Interactions, evaporation, & non–ergodicity of assemblies of cold and Rydberg atoms

Habilitation to Direct Research

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chargé de recherche CNRS [2015–, CRCN 7], LPTM, Cergy–Pontoise

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cnrs

LPTM
Laboratoire de Physique Théorique et Modélisation

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Outline

1. Overview :

- Curriculum, research, and teaching
- Three earlier contributions (2016–) :

atomic interactions : Rydberg blockade

collective phenomena 1/2 : evaporation from a cold gas

collective phenomena 2/2 : evaporation from a Rydberg chain

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2. Chaos and semiclassical physics :

Three Rydberg atoms in a circular trap (2023 & 2024)

Curriculum Vitæ : France, Italy, and the USA

- **2015—** Chargé de recherche au CNRS, currently CRCN 7
  Laboratoire de Physique Théorique et Modélisation, Cergy–Pontoise
- **2011—2015** Post–doctoral appointment, BEC Center, Univ. Trento, Italy
  Advisers : Profs. L.P. Pitaevskii and S. Stringari
- **2007–2011** PhD student, LPTMS, Univ. Paris–Sud, Orsay
  Adviser : Prof. G.V. Shlyapnikov
  PhD defended on 11/07/2011 : "Manipulation of Interactions in Quantum Gases"
- **2006** six-month Masters internship at NIST Gaithersburg (MD, USA)
  in Prof. W.D. Phillips's 'Laser cooling and trapping' group
- **2004—2008** Elève à l'Ecole Normale Supérieure, Ulm (concours Maths/Phys)
- **2001–2004** Classes préparatoires MPSI & MP*, Lycée Louis le Grand, Paris 5

Within LPTM

J. Avan, director of LPTM
A. Honecker, deputy director

Theme A:
Condensed matter,
quantum phenomena

Theme B/C:
Integrability,
dynamics, stochasticity

Theme D:
Physics of
complex systems

10 faculty members

D. Papoular ⟷ collaboration with M. Brune's experimental group (LKB/Collège de France, Paris)

B. Zumer, PhD student

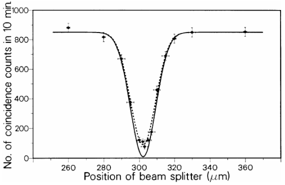
- Representative for one of the two QuanTiP teams of the lab :
  Quantum matter : strong correlations, topology and out–of–equilibrium phenomena
  at the federation for quantum technologies in Île–de–France
  SIRTEQ (2017–2022), QuanTiP (2022–)

Teaching : Quantum Physics at the M2 (graduate) level

- **2018—** M2 ICFP–quantum physics track, ENS Paris
  Exercise sessions, “Advanced quantum mechanics” course
- **2017—** M2 in Theoretical Physics, Cergy–Pontoise
  Formal lectures, “Advanced quantum mechanics” course

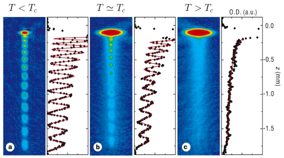
Illustrate the roles of correlations and interactions of identical quantum particles
in recent experiments involving atomic systems, e.g. :

Two–particle interference



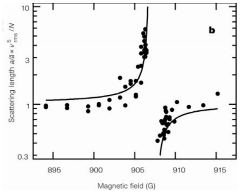
[Hong, Ou, Mandel, PRL 1987]

Quantum coherence



[Bloch, Hänsch, Esslinger, Nature (2000)]

Low–energy scattering resonances

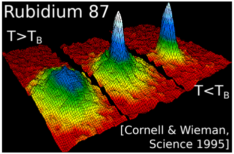


[Ketterle Nature 1998]

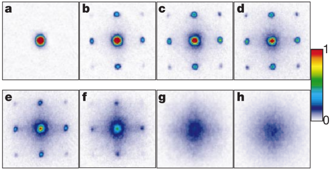
- Earlier teaching appointments : undergraduate physics courses
  2008—2011 : Tutor at Université Paris–Sud, Orsay
  2005—2008 : Tutor, classes préparatoires MPSI & MP*, Lycée Louis le Grand, Paris 5

