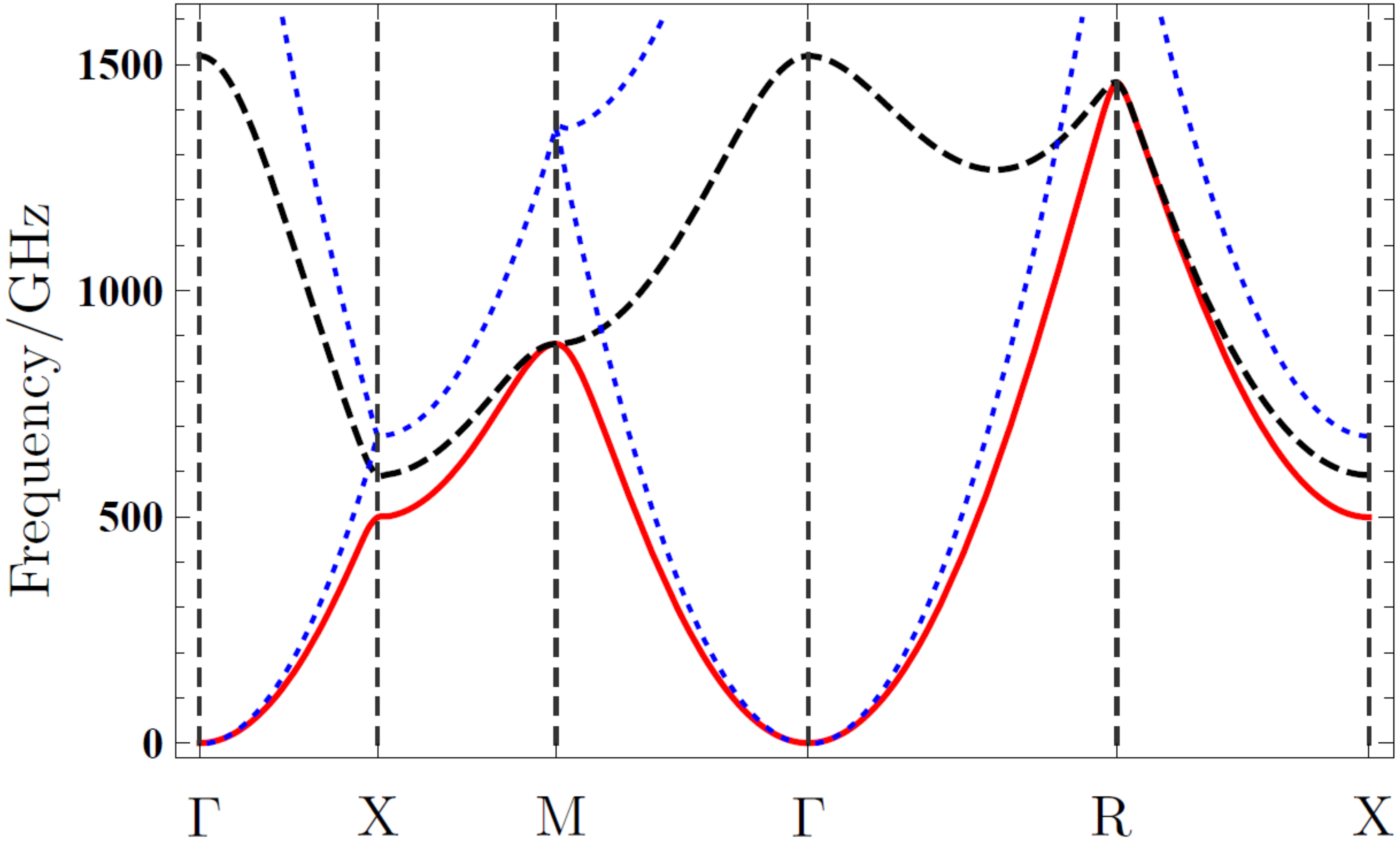


Rydberg matter – norm conserving pseudopotentials



$n = 8$, $l = 0$, norm conserving and simple pseudo-potentials

Rydberg matter – DFT band structure calculations



$n = 8$, homogeneous electron gas approximation, effective mass $m^* \approx 1.2 m_0$, plane wave approx.

