Correlated Quantum Dynamics of Ultracold Bosons: From Few- to Many-Body Systems

Peter Schmelcher
Zentrum für Optische Quantentechnologien
Universität Hamburg

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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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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

$\Rightarrow$ **Matter wave physics has been and still is a rapidly developing field with an extremely rich diversity !**

DIFFERENT DIRECTIONS (INCOMPLETE !):

- Atom laser
- Nonlinear excitations: Solitons, vortices etc.
- Quantum phase transitions (Mott insulator, Kosterlitz-Thouless,...) and superfluidity
- Various directions in strongly interacting systems: Disorder, correlations, 'exotic' lattices, etc.
- Ultracold spinor gases, Fermi gases, Bose-Fermi mixtures
- Quantum simulations
- Single atom control and processing
- Quantum information processing
- Ultracold molecules
- Ultracold Rydberg atoms
- First applications: Sensoring of magnetic fields and accelerations,...

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

Hamiltonian: $\mathcal{H} = \sum_i \left(\frac{\mathbf{p}_i^2}{2m_i} + V(\mathbf{r}_i) \right) + \frac{1}{2} \sum_{i,j,i \neq j} W(\mathbf{r}_i - \mathbf{r}_j)$

V is the trap potential: harmonic, optical lattice, etc.

W describes interactions: contact $g\delta(\mathbf{r}_i - \mathbf{r}_j)$, dipolar, etc.

Dynamics is governed by TDSE: $i\hbar\partial_t \Psi(\mathbf{r}_1, ..., \mathbf{r}_N, t) = \mathcal{H}\Psi(\mathbf{r}_1, ..., \mathbf{r}_N, t)$

Ideal Bose-Einstein condensate: no interaction $g = 0 \Rightarrow$ Macroscopic matter wave.

$$\Phi(\mathbf{r}_1, ..., \mathbf{r}_N) = \prod_{i=1}^{N} \phi(\mathbf{r}_i)$$

Hartree product: bosonic exchange symmetry.

Interaction $g \neq 0$: Mean-field description leads to Gross-Pitaevskii equation with cubic nonlinearity, exact for $N \to \infty, g \to 0$.

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

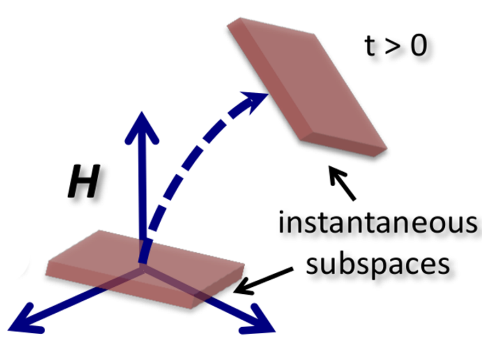
Multi-Layer Multi-Configuration Time-Dependent Hartree for Bosons (ML-MCTDHB) is a significant step in this direction !

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



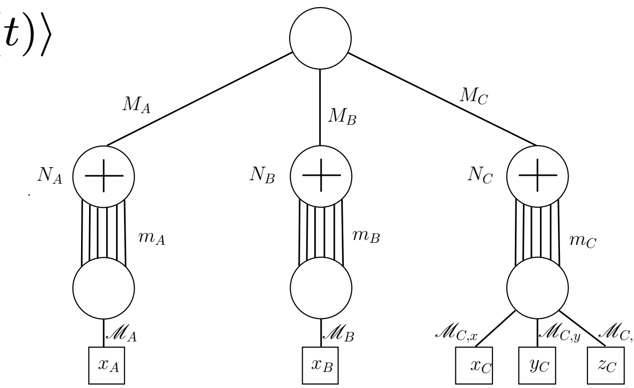
Hierarchy within ML-MCTDHB

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:

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

$\Rightarrow$ 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. Tunneling mechanisms in the double and triple well

Few-boson systems - Perspectives

- Extensive experimental control of few-boson systems possible: Loading, processing and detection

  [I. Bloch *et al*, Nature **448**, 1029 (2007)]
- Bottom-up understanding of tunneling processes and mechanisms
- Atomtronics perspective providing us with controllable atom transport on individual atom level:
  - Diodes, transistors, capacitors, sources and drains
- Double well, triple well, waveguides, etc.

Symmetric Double Well

General remarks

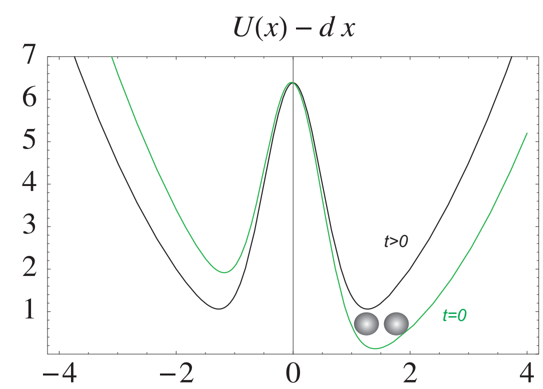
- DW: Paradigm for fundamental quantum process: Tunneling !
- Bose-Einstein condensates
  - Observation of Josephson oscillations (Milburn 1997, Albiez 2005, Smerzi 1997)
  - Nonlinear self-trapping (Albiez 2005, Anker 2005, Javanainen 1986)
- Optical lattices
  - Repulsively bound atom-pairs moving in a lattice (Winkler, 2006)
  - Mechanism: First and second order tunneling (Fölling, 2007)
- Above addresses exclusively the weak interaction regime

What about the few-body tunneling dynamics as we follow the pathway from weak to strong interactions ?

