Nonequilibrium Quantum Dynamics of Ultracold Systems: Interplay of Interference, Interactions and Nonlinearity

Peter Schmelcher
Zentrum für Optische Quantentechnologien
Hamburg Center for Ultrafast Imaging
Universität Hamburg

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The Center for Optical Quantum Technologies

Experiment and Theory -
Workshop and Guest Program

in collaboration with

- L. Cao, S. Krönke, O. Vendrell (ML-MCTDHB)
- L. Cao, S. Krönke, R. Schmitz, J. Knörzer and S. Mistakidis (Applications)

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Contents

1. Introduction and Motivation

Introduction and Motivation

An exquisite control over the external and internal degrees of freedom of atoms developed over decades lead to the realization of **Bose-Einstein Condensation** in dilute alkali gases at nK temperatures.

Worldwide ≈ 170 atom trap experiments
Condensed Species:
$H, Li, Na, K, Rb, Cs, Yb, He^{\star}, Cr, ..., Dy$

Key tools available:

- Laser and evaporative cooling
- Magnetic, electric and optical dipole traps
- Optical lattices and atom chips
- Feshbach resonances (mag-opt-conf) for tuning of interaction

Introduction and Motivation

Enormous degree of control concerning preparation, processing and detection of ultracold atoms !

Weak to strongly correlated **many-body** systems:

- BEC nonlinear mean-field physics (solitons, vortices, collective modes,...)
- Strongly correlated many-body physics (quantum phases: MI etc.; Kondo- and impurity physics, disorder, Hubbard model physics, high T_c superconductors,...)

Few-body regime:

- Novel mechanisms of transport and tunneling
- Atomtronics (Switches, diodes, transistors, ...)
- Quantum information processing

In particular: Links between these regimes !

Introduction: Some facts

Finite, and in particular 'stronger' interactions:

- **Correlations are ubiquitous**
- A multiconfigurational ansatz is necessary

$$\Psi(\mathbf{r}_1, ..., \mathbf{r}_N, t) = \sum_i c_i \Phi_i(\mathbf{r}_1, ..., \mathbf{r}_N, t)$$

$\Rightarrow$ Ideal laboratory for exploring the dynamics of correlations (beyond mean-field):

- Preparation of correlated initial states
- Spreading of localized/delocalized correlations ?
- Time-dependent 'management' and control of correlations ?
- Is there universality in correlation dynamics ?

Introduction and Motivation

Calls for a versatile tool to explore the (nonequilibrium) quantum dynamics of ultracold bosons: **Wish list**

- Take account of all correlations (numerically exact)
- Applies to different dimensionality
- Time-dependent Hamiltonian: Driving
- Weak to strong interactions (short and long-range)
- Few- to many-body systems
- Mixed systems: different species, mixed dimensionality
- Efficient and fast

Introduction and Motivation

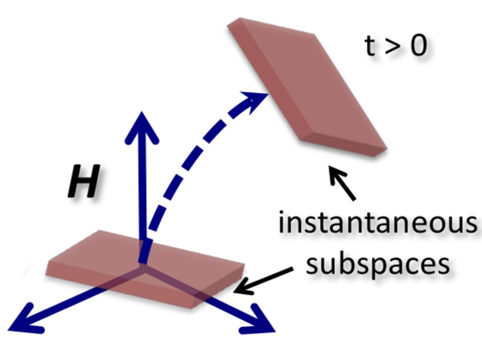
Multi-Layer Multi-Configuration Time-Dependent Hartree for Bosons (ML-MCTDHB) is a significant step in this direction !

In the following: Some selected diverse applications to ultracold bosonic systems.

2. Methodology: The ML-MCTDHB Approach

The ML-MCTDHB Method

- **aim:** numerically exact solution of the time-dependent Schrödinger equation
  for a quite general class of interacting many-body systems
- **history:** [H-D Meyer. *WIREs Comp. Mol. Sci.* **2**, 351 (2012).]
  MCTDH (1990): few distinguishable DOFs, quantum molecular dynamics
  ML-MCTDH (2003): more distinguishable DOFs, distinct subsystems
  MCTDHF (2003): indistinguishable fermions
  MCTDHB (2007): indistinguishable bosons
- **idea:**
  use a time-dependent, optimally moving basis in the many-body Hilbert space



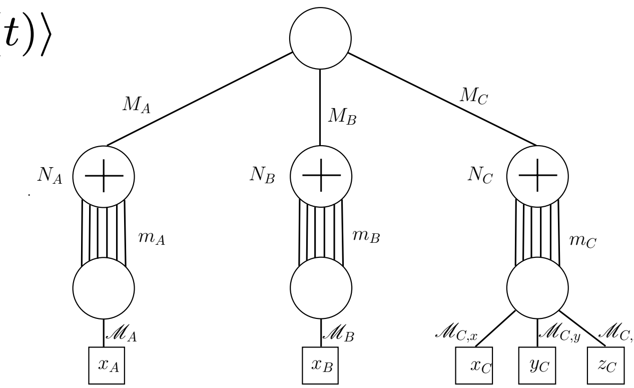
Hierarchy within ML-MCTDHB

We make an ansatz for the state of the total system $|\Psi_t\rangle$ with time-dependencies on different *layers*:

top layer $|\Psi_t\rangle = \sum_{i_1=1}^{M_1} \dots \sum_{i_S=1}^{M_S} A_{i_1,\dots,i_S}(t) \bigotimes_{\sigma=1}^{S} |\psi_{i_\sigma}^{(\sigma)}(t)\rangle$

species layer $|\psi_k^{(\sigma)}(t)\rangle = \sum_{\vec{n}|N_\sigma} C_{k;\vec{n}}^{\sigma}(t)\, |\vec{n}\rangle(t)$

particle layer $|\phi_k^{(\sigma)}(t)\rangle = \sum_{i=1}^{n_\sigma} B_{k;i}^{\sigma}(t)|u_i\rangle$



- Mc Lachlan variational principle: Propagate the ansatz $|\Psi_t\rangle \equiv |\Psi(\{\lambda_t^i\})\rangle$, $\lambda_t^i \in \mathbb{C}$ according to $i\partial_t|\Psi_t\rangle = |\Theta_t\rangle$ with $|\Theta_t\rangle \in \text{span}\{\frac{\partial}{\partial\lambda_t^k}|\Psi(\{\lambda_t^i\})\rangle\}$ minimizing the error functional $|||\Theta_t\rangle - \hat{H}|\Psi_t\rangle||^2$
  [AD McLachlan. *Mol. Phys.* **8**, 39 (1963).]
- In this sense, we obtain a *variationally* optimally moving basis!
- Dynamical truncation of Hilbert space on all layers
- Single species, single orbital on particle layer $\rightarrow$ Gross-Pitaevskii equation ! (Nonlinear excitations: Solitons, vortices,...)

The ML-MCTDHB equations of motion

- top layer EOM:

$$i\partial_t A_{i_1,\dots,i_S} = \sum_{j_1=1}^{M_1} \dots \sum_{j_S=1}^{M_S} \langle \psi_{i_1}^{(1)} \dots \psi_{i_S}^{(S)} |\ \hat{H}\ | \psi_{j_1}^{(1)} \dots \psi_{j_S}^{(S)} \rangle\, A_{j_1,\dots,j_S}$$

$$\text{with} \quad |\psi_{j_1}^{(1)} \dots \psi_{j_S}^{(S)}\rangle \equiv |\psi_{j_1}^{(1)}\rangle \otimes \dots \otimes |\psi_{j_S}^{(S)}\rangle$$

$\Rightarrow$ system of coupled linear ODEs with time-dependent coefficients due to the time-dependence in $|\psi_j^{(\sigma)}(t)\rangle$ and $|\phi_j^{(\sigma)}(t)\rangle$

$\Rightarrow$ reminiscent of the Schrödinger equation in matrix representation

- species layer EOM:

$$i\partial_t C^{\sigma}_{i;\vec{n}} = \langle \vec{n} | (\mathbb{1} - \hat{P}^{spec}_{\sigma}) \sum_{j,k=1}^{M_\sigma} \sum_{\vec{m}|N_\sigma} [(\rho^{spec}_{\sigma})^{-1}]_{ij} \langle \hat{H} \rangle^{\sigma,spec}_{jk} | \vec{m} \rangle\ C^{\sigma}_{k;\vec{m}}$$

$\Rightarrow$ system of coupled non-linear ODEs with time-dependent coefficients due to the time-dependence of the $|\phi_j^{(\sigma)}(t)\rangle$ and of the top layer coefficients

The ML-MCTDHB equations of motion

- particle layer EOM:

$$i\partial_t|\phi_i^{(\sigma)}\rangle = (\mathbb{1} - \hat{P}_\sigma^{part}) \sum_{j,k=1}^{m_\sigma} [(\rho_\sigma^{part})^{-1}]_{ij} \langle \hat{H} \rangle_{jk}^{\sigma,part} |\phi_k^{(\sigma)}\rangle$$

$\Rightarrow$ system of coupled non-linear partial integro-differential equations (ODEs, if projected on $|u_k^{(\sigma)}\rangle$, respectively) with time-dependent coefficients due to time-dependence of the $C_{i;\vec{n}}^{\sigma}$ and $A_{i_1,\ldots,i_S}$

Lowest layer representations:

- **Discrete Variable Representation (DVR):**
  implemented DVRs: harmonic, sine (hardwall b.c.), exponential (periodic b.c.), radial harmonic, Laguerre
- Fast Fourier Transform

Stationary states via improved relaxation involving imaginary time propagation !