Model atomic systems comprised of trapped atoms

- Traps containing 10^5 atoms, or 2 atoms, or 1 single atom
  Control over dimensionality and trapping geometry
  Control over interactions : weak or strong, repulsive or attractive
- **Quantum simulation :** well–controlled systems analogous to more complicated ones
  including minimal ingredients leading to considered effect
- Cold atomic **gases :** dilute, i.e. interaction range $\ll$ interatomic distance

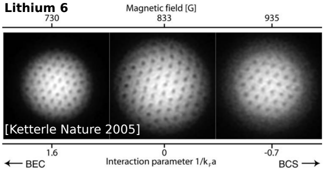


Bose–Einstein condensate



[Greiner, Esslinger, Hänsch, Bloch, Nature 2002]

superfluid to Mott–insulator transition



transition between BEC and BCS superfluidity

More examples may be found in [Cl. Cohen–Tannoudji & D. Guéry–Odelin, *Advances in atomic physics*, World Scientific (2011)]

- **For longer–ranged interactions,** exploit dipole–dipole interaction
  magnetic atoms ; heteronuclear molecules carrying an electric dipole ; **Rydberg atoms**

Cold ground–state versus Rydberg atoms

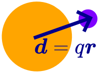
- **'Cold'** is a statement about the **spatial motion** of the atom as a whole

"Sufficiently cold to be confined in an optical trap" : **All atoms considered in this talk**

[Cohen–Tannoudji & Guéry–Odelin, World Scientific 2011, ch. 7] [S.E. Anderson PRL 2011] [Barredo PRL 2020] [Cortiñas PRL 2020]

- Alkali atoms, e.g. $^{87}\mathrm{Rb}$, have one outer electron : principal quantum number n

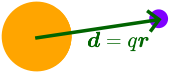
$n = 5$: **electronic ground state**



SMALL off–diagonal electric dipole **d**

Stable

$n = 50$: **Rydberg state**



LARGE off–diagonal electric dipole **d**

Long lifetime $\sim 30\,\mathrm{ms}$ for 'circular' state $|n, l = m = n - 1\rangle$

- **Motivation :** interaction between two atoms in the same electronic state

Van der Waals interaction, range $l_{vdW} = (m|C_6|/\hbar^2)^{1/2}$

$l_{vdW} = 10\,\mathrm{nm} \ll$ mean distance $100\,\mathrm{nm}$

"**Contact interaction** $g\,\delta(\mathbf{r})$"

Many–body ground state is usually a gas

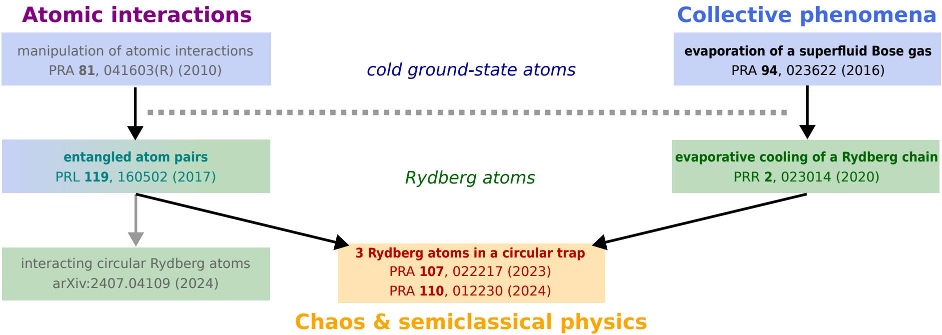
$l_{vdW} = 70\,\mu\mathrm{m} >$ mean distance $10\,\mu\mathrm{m}$

Longer–ranged interaction

Many–body ground state is a crystal

3 connected scientific interests, from 2015 onwards

- All considered systems are experimentally accessible
  They are comprised of cold ground–state atoms and/or Rydberg atoms