From Uncorrelated to Pair Tunneling

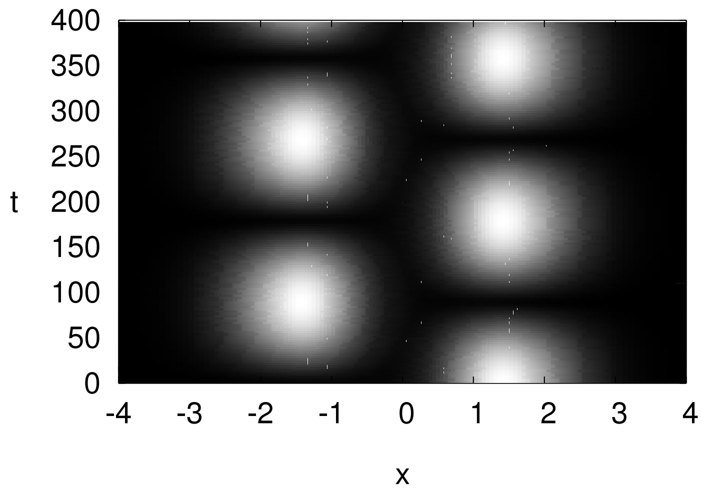
Setup and Perspective

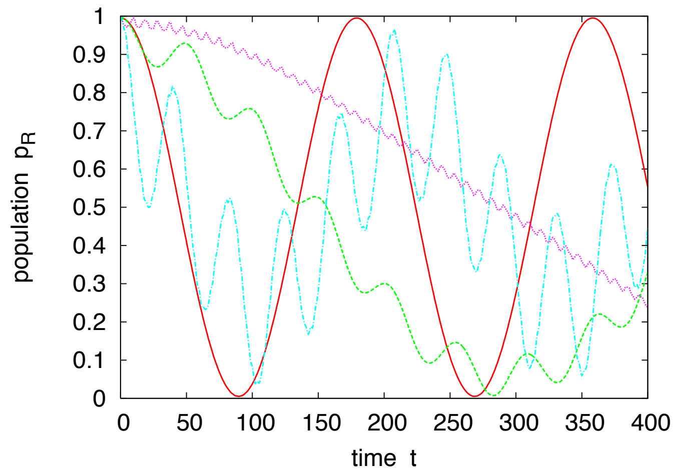
- Preparation of the initial state $\Psi(0)$ with a population imbalance
  - Add a linear external potential and let the system relax to its ground state $\Psi_0^{(d>0)}$
  - Ramp down asymmetry d to $d(t) \rightarrow 0$ nonadiabatically
- Conceptually clearest situation: $N = 2$ atoms, tunneling versus few-body spectrum versus two-body correlations
- More complicated dynamics of $N = 3, 4, \ldots$ atoms



From Uncorrelated to Pair Tunneling

Overview of Features

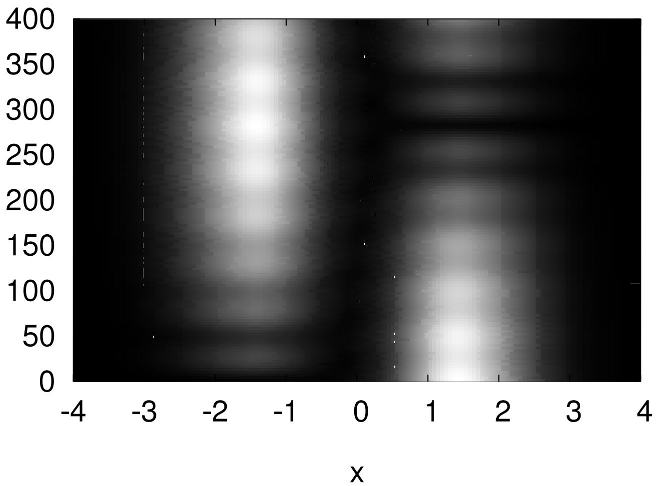


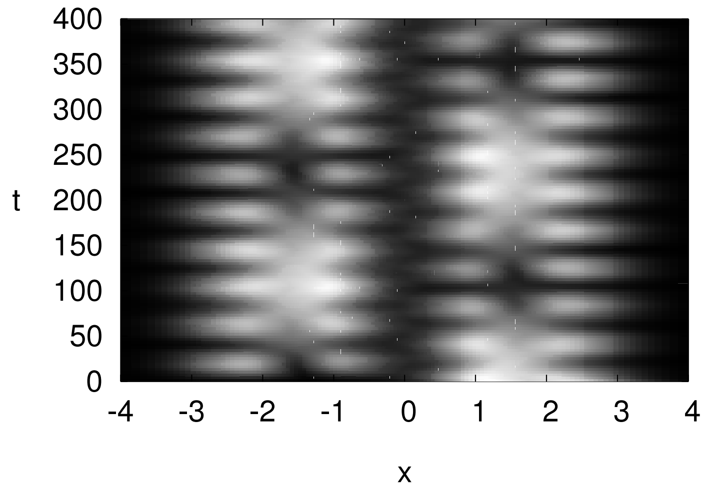


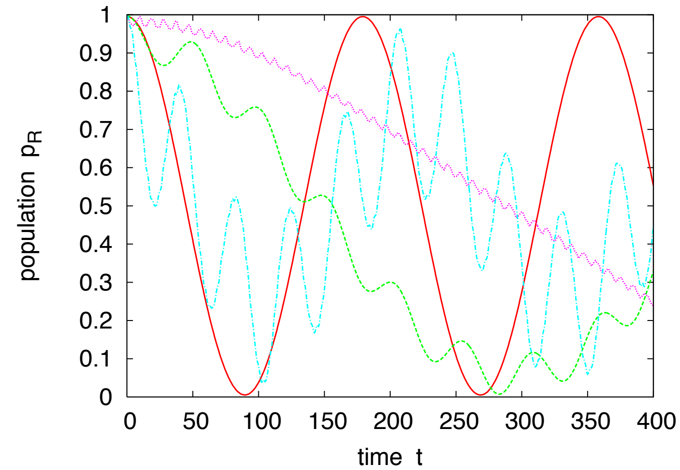
- $g = 0$: Atoms *Rabi*-oscillate between wells monitored by $p_{\mathrm{R}}(t) = \langle \Theta(x) \rangle_{\Psi(t)} = \int_0^\infty \rho(x;t)dx$ or the population imbalance $\delta = p_{\mathrm{R}} - p_{\mathrm{L}} = 2p_{\mathrm{R}} - 1$.
- p_{R} harmonically oscillates between 1 and 0.