S Krönke, L Cao, O Vendrell, P S, *New J. Phys.* **15, 063018 (2013).**

L Cao, S Krönke, O Vendrell, P S, *J. Chem. Phys.* **139, 134103 (2013).**

3. Collective dynamics at the crossover from few- to many-body systems

Collective Dynamics...

Follow a bottom-up approach in the emergence of collective dynamics with increasing atom number: From few to many.

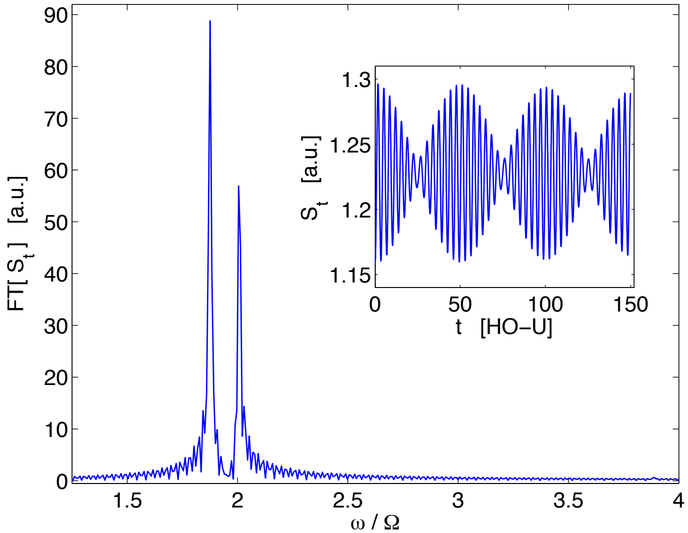
Prototype example and first application of ML-MCTDHB.

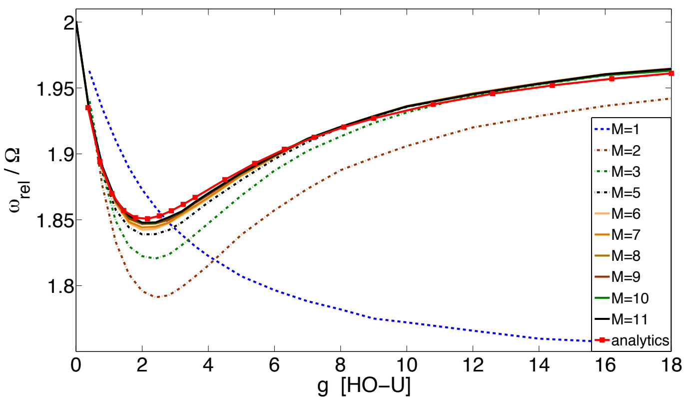
Quench-induced breathing dynamics of ultracold bosons in a harmonic trap.

Answer the question:

- Discrete structure and frequency spectrum transform into collective behaviour
- Correlations change the simple mean-field picture

Start with two atoms...

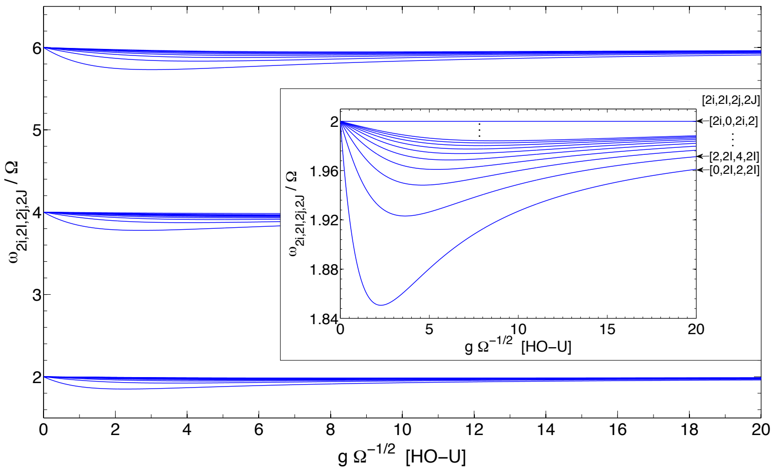




- Beating and breathing dynamics of $< X^2 >$
- Two dominant peaks in a background of frequencies: Relative + CM motion
- Relative motion breathing mode frequency varies with g whereas CM one not.

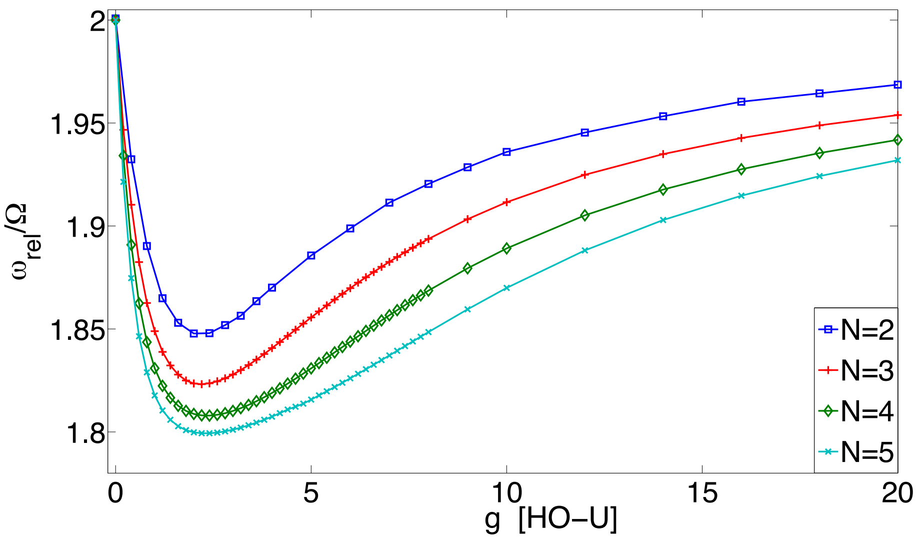
Rich breathing spectrum: Infinite sets of bands around $2n\Omega$ - but strongly suppressed !

A more detailed view...

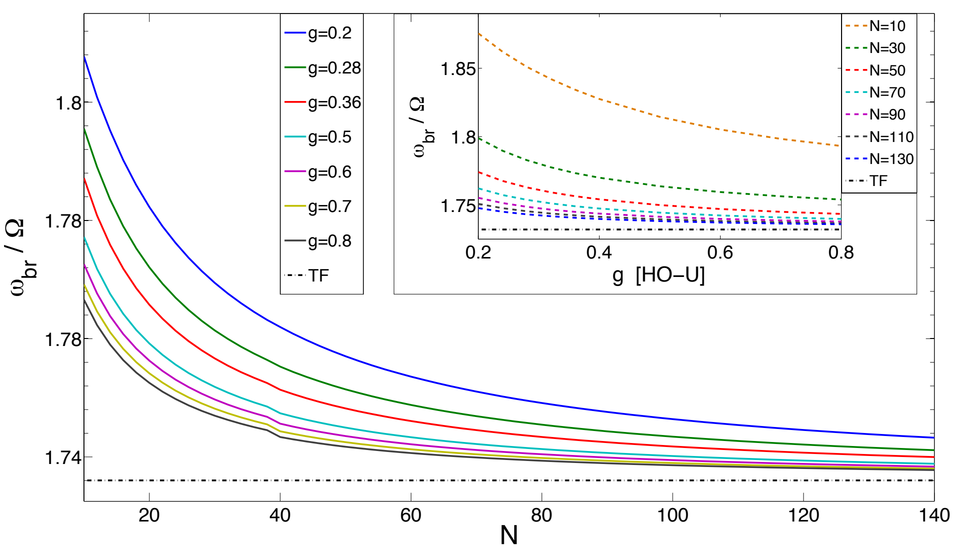


- Full breathing/beating mode spectrum up to 20 quanta at any interaction strength up to $\approx 6\Omega$.
- Inset: detailed view on the lowest band.
- Frequencies: $\omega_{2i,2I,2j,2J}$ which refers to the frequency arising from $\langle \Phi_{2I}\phi_{2i}|\, \hat{X}^2 \,|\Phi_{2J}\phi_{2j}\rangle$.