using Quantum Espresso

Rydberg matter – lifetime

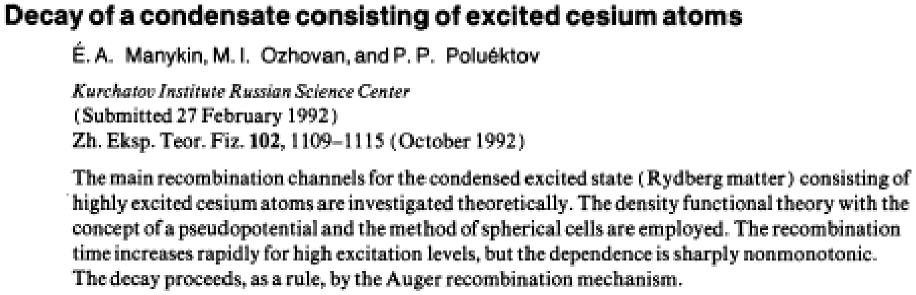
- Non-radiative Auger decay rates decrease fast with lattice period

$$\gamma_{nr} \propto \rho^2 \propto \epsilon^6$$

- Radiative decay rates also decrease

$$\gamma_r \propto \rho \propto \epsilon^3$$

Lifetime further increased by electron localization

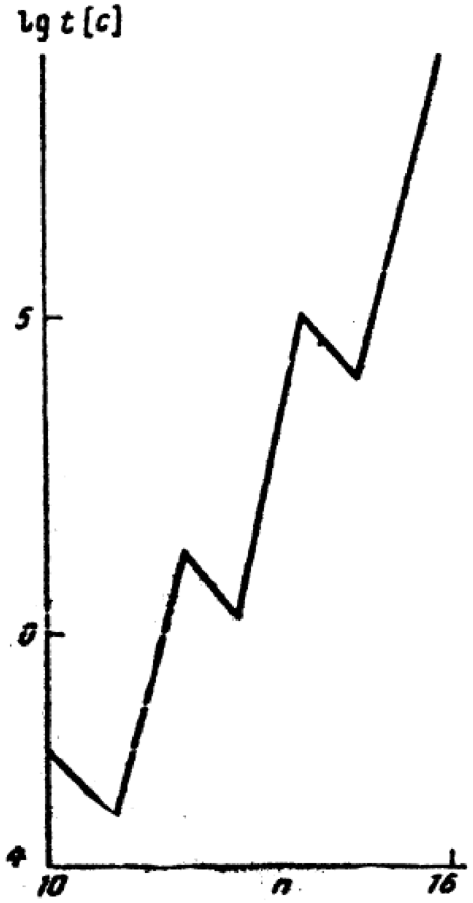


Decay of a condensate consisting of excited cesium atoms

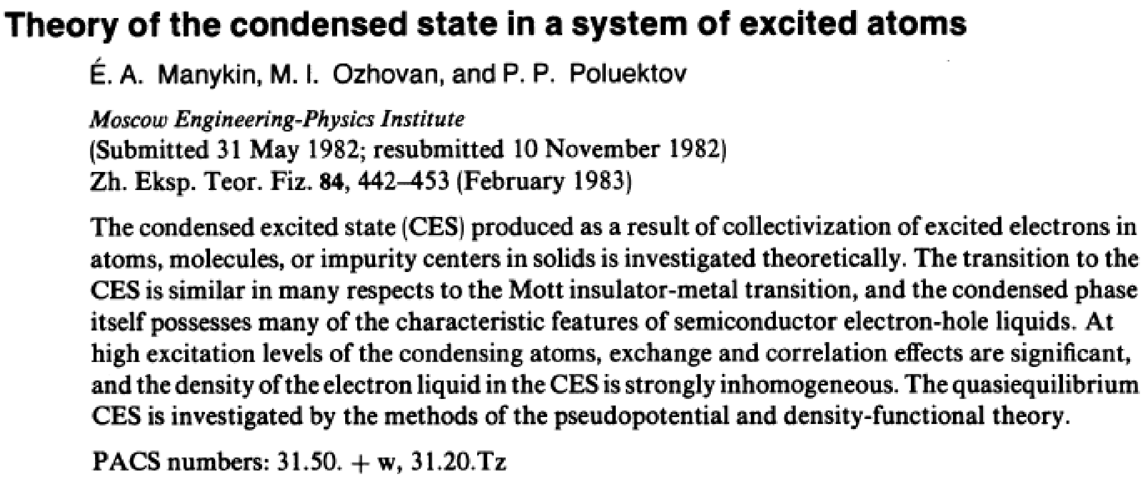
É. A. Manykin, M. I. Ozhovan, and P. P. Poluéktov