From Uncorrelated to Pair Tunneling

Overview of Features



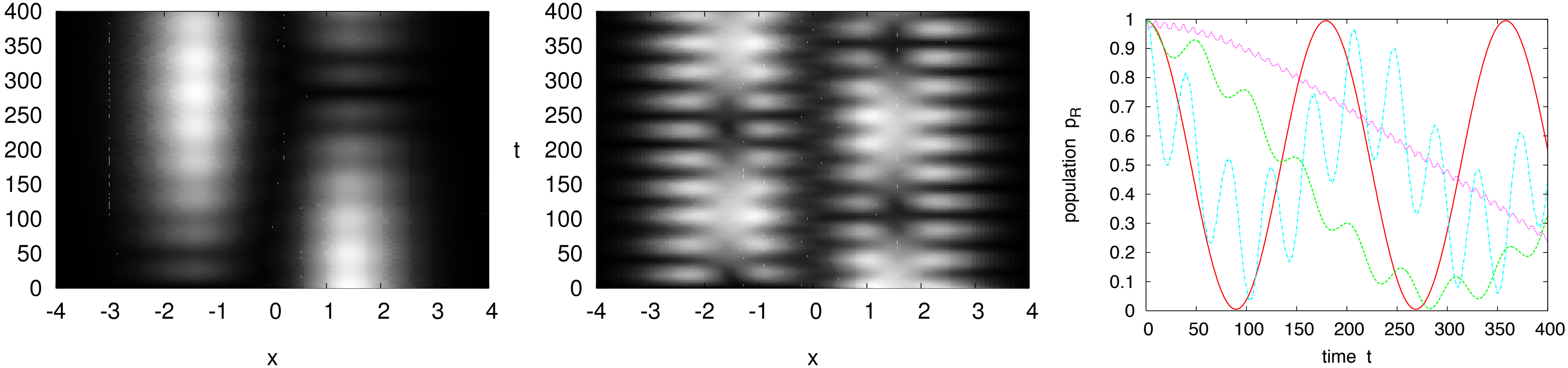




- $g = 0.2$ - Naive expectation: Tunneling is enhanced due to repulsive interaction.
- Facts:
  - For short times: minute small amplitude oscillations
  - Complete population transfer on much longer time scales $T/2 \sim 300$
  - Tunneling oscillations have become a two-mode process.
- $g = 1.3$: Tunneling period becomes as large as 2×10^3: **Few-body analog of quantum self-trapping**

From Uncorrelated to Pair Tunneling

Overview of Features



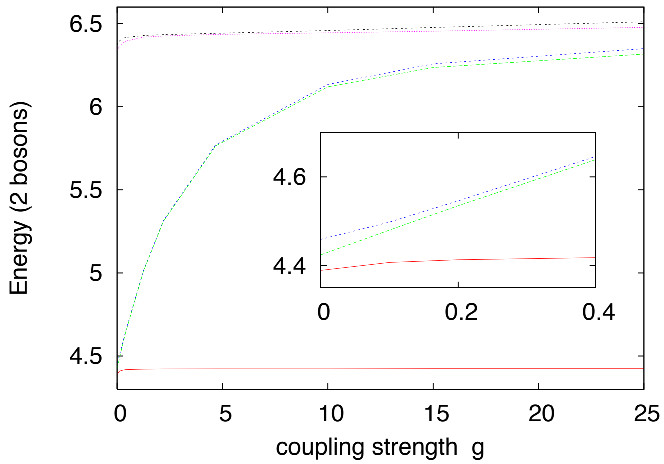
- $g = 4.7$: Time evolution becomes more complex: p_{R} doesnt capture this !
- $g = 25$ (near fermionization limit) again a simple picture: Tunneling with Rabi period is superimposed by a faster, large-amplitude motion. Strongly repulsive atoms coherently tunnel back and forth as a *fragmented pair*.

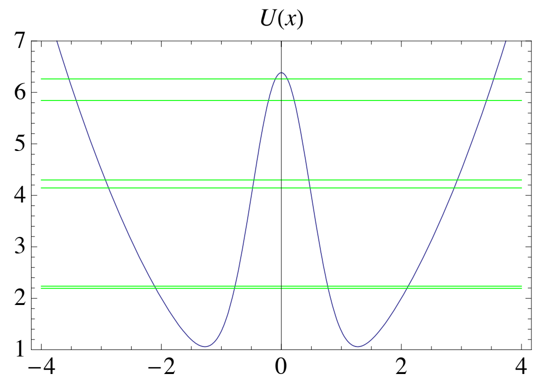
SPECTRAL ANALYSIS

Spectral Analysis

- Understanding of the very different time scales of the dynamics $\Leftrightarrow$ Analyze the evolution of the spectrum $\{E_m(g)\}$
- $g = 0$: Occupy lowest doublet $\Rightarrow N + 1$ energies $\{E_m = E_0 + m\Delta^{(0)} \mid m = 0, \ldots, N\}$ with energy gap (width of lowest band) $\Delta^{(0)} = \epsilon_1^{(0)} - \epsilon_0^{(0)}$

Spectral Analysis



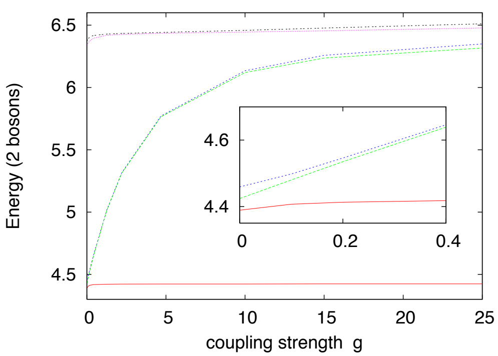


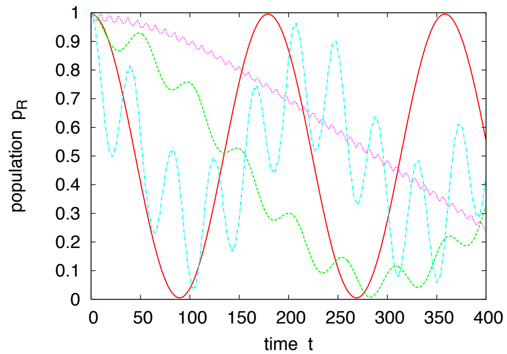
- Small g: Lowest band approximation
  - $\Psi(t) = \sum_m e^{-iE_m t} c_m \Psi_m \Rightarrow$ Imbalance $\delta(t) \equiv \langle \Theta(x) - \Theta(-x) \rangle_{\Psi(t)}$ gives

$$\delta(t) = \delta^{(01)} \cos(\omega_{01} t) + \delta^{(12)} \cos(\omega_{12} t)$$

    $\omega_{mn} = E_m - E_n$ and $\delta^{(mn)} = 4 \langle \Psi_m | \Theta(x) | \Psi_n \rangle c_m c_n$
    Note: $(mn) = (02)$-contribution vanishes due to symmetry.
  - $g = 0$: Single mode with Rabi frequency $\omega_{01} = \omega_{12} = \Delta^{(0)}$
  - $g \gtrsim 0$ Equidistance is lifted: Additional small beat frequency $\omega_{01} - \omega_{12}$
  - Further increasing g: Upper $E_{1,2}(g)$ form a neardegenerate doublet and the gap to E_0 increases