- Joint papers with experimentalists : WIPM, Wuhan (China) ; CQED, LKB (Paris)
- Supervision of one PhD student : B. Zumer, Cergy, 2021–2024 (2 papers in PRA)

Entanglement of two **distinguishable atoms**

[Zeng, Zhan, Papoular, Shlyapnikov et al, Phys. Rev. Lett. **119**, 160502 (2017)]

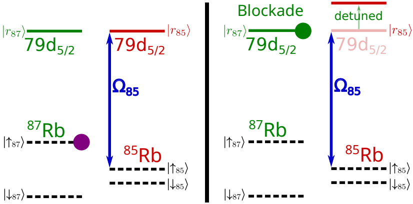
Collaboration between Wuhan, LPTM, and LPTMS, cited 173 times (Google Scholar)

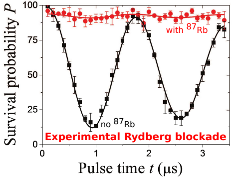
- One $^{87}\mathrm{Rb}$ atom and one $^{85}\mathrm{Rb}$ atom, each in its own microtrap, $\sim 4\ \mu\mathrm{m}$ apart

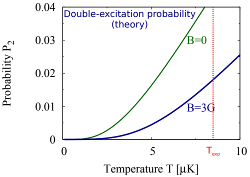
2 states per atom in ground hyperfine manifold : $|\uparrow_{87}\rangle$, $|\downarrow_{87}\rangle$ for $^{87}\mathrm{Rb}$; $|\uparrow_{85}\rangle$, $|\downarrow_{85}\rangle$ for $^{85}\mathrm{Rb}$; 1 Rydberg state per atom : $|r_{87}\rangle$, $|r_{85}\rangle$

- The states $|\uparrow_{85}\rangle$ and $|r_{85}\rangle$ of $^{85}\mathrm{Rb}$ are Rabi–coupled by a two–photon transition
- Prepare $^{87}\mathrm{Rb}$ in $|r_{87}\rangle$ to push $|r_{85}\rangle$ out of resonance

Rydberg blockade







Calculation of double–excitation probability

- accounts for 437 internal states
  external magnetic field,
  thermal atomic motion within microtraps

Agrees with measured Rabi oscillation amplitude

- Rydberg blockade is *conditional* on $^{87}\mathrm{Rb}$ being in its Rydberg state $|r_{87}\rangle$

Start from superposition state to achieve **2–atom entangled state** $(|\uparrow_{87}\uparrow_{85}\rangle + |\downarrow_{87}\downarrow_{85}\rangle)/\sqrt{2}$

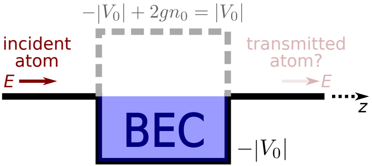
Quantum evaporation of a Bose gas

[Papoular, Pitaevskii & Stringari, Phys. Rev. A **94**, 023622 (2016)] collaboration LPTM / Trento (Italy)

Cold atomic gas : Identical bosonic atoms, e.g. $^{87}\mathrm{Rb}$, in their ground electronic state

- The trap is filled with a weakly–interacting Bose–Einstein condensate, $g\, n_0 \approx |V_0|$
  An atom with a given energy $E < |V_0|$ impinges on it

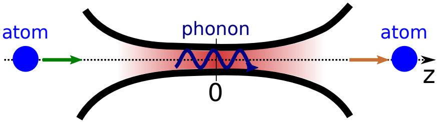
n_0 = condensate density, $g = 4\pi\hbar^2 a/m > 0$ is the interaction strength, a = scattering length



- In the absence of a collective mechanism,
  The atom would experience the mean–field shift $2gn_0$
  potential barrier $-|V_0| + 2gn_0 = |V_0|$: atom blocked
  $2gn_0$ because incident and condensate atoms are in different states

- **Collective transport mechanism :**

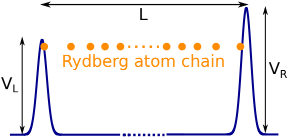
The atom impinges on one end of the constriction,
Excites a phonon : **condensation,**
which propagates to the other end,
where an atom is emitted : **evaporation.**