Kurchatov Institute Russian Science Center
(Submitted 27 February 1992)
Zh. Eksp. Teor. Fiz. **102**, 1109–1115 (October 1992)

The main recombination channels for the condensed excited state (Rydberg matter) consisting of highly excited cesium atoms are investigated theoretically. The density functional theory with the concept of a pseudopotential and the method of spherical cells are employed. The recombination time increases rapidly for high excitation levels, but the dependence is sharply nonmonotonic. The decay proceeds, as a rule, by the Auger recombination mechanism.



Rydberg matter – simple model



Theory of the condensed state in a system of excited atoms

É. A. Manykin, M. I. Ozhovan, and P. P. Poluektov

Moscow Engineering-Physics Institute

(Submitted 31 May 1982; resubmitted 10 November 1982)
Zh. Eksp. Teor. Fiz. **84**, 442–453 (February 1983)

The condensed excited state (CES) produced as a result of collectivization of excited electrons in atoms, molecules, or impurity centers in solids is investigated theoretically. The transition to the CES is similar in many respects to the Mott insulator-metal transition, and the condensed phase itself possesses many of the characteristic features of semiconductor electron-hole liquids. At high excitation levels of the condensing atoms, exchange and correlation effects are significant, and the density of the electron liquid in the CES is strongly inhomogeneous. The quasiequilibrium CES is investigated by the methods of the pseudopotential and density-functional theory.

PACS numbers: 31.50. + w, 31.20.Tz

- Self-trapping of electrons outside the core region
- Exchange and correlation enhances lifetime/stability

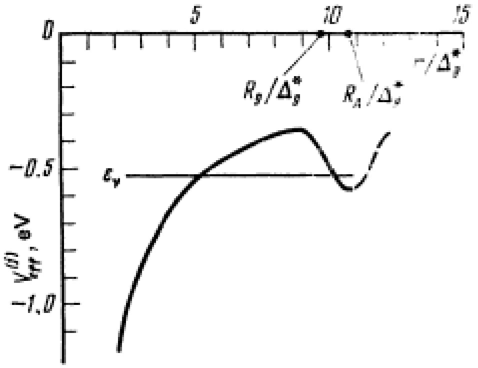
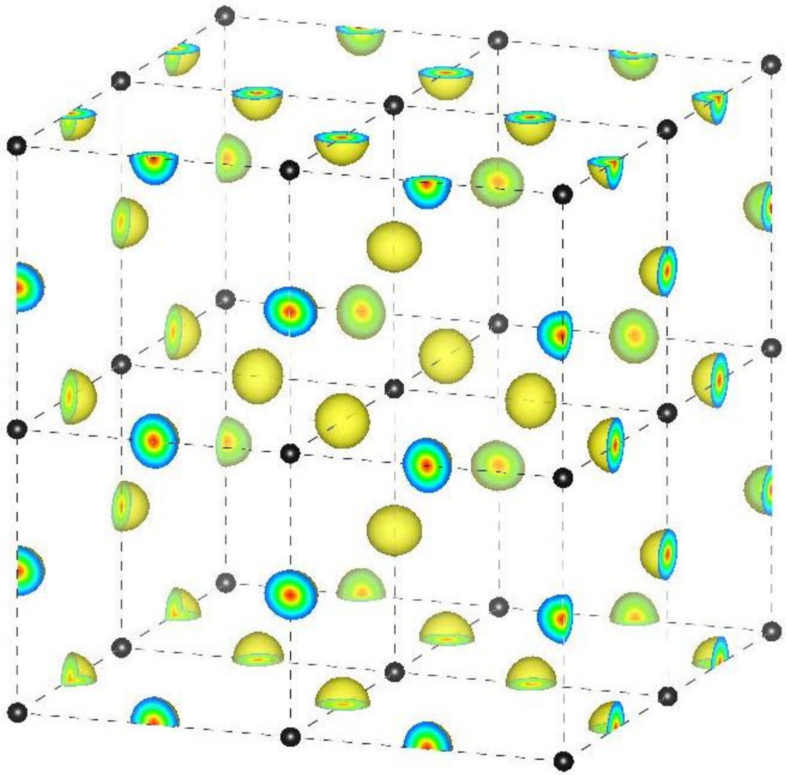