Spectral Analysis



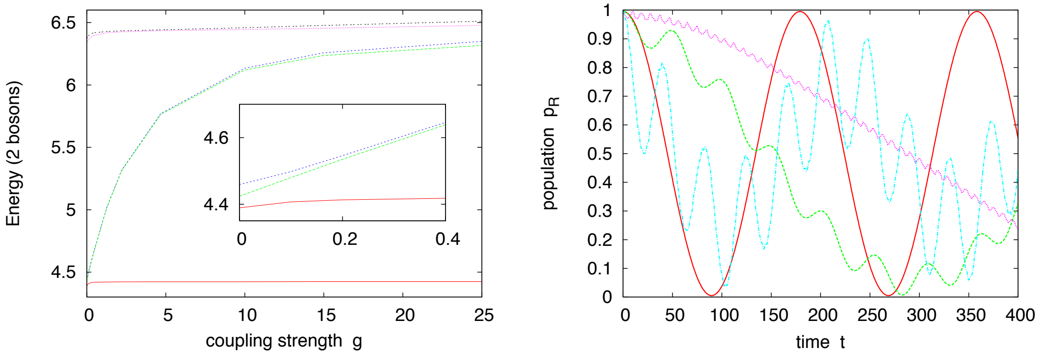


- Small g: Lowest band approximation with Imbalance

$$\delta(t) = \delta^{(01)} \cos(\omega_{01} t) + \delta^{(12)} \cos(\omega_{12} t)$$

- For $t \ll T_{12} \equiv 2\pi/\omega_{12}$, we only see an oscillation period $T_{01} \ll T_{12}$, offset by $\delta^{(12)}$.
- Longer timescale: *Slow* tunneling of period T_{12} modulated by T_{01} oscillations.
- Small initial imbalances: $\left|\delta^{(01)}/\delta^{(12)}\right| \propto |c_0/c_2| \gg 1$; i.e. for short times we observe the few-body analog of Josephson tunneling
- Almost complete imbalance: $|\delta^{(12)}|$ dominates $\Rightarrow$ Extremely long tunnling times ($\Leftrightarrow$ *self-trapping*)
- *Ab initio* picture for the few-body counterpart of the crossover from Rabi oscillations to self-trapping.

Spectral Analysis



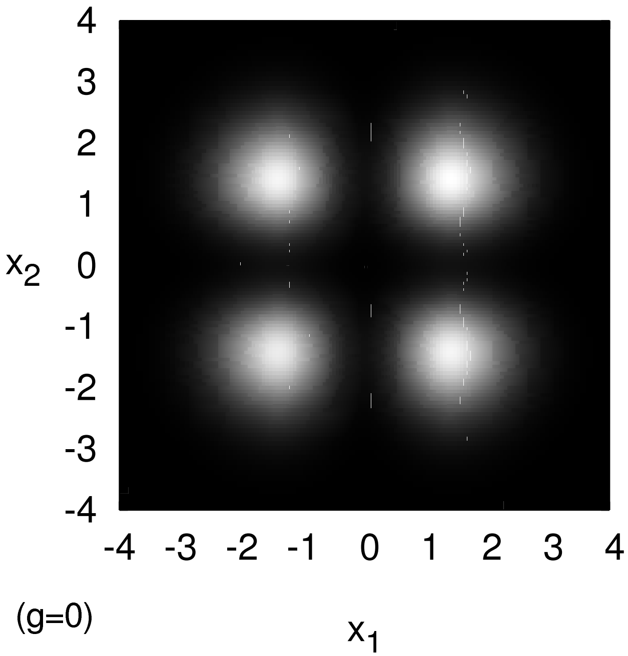
- Stronger Interactions g: Two-frequency description breaks down as the gap to higher-lying states melts.
  - Quasi-degenerate doublet will break up again: Imbalance dynamics: “self-trapping” scenario will give way to much shorter tunnel periods again.
  - States emerging from higher bands will be admixed: Multi-band dynamics. This most clearly manifests towards fermionization, $g = 25$
- $g \to \infty$: Free fermions. An analysis of the imbalance dynamics yields for two atoms: Only participating frequencies are $\Delta^{(0)}$ (the lowest-band Rabi frequency) and $\Delta^{(1)}$ (the larger tunnel splitting of the first excited band).
- Link of the strongly interacting dynamics to the noninteracting Rabi oscillations.

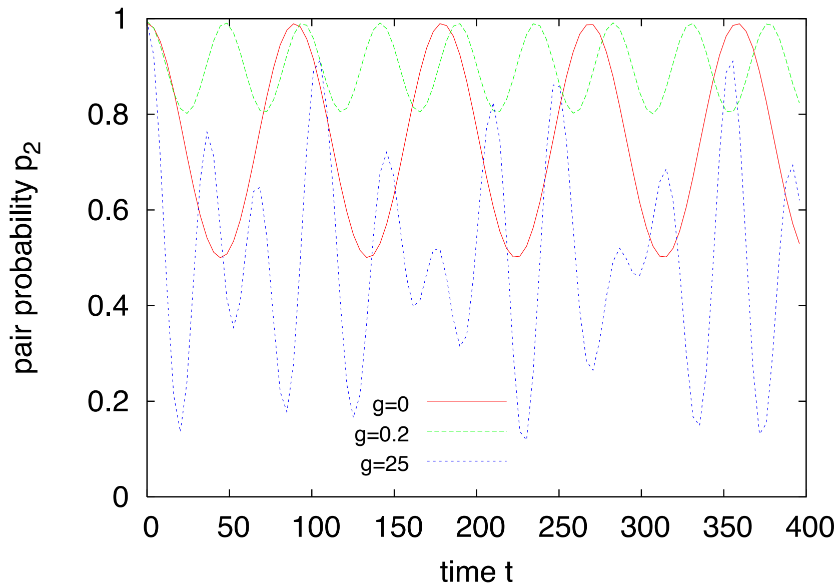
ROLE OF CORRELATIONS

Role of Correlations

Two-body correlation density $\rho_2(x_1, x_2; t_*)$ at equilibrium points t_*, for $g = 0$ $(t_* = 44)$

and pair probability $p_2(t) = \langle \Theta(x_1)\Theta(x_2) + \Theta(-x_1)\Theta(-x_2)\rangle_t$