For superfluid Helium 4 : [Johnston & King PRL 1966] [Anderson Phys. Lett. A 1969] [Dalfovo PRL 1995]

Evaporative cooling of a chain of Rydberg atoms

[Brune & Papoular, Phys. Rev. Research **2**, 023014 (2020)] collaboration LPTM / LKB

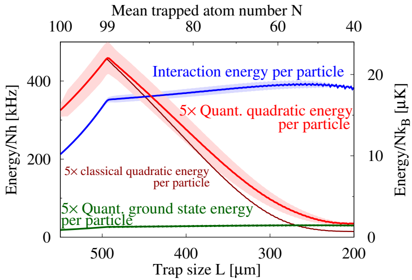


- Trapped chain of circular Rydberg atoms, mean spacing 5 μm
  Repulsive interatomic interaction C_6/x^6, range 70 μm ;
- Slowly bring plugs closer : the leftmost atom evaporates
  The remaining trapped chain thermalises to a lower temperature

Initially proposed in [Nguyen, Brune et al, PRX 2018]

- **Thermodynamic description**
  valid both in classical and quantum regimes
- **long 1D crystal,** comprising > 700 atoms
  close to quantum ground state

Spatial order, even though no spatially periodic potential is used



- As for cold gases, classical regime described by **truncated Boltzmann distribution**
  [Luiten, Reynolds, & Walraven, PRA 1996]
- **One important difference** with respect to cold gases :
  The partition function of the chain does not factorise in terms of atoms or modes
  Hence, the quantum regime is not described by a truncated Bose–Einstein distribution

Three Rydberg atoms in a circular trap

[D.J. Papoular & B. Zumer, Phys. Rev. A **107**, 022217 (2023)]

[D.J. Papoular & B. Zumer, Phys. Rev. A **110**, 012230 (2024)]

- An experimentally accessible system analysed using well–established tools

  Heller's quantum scar, Gutzwiller's trace formula, EBK theory, . . .

- Quantum energy levels satisfy Berry–Robnik statistics [Berry & Robnik, J. Phys. A **17**, 2413 (1984)]

- Two mechanisms impeding ergodicity : quantum scar, classical localisation

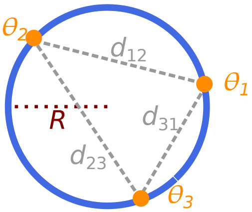
  [Heller, *The semiclassical way to dynamics and spectroscopy*, Princeton (2018), chap. 22]

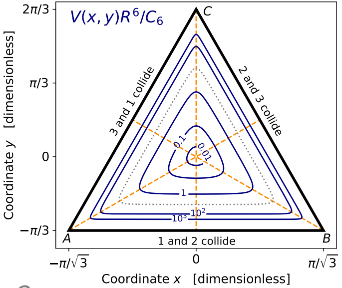
- Links with the Hénon–Heiles Hamiltonian and recent many–body experiments

  [Hénon & Heiles, Astron. J. **69**, 73 (1964)] [Bernien, Lukin et al, Nature **551**, 579 (2017)]

Three Rydberg atoms in a circular trap

- No longitudinal potentials : dynamics due to interaction between particles
  Interacting particles are e.g. trapped circular Rydberg atoms





$$H = \frac{l_1^2 + l_2^2 + l_3^2}{2mR^2} + \frac{C_6}{d_{12}^6} + \frac{C_6}{d_{23}^6} + \frac{C_6}{d_{31}^6}$$

(l_i= angular momentum of atom i)