Moving up to 140 atoms...

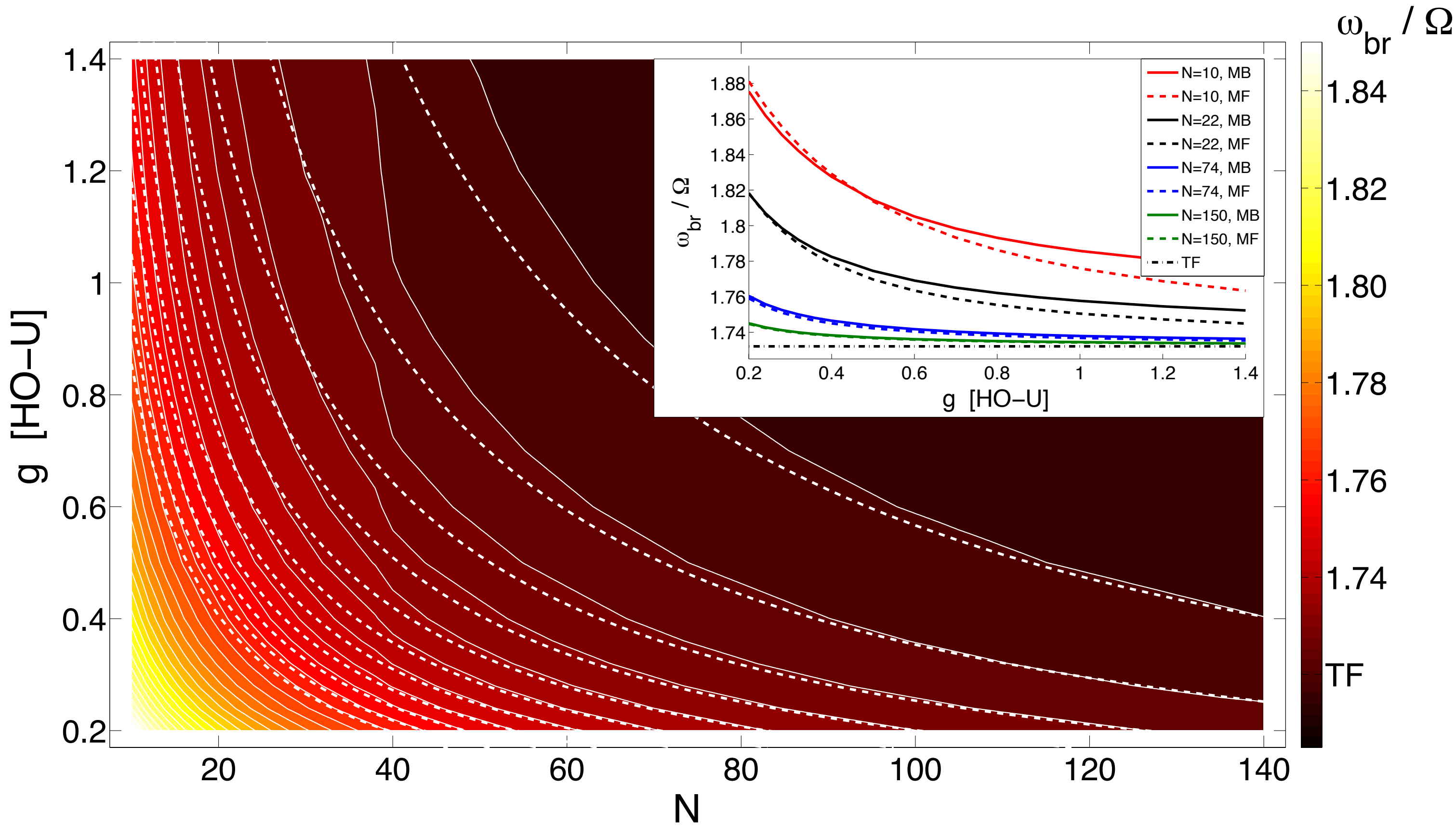


- CM breathing mode becomes strongly suppressed
- Breathing of the relative motion becomes dominant !



- Breathing mode frequency with varying particle number for various interaction strength g

Moving up to 140 atoms...



- Many-body versus mean-field breathing mode frequency.

See: R. Schmitz, S. Krönke, L. Cao and P.S., PRA 88, 043601 (2013)

4. Multi-mode quench dynamics in optical lattices

Main features

Focus: Correlated non-equilibrium dynamics of in one-dimensional finite lattices following a sudden interaction quench from weak (SF) to strong interactions!

Phenomenology: Emergence of density-wave tunneling, breathing and cradle-like processes.

Mechanisms: Interplay of intrawell and interwell dynamics involving higher excited bands.

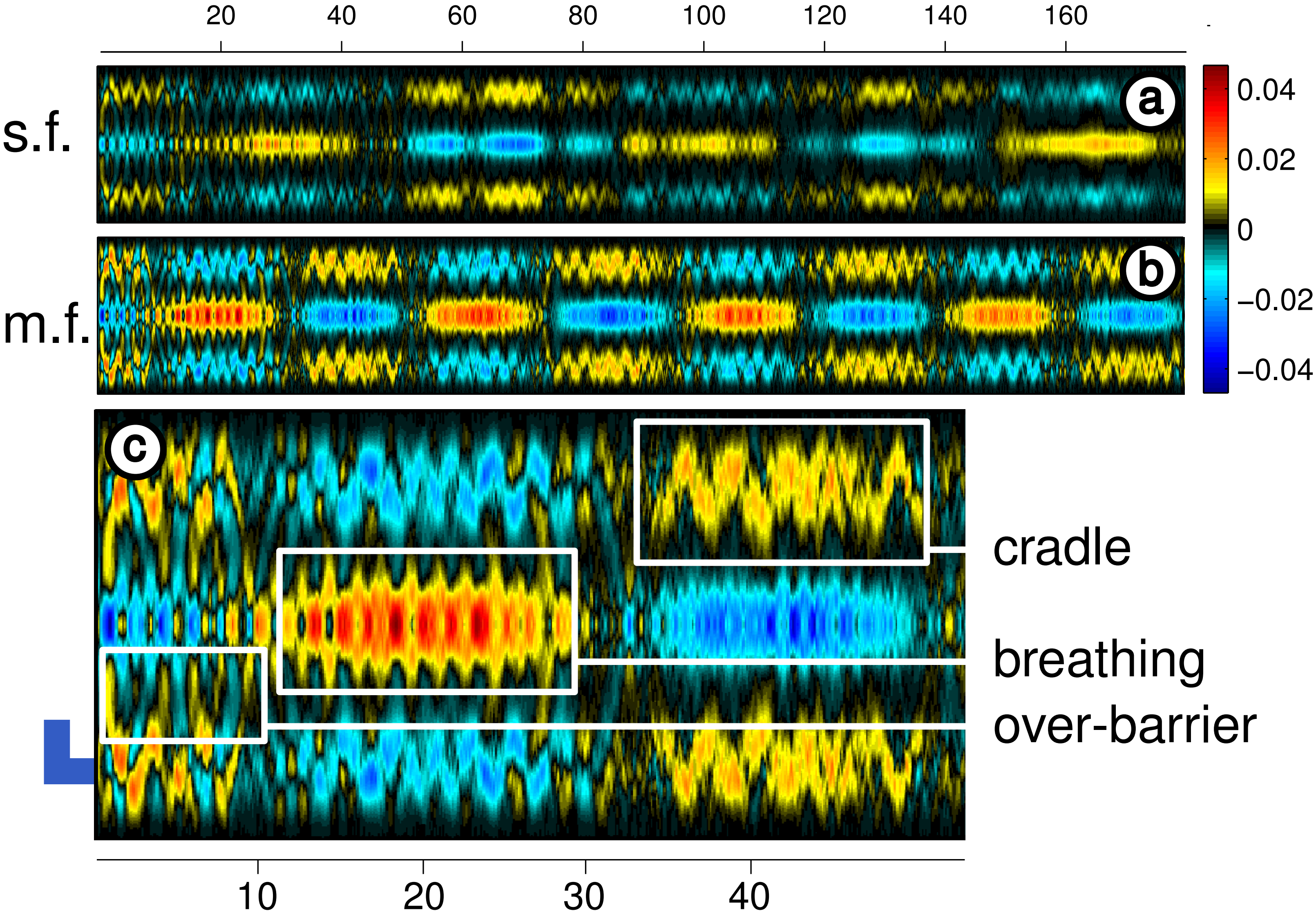
Resonance phenomena: Coupling of density-wave and cradle modes leads to a corresponding beating phenomenon !

$\Rightarrow$ Effective Hamiltonian description and tunability.