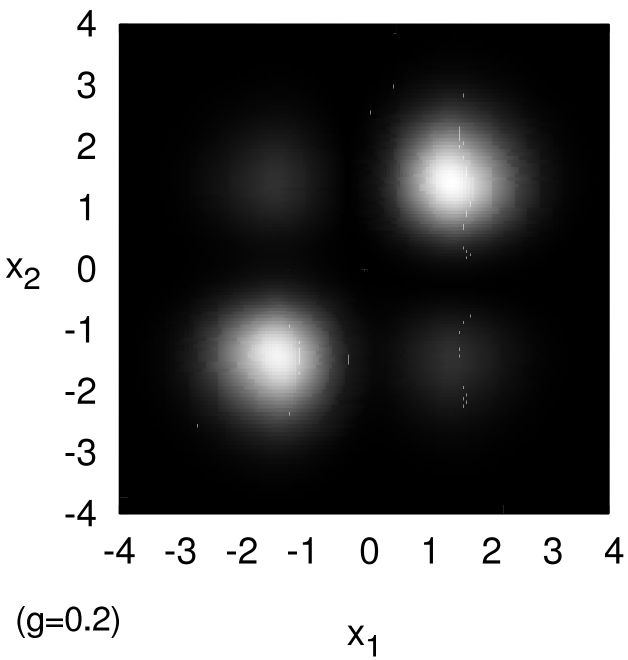


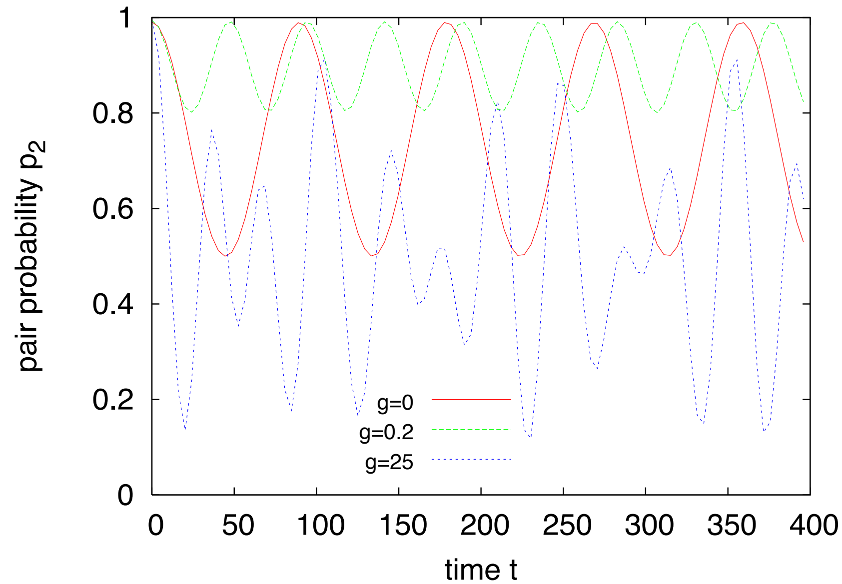


- $g = 0$: Noninteracting bosons tunnel independently: Starting in one well, at the equilibrium point ($p_{\mathrm{L,R}}(t_*) \stackrel{!}{=} \frac{1}{2}$), the probability for finding them in the same and different wells is equal.

Role of Correlations

$\rho_2(x_1, x_2; t_*)$ for $g = 0.2$ ($t_* = 128$) and $p_2(t)$

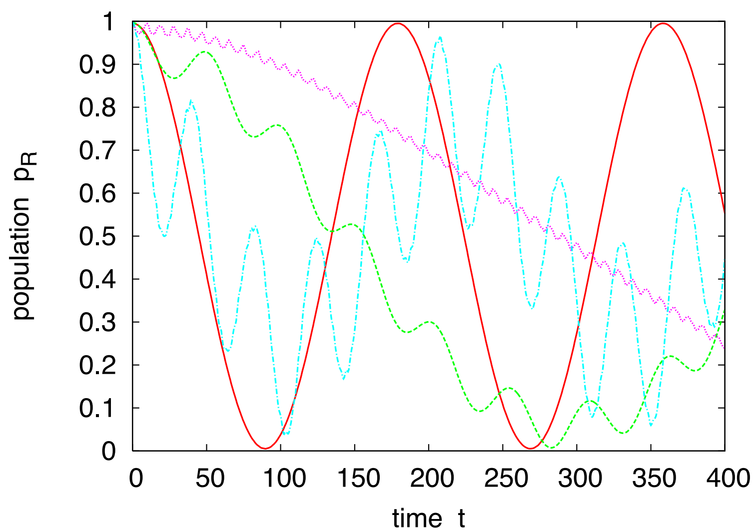


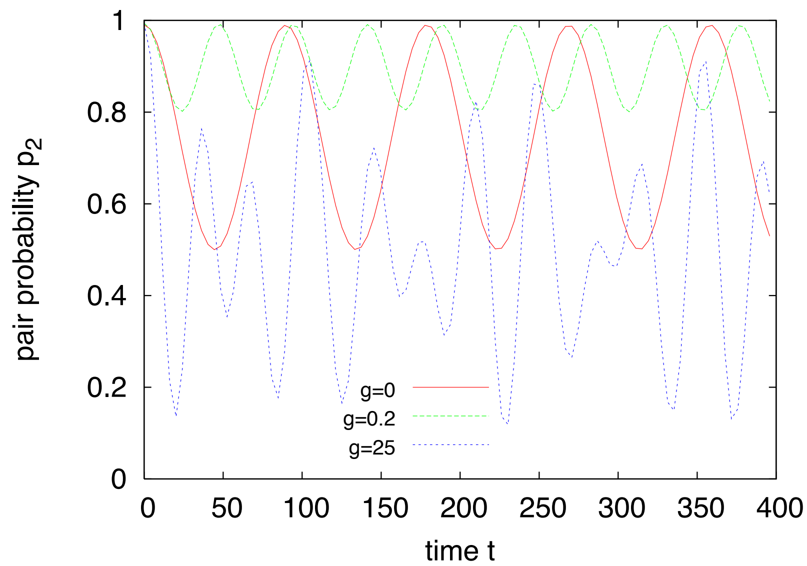


- Weak interactions: Pair probability stays close to 100%. Both atoms can essentially be found in the *same* well in the course of tunneling, *they tunnel as pairs*.
- In terms of eigenstate analysis: While the $g = 0$ eigenstates $\Psi_{1,2}$ are *delocalized*, at intermediate $g = 0.2$ they have basically evolved into superpositions $|N_\mathrm{L} = 2, N_\mathrm{R} = 0\rangle \pm |0, 2\rangle$ of pair states *localized in each well*. In this light, the dynamics solely consists in shuffling the population back and forth between these two pair states.