- Conservation of total angular momentum : reduction to 2 degrees of freedom

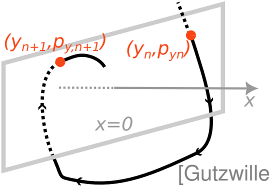
$$H_{2\mathrm{D}} = \frac{p_x^2 + p_y^2}{4m\,R^2} + \frac{C_6}{(2R)^6}\left(\frac{1}{\sin^6\left[\frac{\pi}{3} + y\right]} + \frac{1}{\sin^6\left[\frac{\pi}{3} - \frac{\sqrt{3}}{2}x - \frac{1}{2}y\right]} + \frac{1}{\sin^6\left[\frac{\pi}{3} + \frac{\sqrt{3}}{2}x - \frac{1}{2}y\right]} - \frac{64}{9}\right)$$

The effective potential $V(x,y)$ within the triangle ABC exhibits triangular symmetry (group C_{3v})

Analogous to $V(x,y) = m\omega_0^2(x^2+y^2)/2 + \alpha(x^2y - y^3/3)$ [Hénon & Heiles (1963)]

Mixed classical phase space

Surface of section at energy ε : intersections of classical trajectories with a plane

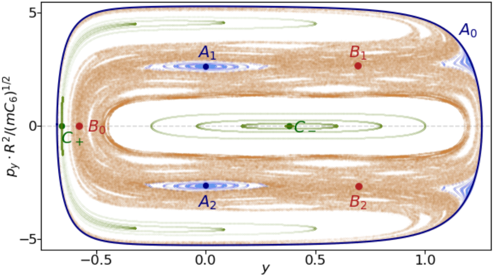


- The brown ergodic zone covers a fraction of the surface
- Non–ergodic tori yield concentric closed curves (blue, green)
- Periodic trajectories yield fixed points (blue, red, green)

[Gutzwiller, *Chaos in classical and quantum mechanics*, Springer (1990), ch. 7&8]

Surface of section drawn for the **given energy** $\varepsilon = 7C_6/R^6$

- Experimentally accessible
- Ergodic region and non–ergodic islands occupy comparable areas



- Classical phase space comprises both an ergodic region and non–ergodic islands
  Stable (blue, green) and unstable (red) periodic trajectories

Consequences in quantum mechanics ? *(i)* energy spectra ; *(ii)* some specific wavefunctions

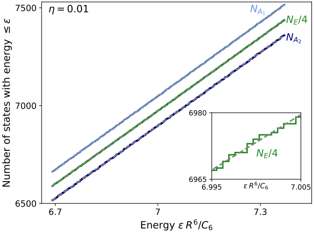
Statistics of the quantum energy levels

- Dimensionless parameter $\eta = \hbar R^2/(mC_6)^{1/2} = 0.01$ experimentally accessible value

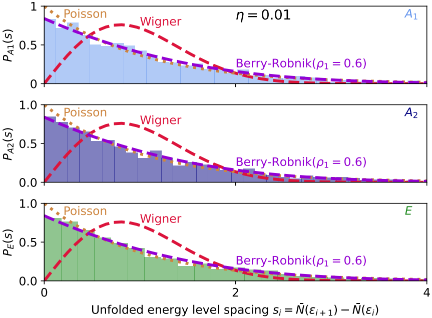
trap radius $R = 7\,\mu\mathrm{m}$, atomic mass $m = m_{^{87}\mathrm{Rb}}$, interaction strength $C_6/h = 3\,\mathrm{GHz}\,\mu\mathrm{m}^6$

- For each irreducible representation $r = A_1, A_2, E$ of C_{3v},

I calculate > 1000 wavefunctions & energies (ε_i) near $7C_6/R^6$ using the Finite Element Method (FreeFEM, open–source)



- The integrated densities of states $N_r(\varepsilon)$ fluctuate about their smooth components $\bar{N}_r(\varepsilon)$



- Unfolded level spacing : $s_i = \bar{N}_r(\varepsilon_{i+1}) - \bar{N}_r(\varepsilon_i)$

[Bohigas, Tomsovic, Ullmo, Phys. Rep. **223**, 43 (1993)]

Integrable : Poisson statistics ; Fully chaotic : Wigner statistics

- Mixed phase space : **Berry–Robnik statistics**

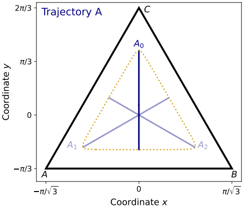
[Berry & Robnik, J. Phys. A **17**, 2413 (1984)]