Incommensurate filling factor $\nu > 1 (\nu < 1)$

Post quench dynamics....

Fluctuations $\delta\rho(x,t)$ of the one-body density for weaker (a) and stronger (b) quench: Spatiotemporal oscillations.

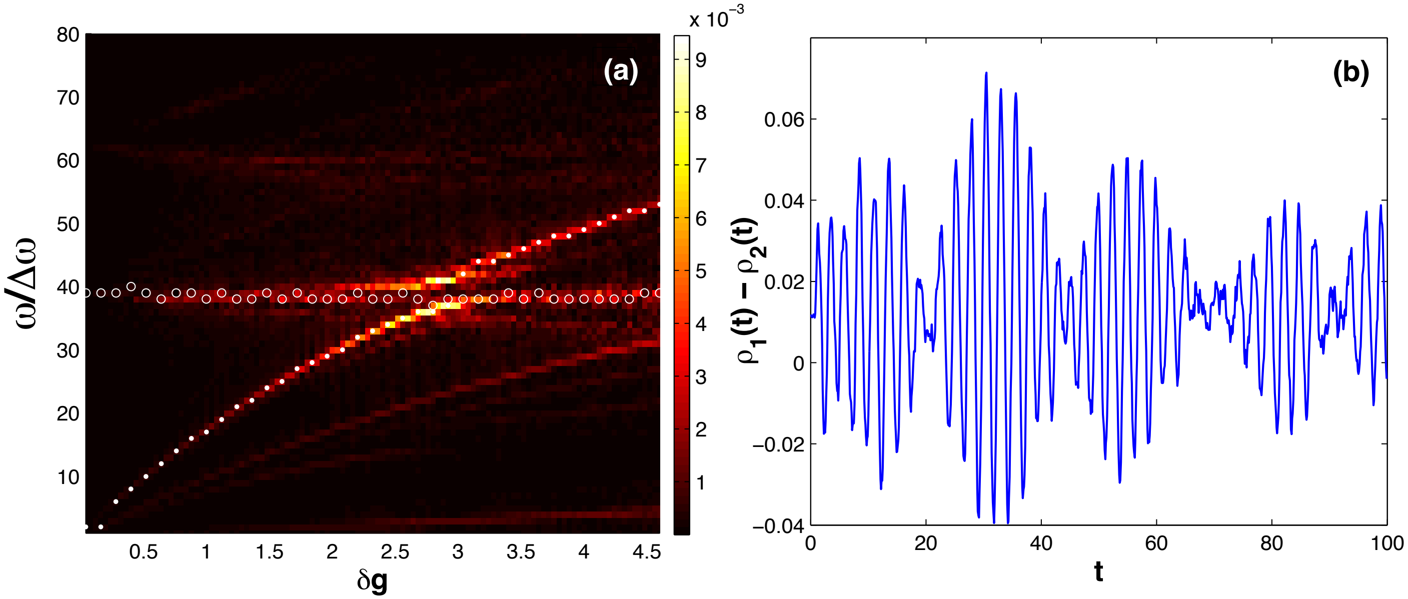


Density waves and their tunneling.

Mode analysis

- Density tunneling mode: Global ’envelope’ breathing
  - Identification of relevant tunneling branches (number state analysis)
  - Fidelity analysis shows 3 relevant frequencies: pair and triple mode processes
  - Transport of correlations and dynamical bunching antibunching transitions
- On-site breathing and craddle mode: Similar analysis possible involving now higher excitations

Craddle and tunneling mode interaction



Fourier spectrum of the intrawell-asymmetry $\Delta\rho_L(\omega)$:

Avoided crossing of tunneling and craddle mode !

$\Rightarrow$ Beating of the craddle mode - resonant enhancement.

S.I. Mistakidis, L. Cao and P. S., JPB 47, 225303 (2014), PRA 91, 033611 (2015)

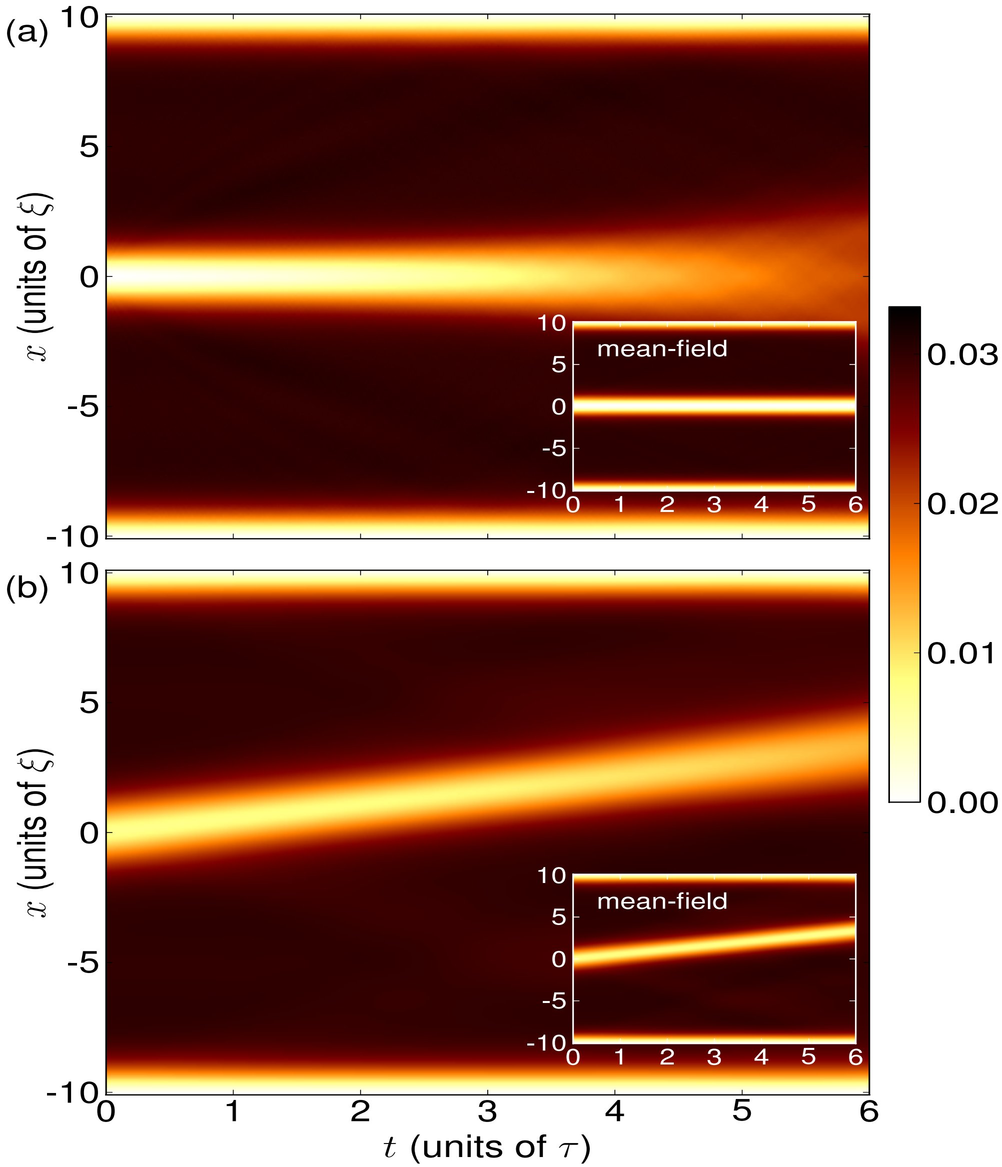
5. Many-body processes in black and grey matter-wave solitons

Setup and preparation

- N weakly interacting bosons in a one-dimensional box
- Initial many-body state: Little depletion, density and phase as close as possible to dark soliton in the dominant natural orbital
- Preparation: Robust phase and density engineering scheme.