FIG. 2. Effective cell potential (25) for CES electrons ($n = 9$).

Rydberg matter – roadmap, preliminary

- Calulate electronic structure with self consistent

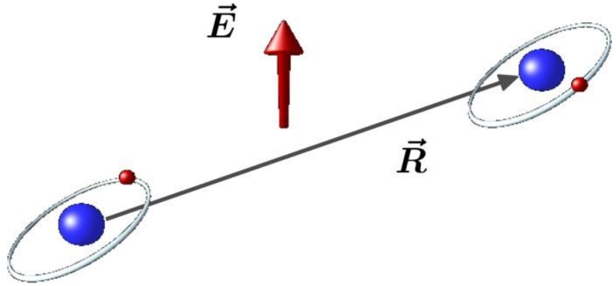
  Density Functional Theory (using Quantum Espresso)



- $n = 8, l = 0$ simple cubic lattice
- strong electron localizatioin
- each “blob” carries charge $e/3$

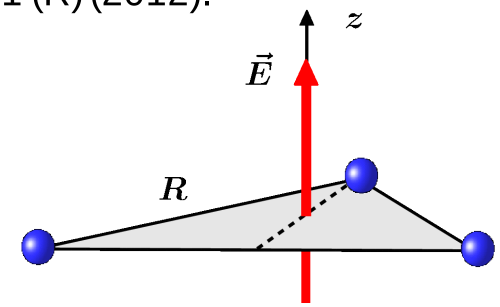
- strong suppression of decay processes

Summary



- **Few-body physics**
  - **Dimer/Trimer**

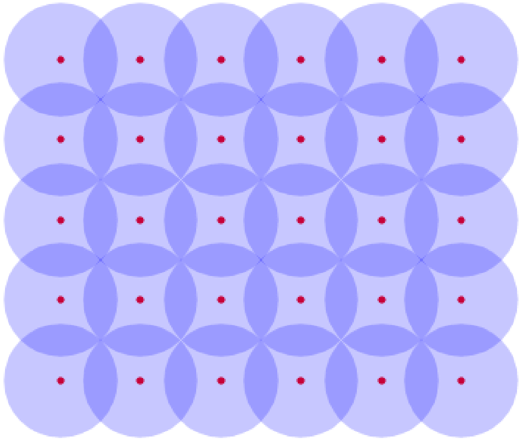
    M. Kiffner, H. Park, W. Li, and T. F. Gallagher, Phys. Rev. A **86**, 031401 (R) (2012).
    M. Kiffner, W. Li, and DJ, Phys. Rev. Lett. **111**, (2013).
    M. Kiffner, M. Huo, W. Li, DJ, Phys. Rev. A **89**, 052717 (2014).



  - **Artificial Gauge Fields**

    M. Kiffner, W. Li, and DJ, Phys. Rev. Lett. **110**, 170402 (2013).
    M. Kiffner, W. Li, and DJ, J. Phys. B: At. Mol. Opt. Phys. **46**, 134008 (2013).

- **Electronic Structure**
  - simple model / scaling
  - Pseudopotentials
  - current step: DFT calculations, preparation, …



People

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  - Sabrina Maniscalco
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  - Stephen Blundell
  - Martin Plenio
  - Javier Prior
  - Tania Monteiro
  - Numerical Algorithms Group

The End

THANK YOU