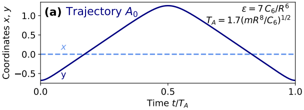
Stable and unstable classical periodic trajectories

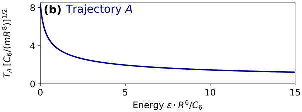
- Three families *A*, *B*, *C* of periodic trajectories found numerically

  using our own C++ implementation of [Baranger et al, Ann. Phys. **186**, 95 (1988)]

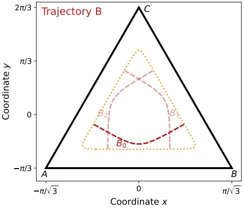
There are multiple trajectories in each family due to discrete symmetries

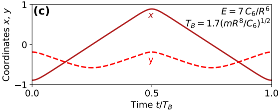


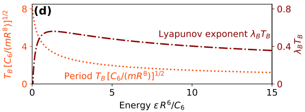




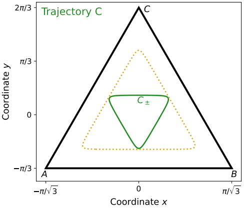
Stable : Lyapunov exponent $\lambda_A = 0$

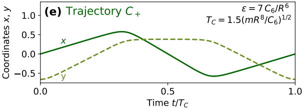


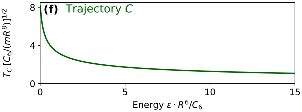




Unstable : Lyapunov exponent $\lambda_B > 0$





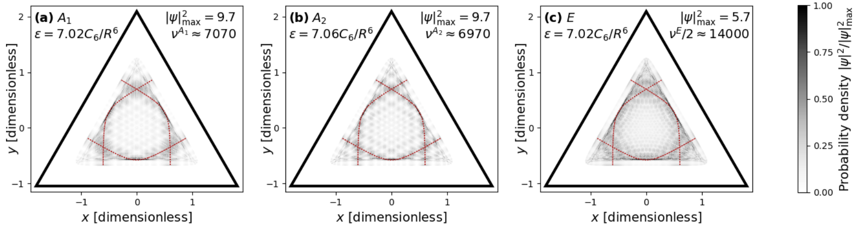


Stable : Lyapunov exponent $\lambda_C = 0$

Quantum scar due to the unstable Trajectory B

- For most eigenstates, the density $|\psi_n(\mathbf{r})|^2$ is unrelated to Trajectory B
- For each irreducible representation $r = A_1, A_2, E$ of C_{3v}, multiple quantum states exhibit enhanced density near the **unstable** trajectory B

Three examples, Finite–Element Method numerical results : (there are other similar states)



- Quantum scar satisfying Heller's definition [Heller, PRL **53,** 1515 (1984)]
- No longitudinal single–particle trapping potential along the circular trap
  The quantum scar is due to interatomic interactions

Quantum scar due to Traj. B : semiclassical analysis

- Impact of unstable periodic trajectory B analysed using *Gutzwiller's trace formula*

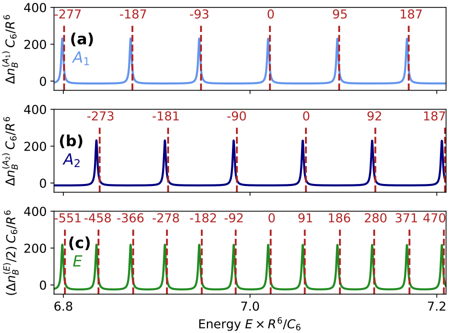
density of states for Representation r : $n^{(r)}(\varepsilon)$ = sum over classical periodic trajectories

[Gutzwiller, *Chaos in classical and quantum mechanics*, Springer (1990), Sec. 17.4]