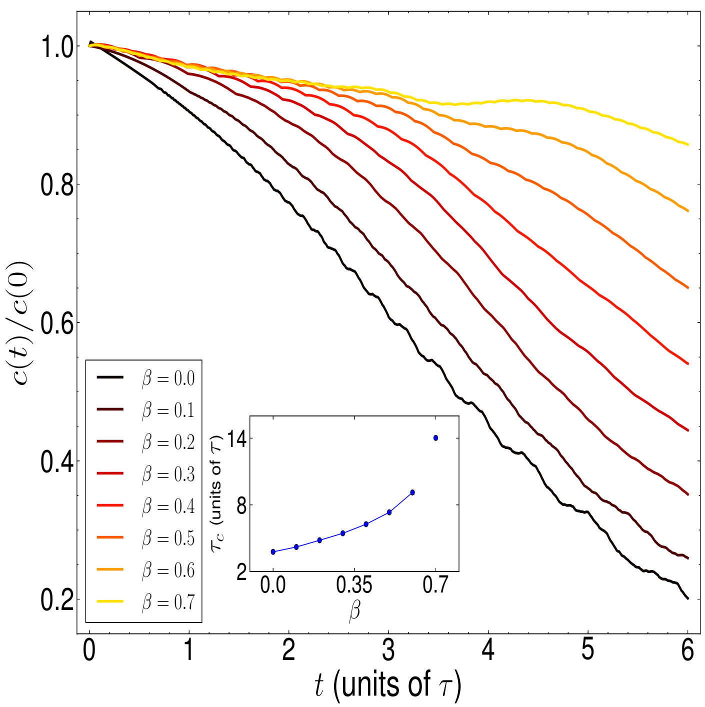
  CARR ET AL, PRL 103, 140403 (2009); PRA 80, 053612 (2009); PRA 63, 051601 (2001); RUOSTEKOSKI ET AL, PRL 104, 194192 (2010)

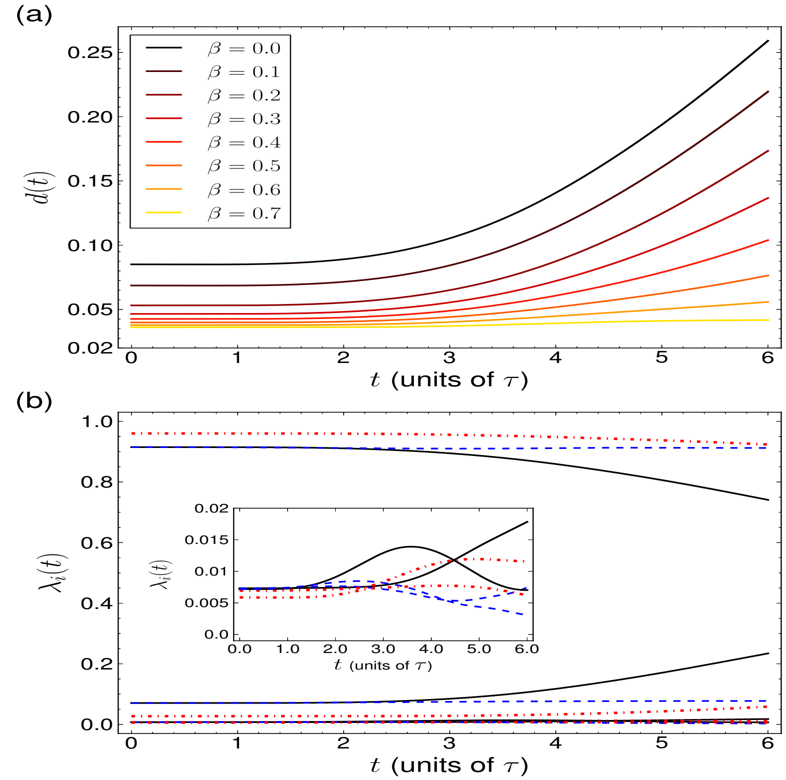
Density dynamics



- Reduced one-body density $\rho_1(x,t)$
- $N = 100$, $\gamma = 0.04$
- Black (top) and grey (bottom) soliton
- $M = 4$ optimized orbitals
- Inset: Mean-field theory (GPE)
- Slower filling process of density dip for moving soliton

Evolution of contrast and depletion

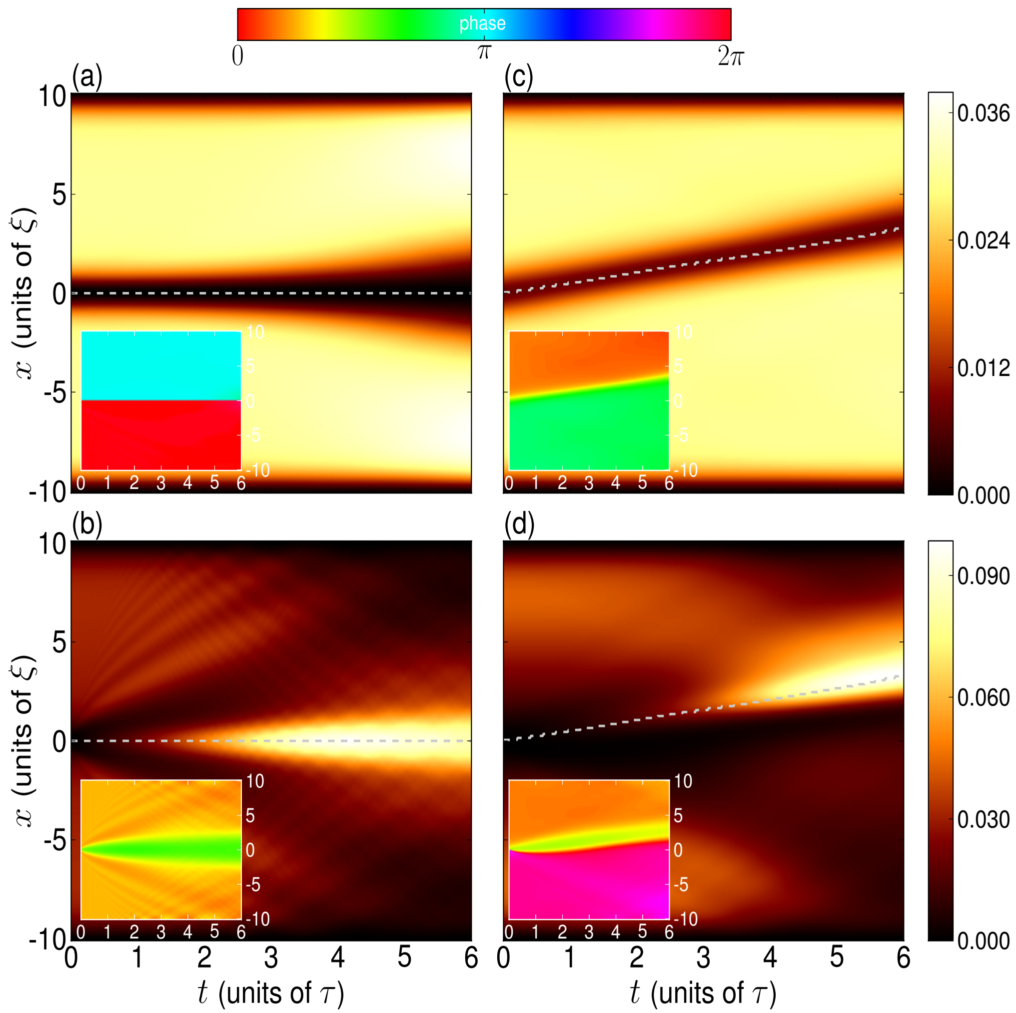




- Relative contrast $c(t)/c(0)$ of dark solitons for various $\beta = \frac{u}{s}$ $\left(c(t) = \frac{\max \rho_1(x,0) - \rho_1(x_t^s,t)}{\max \rho_1(x,0) + \rho_1(x_t^s,t)}\right)$

- Dynamics of quantum depletion $d(t) = 1 - \max_i \lambda_i(t) \in [0,1]$ and evolution of the natural populations $\lambda_i(t)$ for $\beta = 0.0$ (solid black lines) and $\beta = 0.5$ (dashed dotted red lines). $\hat{\rho}_1(t) = \sum_{i=1}^{M} \lambda_i(t)\, |\varphi_i(t)\rangle\langle\varphi_i(t)|$