Role of Correlations

$\rho_2(x_1, x_2; t_*)$ for $g = 0.2$ ($t_* = 128$) and $p_2(t)$

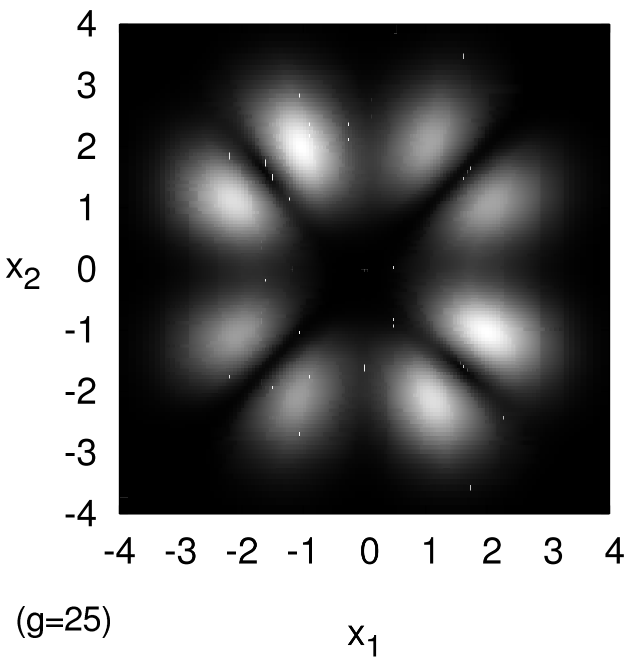


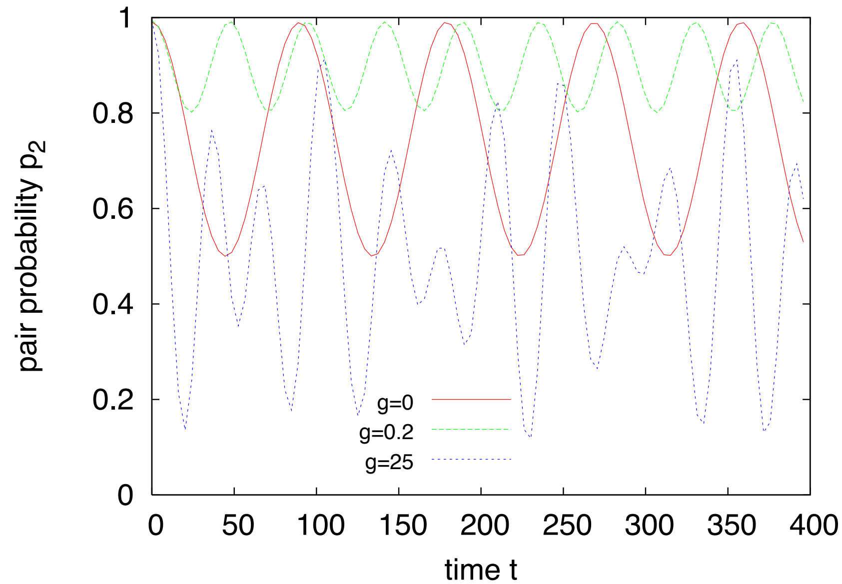


- Fast (small-amplitude) modulations of p_{R} encountered in are linked to temporary reductions of the pair number p_2: Attempted one-body tunneling.

Role of Correlations

$\rho_2(x_1, x_2; t_*)$ for $g = 25$ ($t_* = 53$) and $p_2(t)$





- $g = 25$: Two-body density pattern is fully fragmented, both in-well as well as at equilibrium point.
- Higher-band excited states also reflect in the evolution of $p_2(t)$, which is determined by the two modes $\omega_\pm = \Delta^{(0)} \pm \Delta^{(1)}$.
- p_2 passes through just about any value from 1 (pair) to almost zero (complete isolation). In analogy to free fermions, it is again tempting to understand this involved pattern as two fermions tunneling independently with different frequencies.

TRIPLE WELL

Triple Well: Interband Tunneling

Here: Bottom-up approach of understanding the tunneling mechanisms !

- Triple well is minimal system analog of a source-gate-drain junction for atomtronics
- Triple well shows novel tunneling scenarios $\Leftrightarrow$ Impact on transport
- Strong correlation effects beyond single band approximation !
- Beyond the well-known suppression of tunneling: Multiple windows of enhanced tunneling i.e. revivals of tunneling: Interband tunneling involving higher bands !

Setup, computational approach and analysis tool

Hamiltonian

$$H = \sum_{j=1}^{N} -\frac{\hbar^2}{2M}\partial_{x_j}^2 + \sum_{j=1}^{N} V_{tr}(x_j) + \frac{1}{2}\sum_{j\neq k} g_{1D}\delta(x_j - x_k)$$

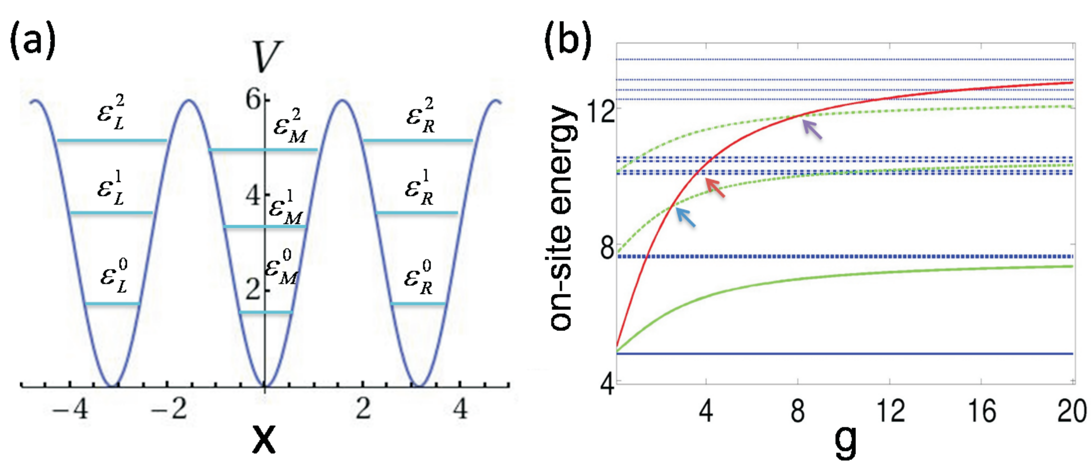
Number-state representation including interaction effects !