- The contribution from Trajectory B exhibits peaks with nonzero width

  Their positions provide approximate energies for the scarred eigenstates

  This approach *does not yield semiclassical wavefunctions*



- We find one scarred eigenstate near the maximum of each peak

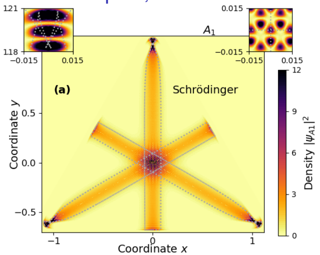
Classical localisation near stable Trajectory *A*

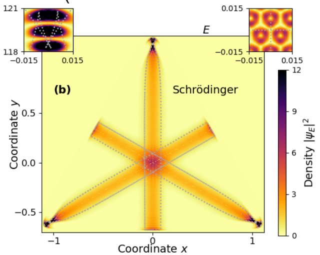
Similar results for Trajectory *C* in [Papoular & Zumer, Phys. Rev. A **110**, 012230 (2024)]

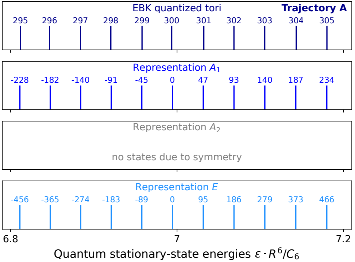
- Some eigenstates are localised near the **stable** periodic Trajectory *A*

  NOT quantum scars : quantum mechanics brings no qualitative change

Two examples, numerical Finite–Element Method results (there are other similar states)







- Energies & *wavefunctions* obtained semiclassically using the *Einstein–Brillouin–Keller approach*

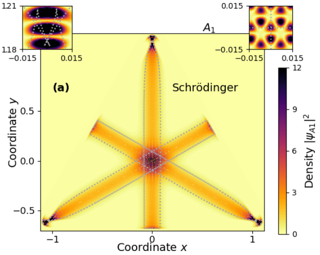
  [Martens & Ezra, J. Chem. Phys. **86**, 279 (1987)]

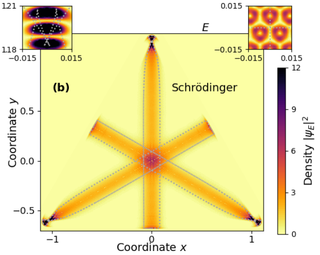
- Selection rules reflecting the symmetries of the classical trajectories : no such states in A_2

Classical localisation near Trajectory A : wavefunctions

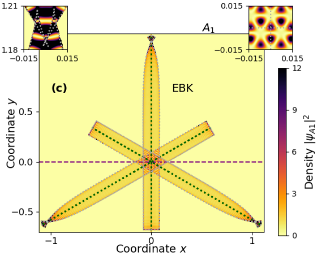
Similar results for Trajectory C in [Papoular & Zumer, Phys. Rev. A **110**, 012230 (2024)]

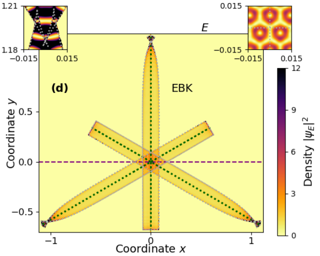
- Numerical solution of the stationary Schrödinger equation (Finite–Element Method)





- Semiclassical Einstein–Brillouin–Keller wavefunctions [Knudson et al, J. Chem. Phys. (1986)]





Differences near the caustics (e.g. dashed gray lines in left insets)

Comparison with **many–body scar** in a Rydberg chain

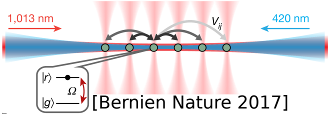
- **Experiment** [Bernien, Lukin, et al, Nature **551**, 579 (2017)]

51 $^{87}\mathrm{Rb}$ ground–state atoms $|\circ\rangle$ in array of optical microtraps

Each atom is coupled to Rydberg state $|\bullet\rangle$ (via Raman transition)

Prepare $|\bullet \circ \bullet \circ \bullet \circ \cdots\rangle$, then observe spin dynamics