Natural orbital dynamics

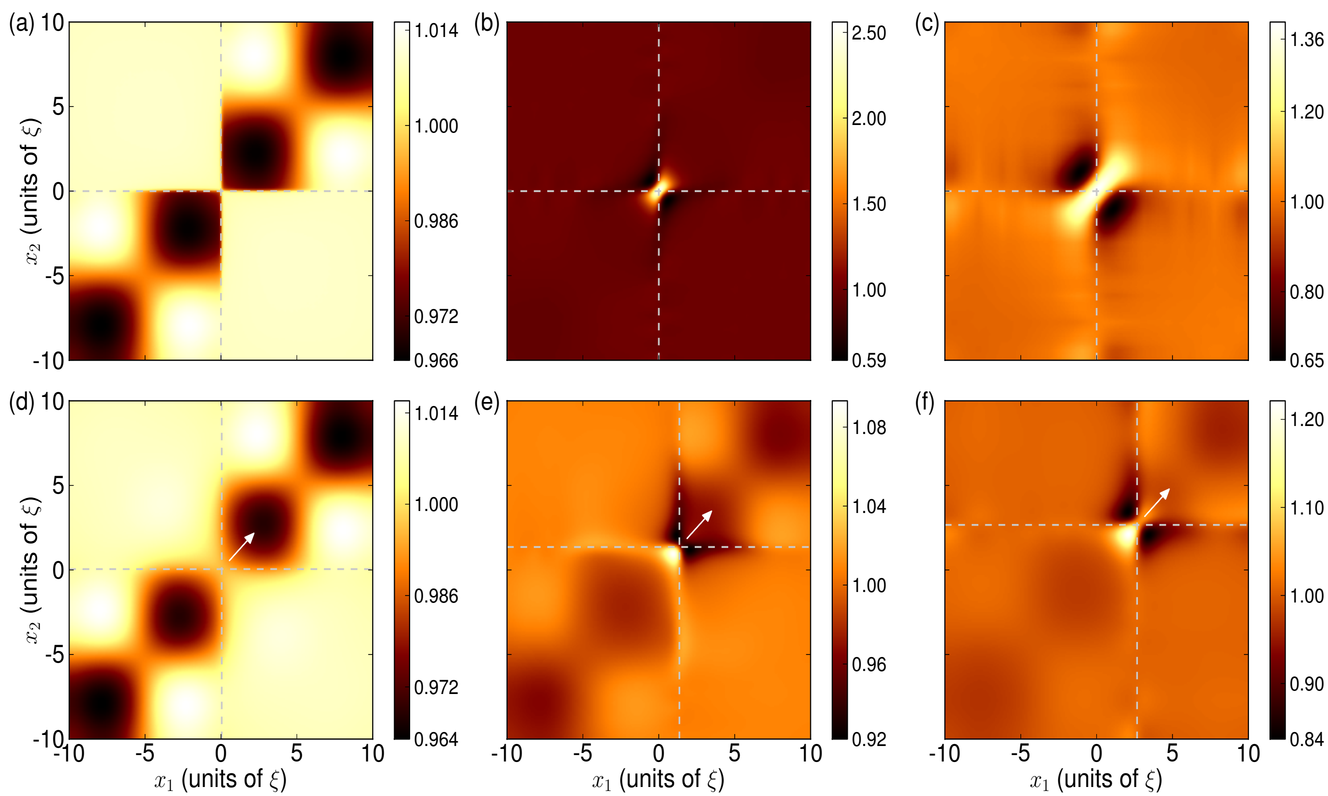


- Density and phase (inset) evolution of the dominant and second dominant natural orbital. (a,b) black soliton (c,d) grey soliton $\beta = 0.5$.

Localized two-body correlations

- Two-body correlation function $g_2(x_1, x_2; t)$ for a black soliton (first row) and a grey soliton $\beta = 0.5$ (second) at times $t = 0.0$ (first column), $t = 2.5\tau$ (second) and $t = 5\tau$ (third).

S. Krönke and P.S., PRA 91, 053614 (2015)



6. Atom-ion hybrid systems: Structure and dynamics

Experiment:

- B. Ruff, T. Kroker, J. Franz, T. Lampe, M. Neundorf, J. Simonet, P. Wessels, K. Sengstock and M. Drescher

Theory:

- J. Schurer, A. Negretti and P. Schmelcher

Motivation

Focusing on the physics of ions in a gas of trapped ultracold atoms: Hybrid atom-ion systems.

- Controlled state-dependent atom-ion scattering
- Novel tunneling and state-dependent transport processes
- Spin-dependent interactions
- Emulate condensed matter systems on a finite scale, including dynamics: polarons, charge-phonon coupling, ... PRL 111, 080501 (2013)
- Mesoscopic molecular ions and ion-induced density bubbles - PRL 89, 093001 (2002); PRA 81, 041601 (2010)

Challenges and Developments

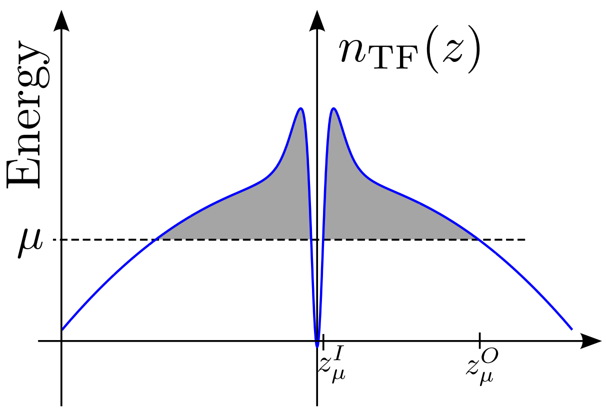
- Atom-ion interaction introduces an additional length scale $R^* = \sqrt{\frac{2C_4\mu}{\hbar^2}}$
- 'Molecular' bound states

- Our toolbox: ML-MCTDHB
- Modelling of ultracold atom-ion collisions:
  - Quantum defect theory links defect parameters to asymptotic scattering properties: Covering a broad range of scattering behaviour
  - Model potential: $V(z) = V_0 e^{-\gamma z^2} - \frac{1}{z^4 + \frac{1}{\omega}}$

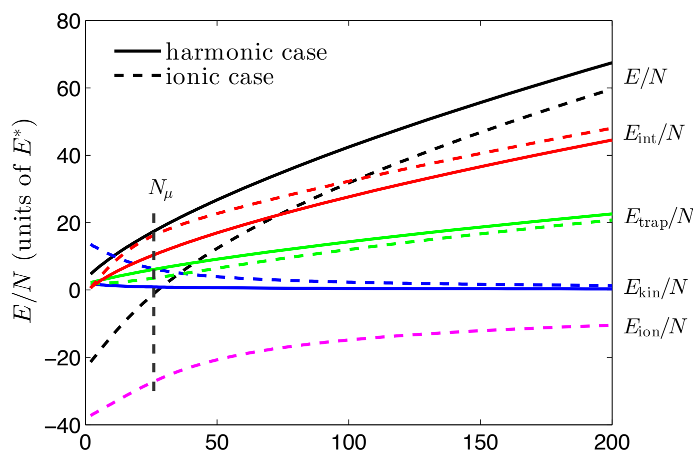
First: Static strongly trapped ion

Ground state of a localized ion in a cloud of ultracold atoms in a harmonic trap

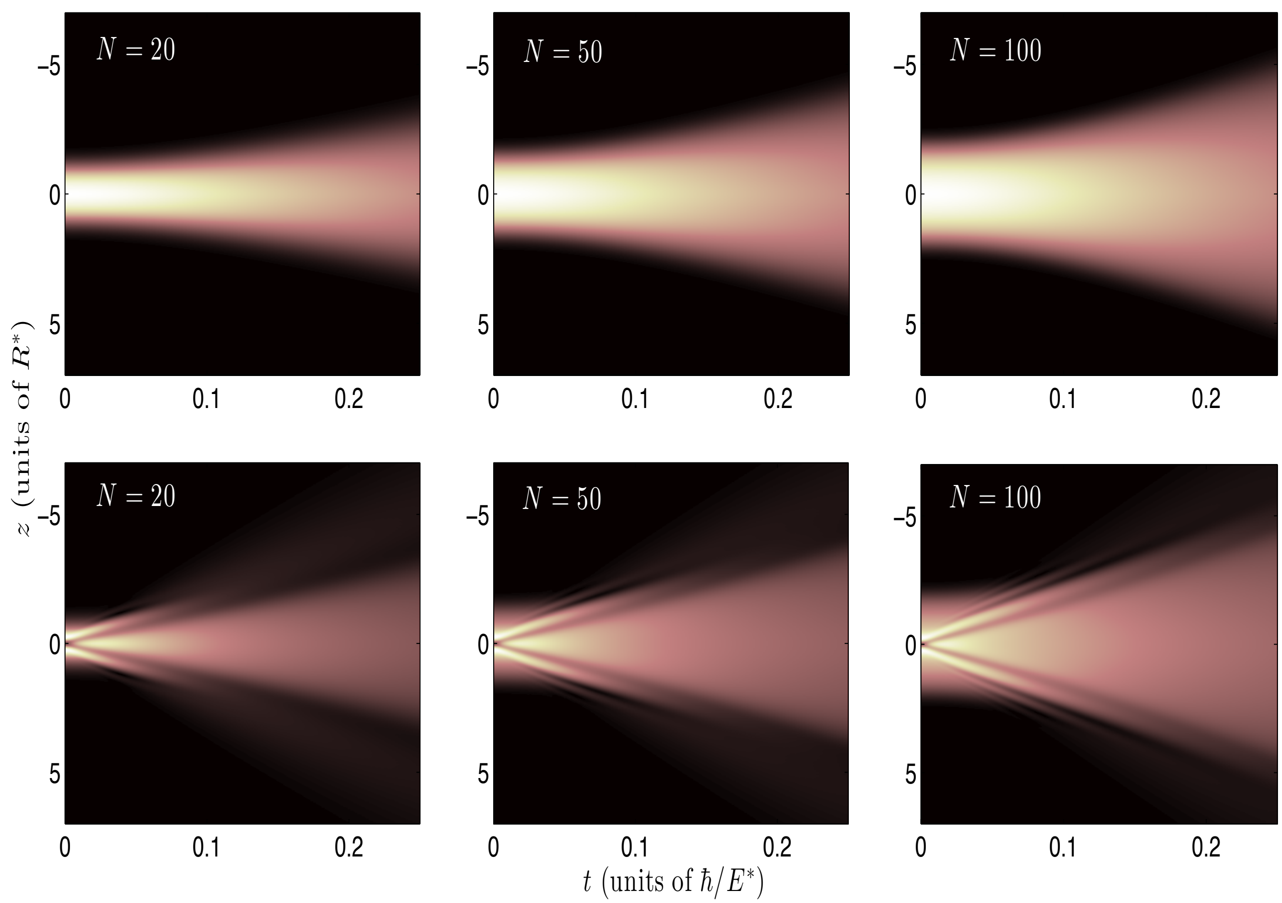
J. SCHURER ET AL, PRA 90, 033601 (2014)