$$|\Psi\rangle = \sum_{\boldsymbol{N},i} C^i_{\boldsymbol{N}} |N_L, N_M, N_R\rangle_i$$

$$\langle \mathbf{x}|N_L, N_M, N_R\rangle_i = S\phi^i_{\boldsymbol{N}}(\mathbf{x} - \mathbf{r}_{\boldsymbol{N}})$$

$$\left(\sum_{j=1}^{N} -\frac{\hbar^2}{2M}\partial_{x_j}^2 + \sum_{j=1}^{N} W(x_j) + V_I(\mathbf{x})\right)\phi^i_{\boldsymbol{N}}(\mathbf{x}) = e^i_{\boldsymbol{N}}\phi^i_{\boldsymbol{N}}(\mathbf{x})$$

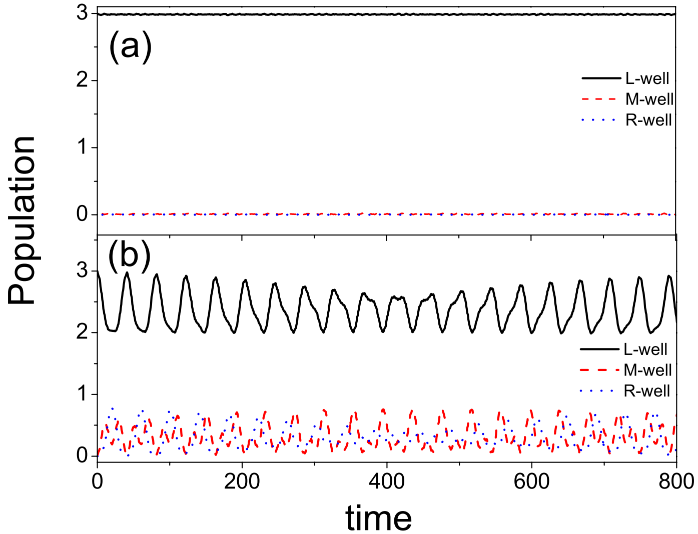
Three bosons: Single, pair and triple modes.



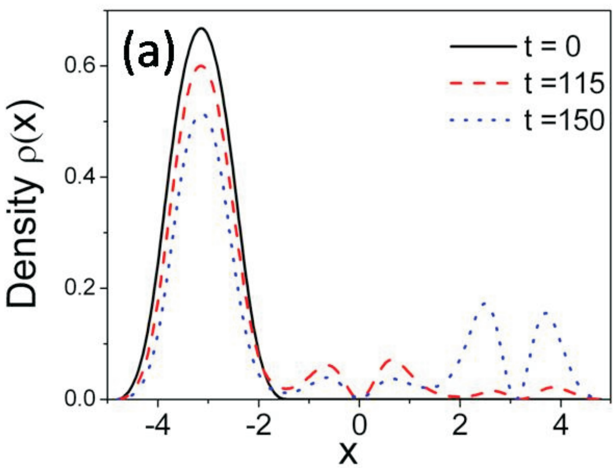
Interband Tunneling: Single boson tunneling

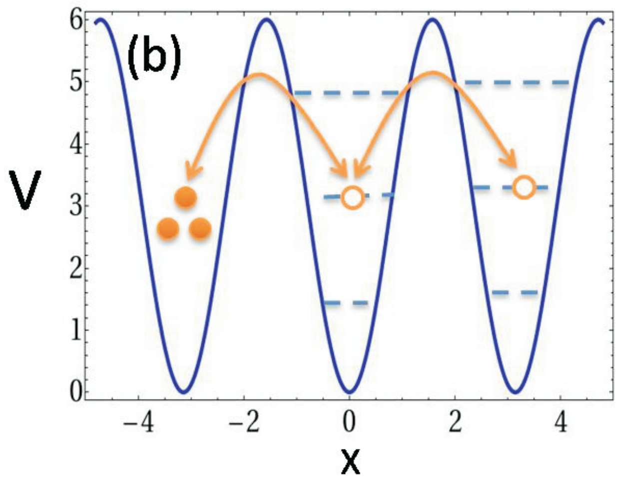
Three bosons initially in the left well: $\Psi \approx |3,0,0\rangle_0$

(a) $g = 0.1$ and (b) $g = 3.26$



Single boson tunneling to middle and right well via $|3,0,0\rangle_0 \Leftrightarrow |2,1,0\rangle_1 \Leftrightarrow |2,0,1\rangle_1$ i.e. via first-excited states !

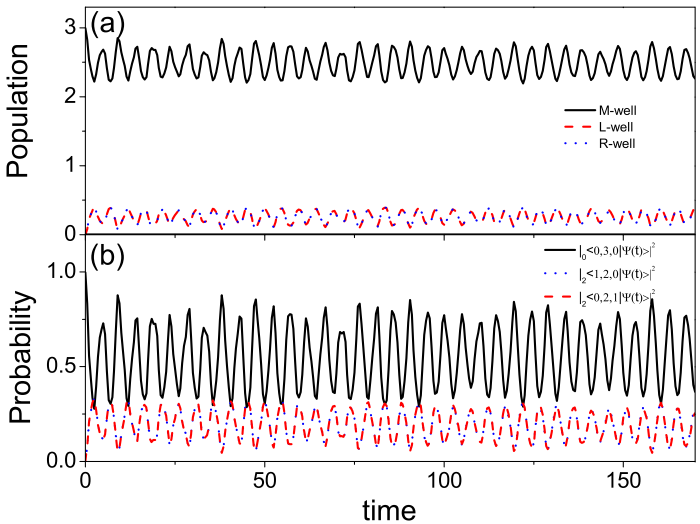




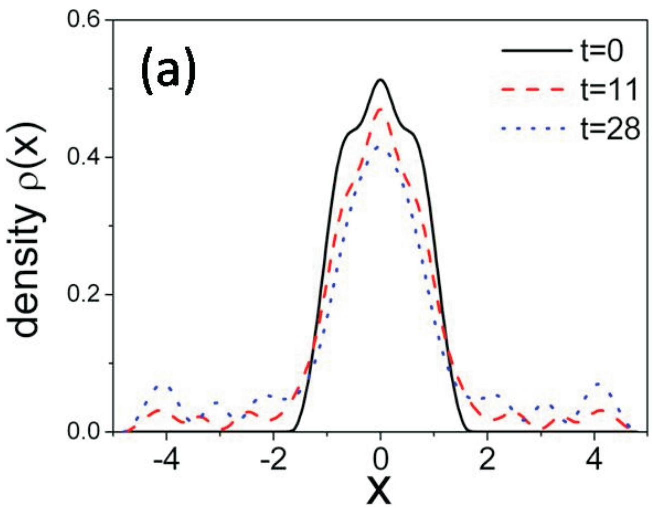
Interband Tunneling: Single boson tunneling