The period–2 chain thermalises only very slowly



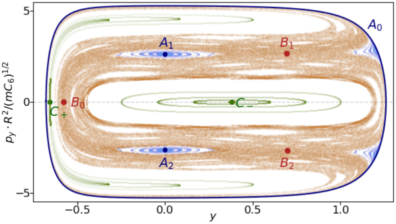
[Bernien Nature 2017]

- **Theoretical description** [Michailidis, Papić et al, Phys. Rev. X **10**, 011055 (2020)]

Approximate many–body dynamics using Hamiltonian system, phase space dimension 4

3 Atoms in a circular trap

exact Hamiltonian description

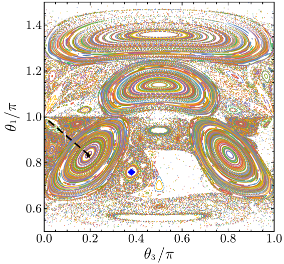


Stable (blue, green) & **unstable** (red) fixed points

[Papoular & Zumer, PRA (2023) & PRA (2024)]

Rydberg atom chain

initial condition different from experiment



Stable fixed points

[Michailidis, Papić et al, PRX 2020]

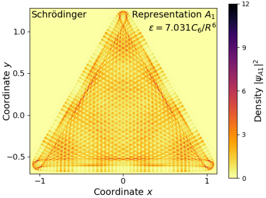
Prospects : Three Rydberg atoms in a circular trap

- **Localised and non–localised quantum eigenstates :**

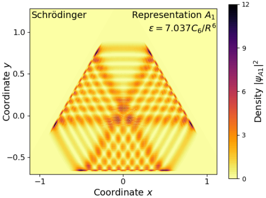
I have calculated $\sim 3 \times 1000$ eigenstate wavefunctions and energies near $7C_6/R^6$

Periodic trajectories beyond families A, B, C may explain other localised quantum states

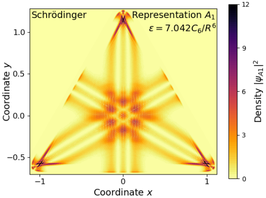
Interpret non–localised quantum states as random Gaussian waves ? [Berry, J. Phys. A (1977)]



Non–localised ?



Bifurcation from family C ?



Bifurcation from family A ?

- **Periodic modulation** e.g. of the **interaction strength** C_6 (RF electric field)

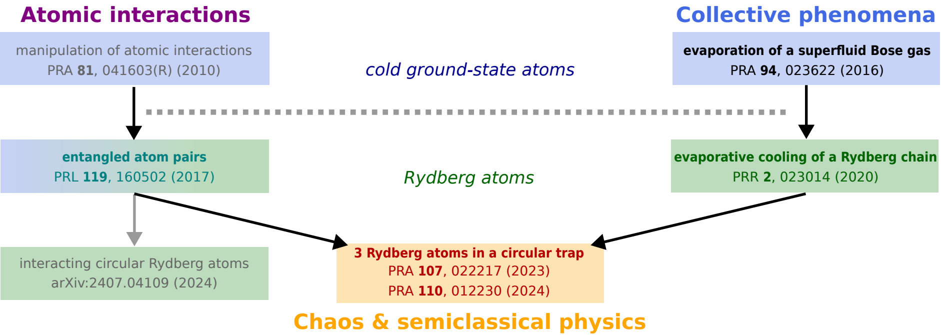
Analogy with a recent experiment by Lukin (Harvard) [Bluvstein et al, Science (2021)]

Does it stabilise the unstable trajectory B ?

If so, is the stabilisation mechanism quantum or classical ?

3 connected scientific interests, from 2015 onwards

- All considered systems are experimentally accessible
  They are comprised of cold ground–state atoms and/or Rydberg atoms



- Joint papers with experimentalists : WIPM, Wuhan (China) ; CQED, LKB (Paris)
- Supervision of one PhD student : B. Zumer, Cergy, 2021–2024 (2 papers in PRA)
- Prospects concerning chaos and semiclassical physics in atomic systems