Thomas-Fermi profile



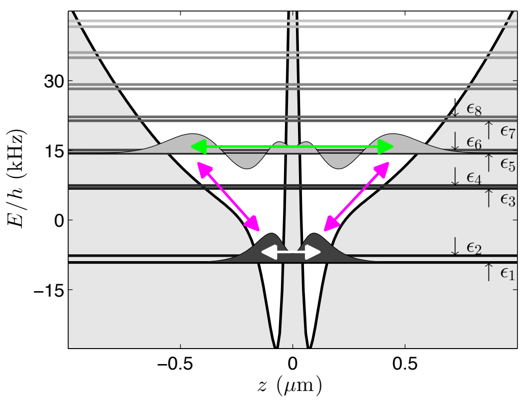
Energetical contributions



Expansion dynamics of the density

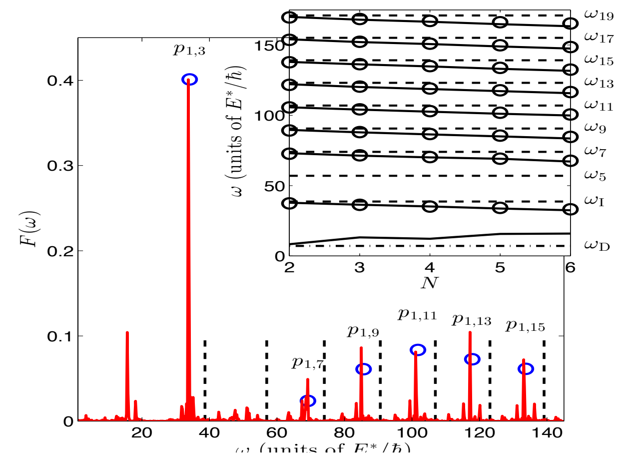
Next: Sudden creation of the ion

Laser pulse creates an ion immersed into a bosonic ensemble of atoms



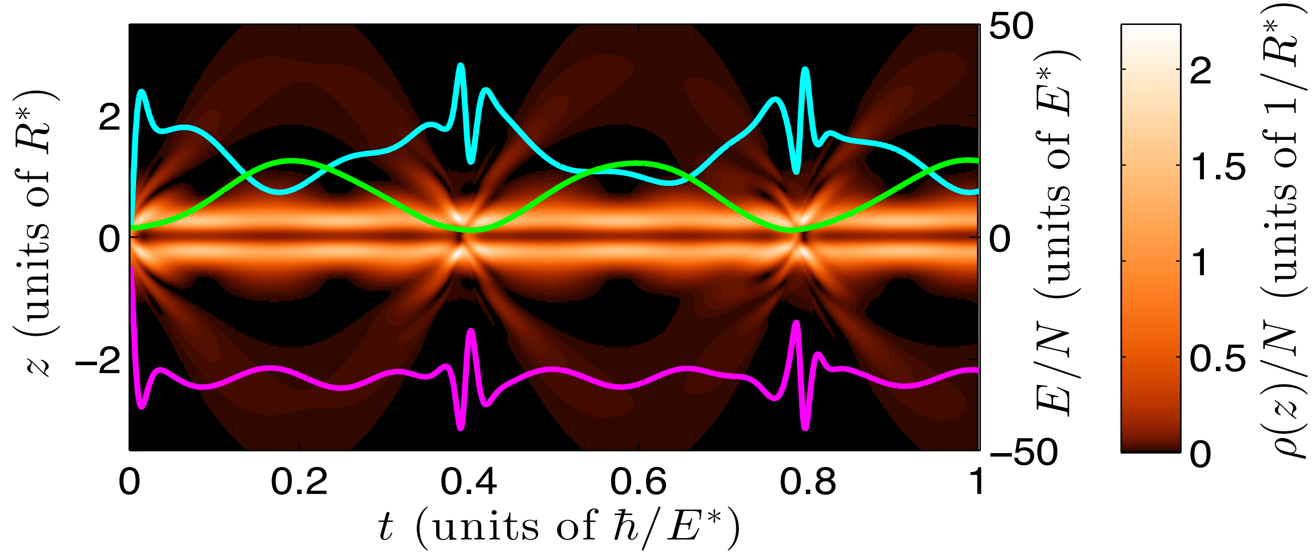
Effective potential, ion-bound

and trap states



Excitation spectrum

J. Schurer et al, NJP 17, 083024 (2015)



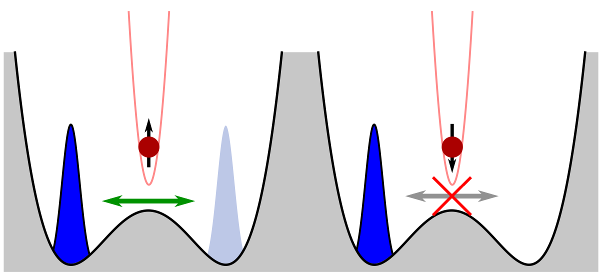
Time evolution of the density and energies per particle

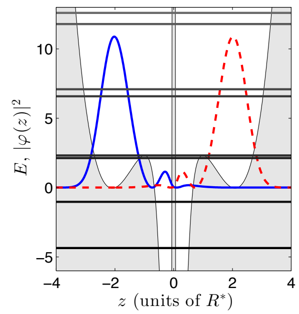
Recent progress: Background

Impact of many-body correlations on the dynamics of an ion-controlled bosonic Josephson junction

Bosonic Josephson junction: Rabi oscillations versus macroscopic quantum self-trapping - suppression of tunneling.

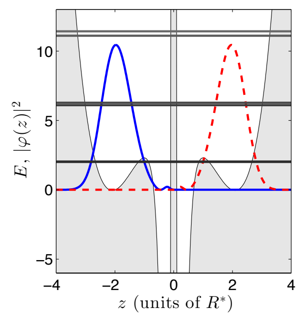
Add an ion: Coupling between the wells can be controlled by the ionic spin state. Ion-bosons entanglement.





R. GERRITSMA ET AL, PRL 109, 083024 (2012)

Unknown impact of many-body correlations on this process !

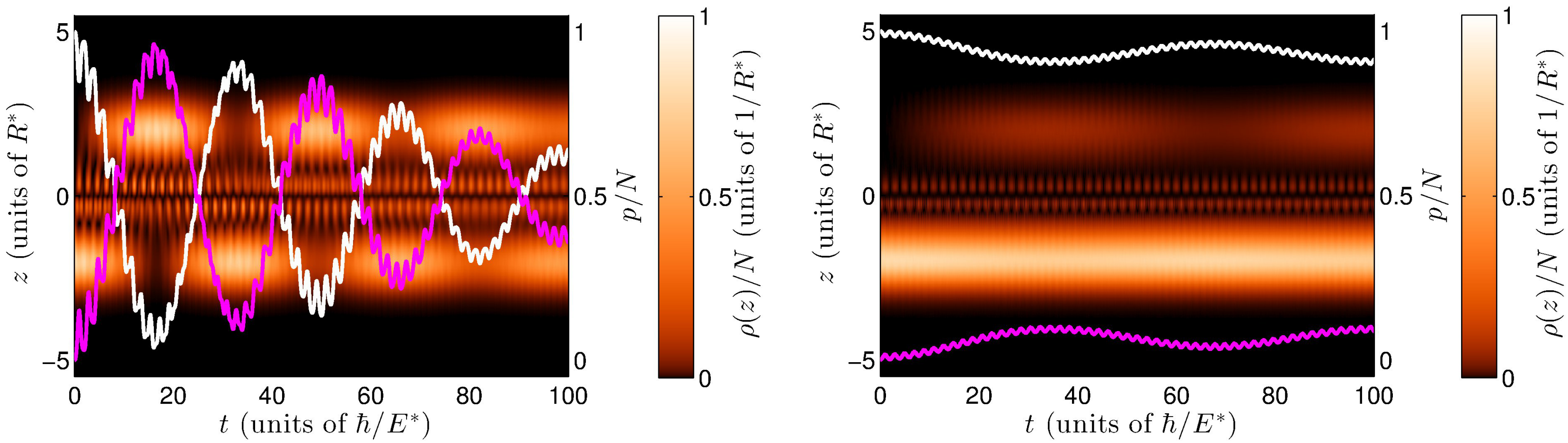


Ion controlled bosonic Josephson junction

Controlled tunneling dynamics for the many-body interacting case: Bosonic ensemble is chosen in the self-trapping regime.

Tunneling regime
Ion state 1

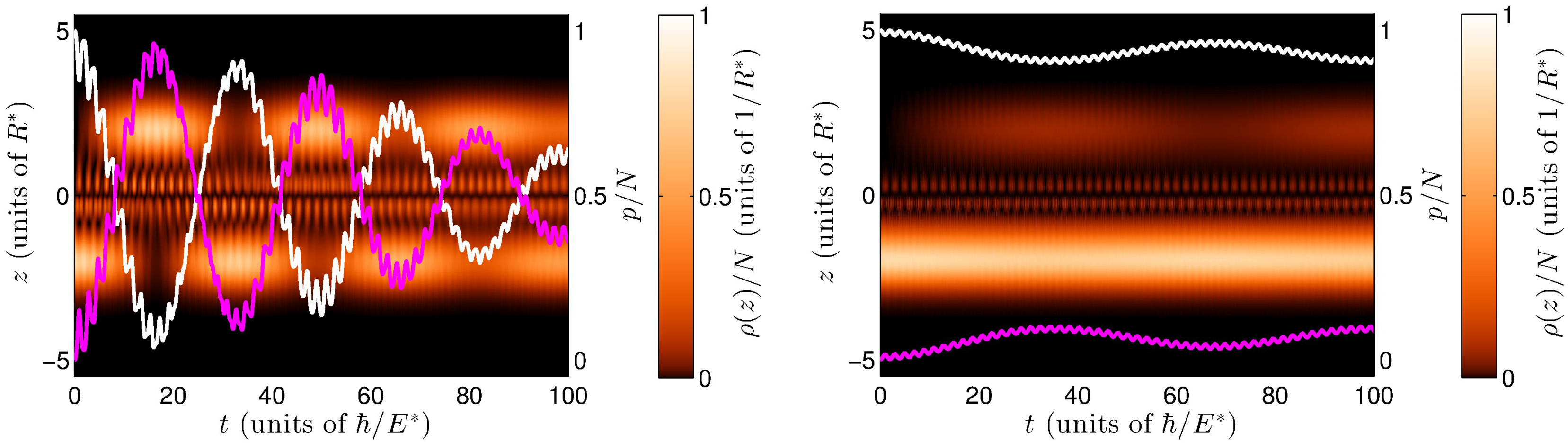
Self-trapping regime
Ion state 2



One-body density $\rho(z,t)$ as well as left well p_L and right well p_R occupation

- Principally: Ion-controlled BJJ is still operational

Ion controlled bosonic Josephson junction

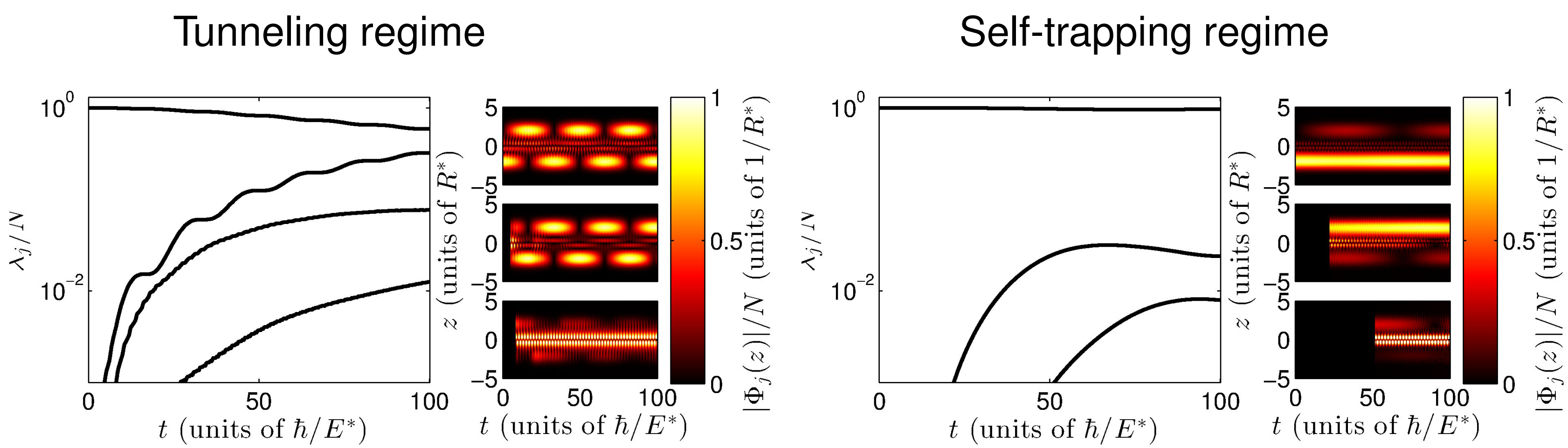


One-body density $\rho(z,t)$ as well as left well p_L and right well p_R occupation

- Major interaction effects present:
  - Damping of low frequency oscillations (collapse and revival): Singlet analysis with two relevant modes.
  - Fast frequency oscillations: In p_L and p_R, mostly due to the ion-bound component. Many modes participate.

Ion controlled bosonic Josephson junction

Build up of correlations: Natural population analysis indicates degree of fragmentation !



Hierarchy of natural orbitals

J. SCHURER, PRA 93, 063602 (2016); HIGHLIGHTED

1. Orbital: Expected TR and STR behaviour
2. Orbital: Mirror image
3. Orbital: Ion bound state dominated contribution

$\Rightarrow$ Entanglement protocol !

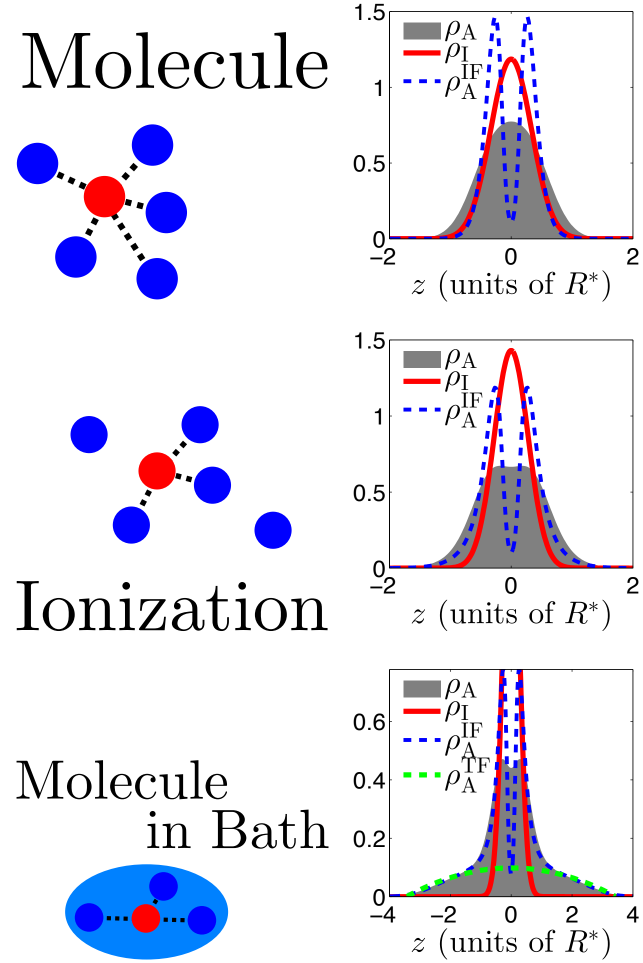
In progress: Mesoscopic charged molecules in a BEC

Challenges:

- Include Motion of Ion
- Many-Body Bound States

Main Observations:

- Formation of Ionic Molecule
- Stabilizing by Shell-Structure Formation
- Dissociation
- Strong Self-Localization of Ion
- Formation of Thomas-Fermi Bath



7. Concluding remarks

Conclusions

- ML-MCTDHB is a versatile efficient tool for the nonequilibrium dynamics of ultracold bosons.
- Few- to many-body systems can be covered: Shown here for the emergence of collective behaviour.
- Many-mode correlation dynamics: From quench to driving.
- Beyond mean-field effects in nonlinear excitations.
- Open systems dynamics, impurity and polaron dynamics, etc.
- Mixtures !

Thank you for your attention !