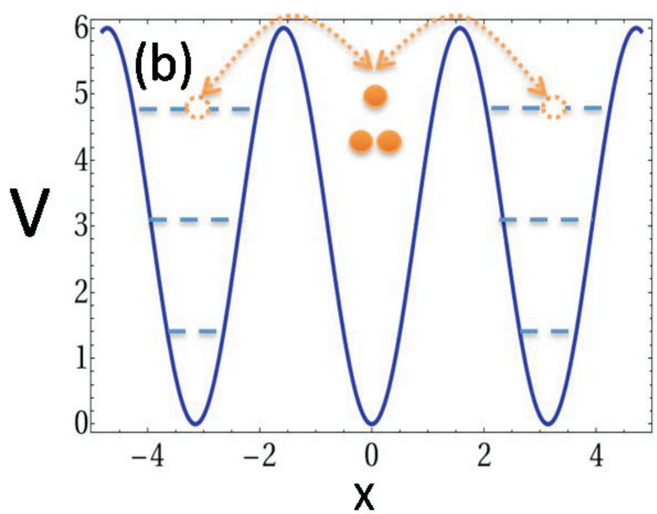
Three bosons initially in the middle well: $\Psi \approx |0,3,0\rangle_0$

(a) $g = 9.85$



Single boson tunneling to left and right well via $|0,3,0\rangle_0 \Leftrightarrow |1,2,0\rangle_3 \Leftrightarrow |0,2,1\rangle_3$ i.e. via second-excited states !

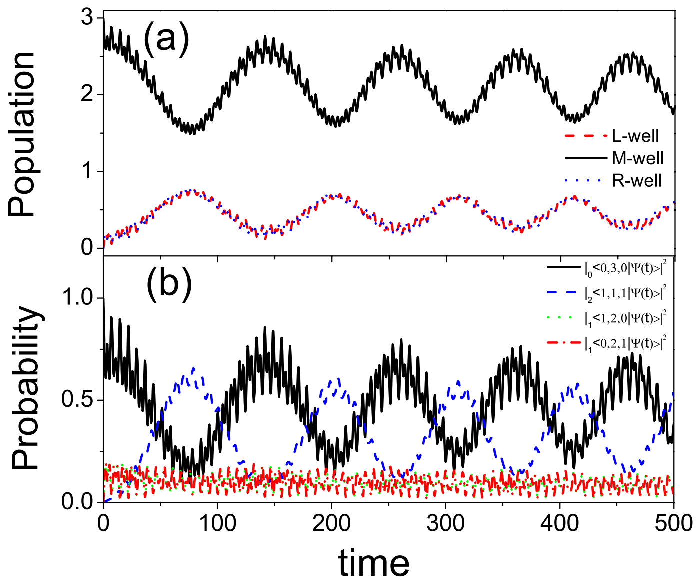




Interband Tunneling: Two boson tunneling

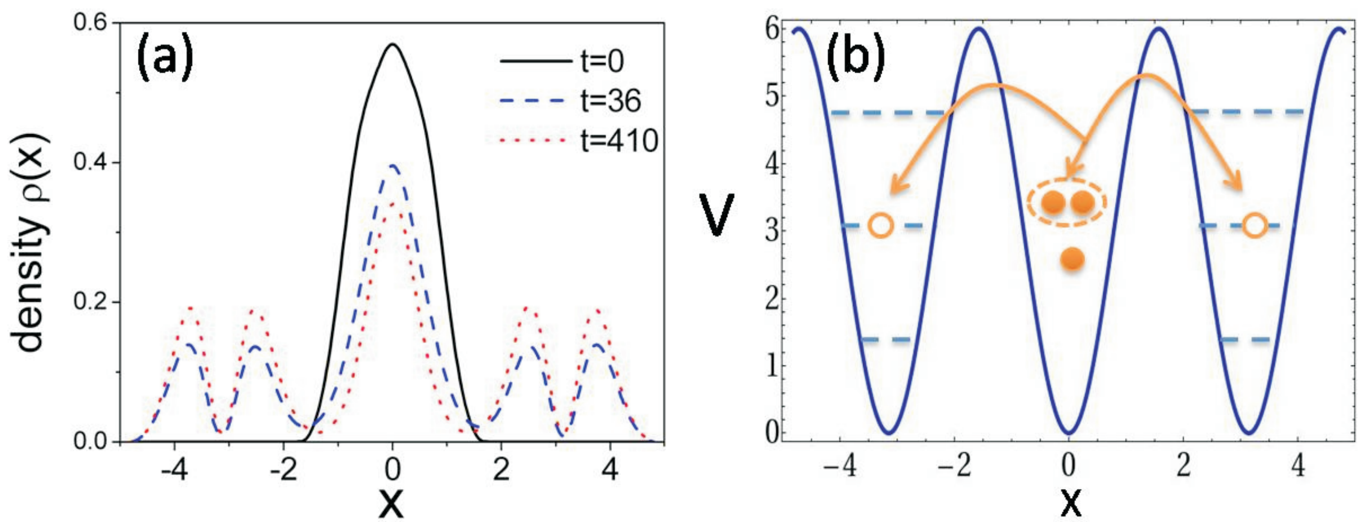
Three bosons initially in the middle well: $\Psi \approx |0,3,0\rangle_0$

(a) $g = 5.8$



Two boson tunneling to the left and right well via $|0,3,0\rangle_0 \Leftrightarrow |1,1,1\rangle_6$ i.e. two first-excited states !

Cao *et al*, NJP **13**, 033032 (2011)



4. 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.

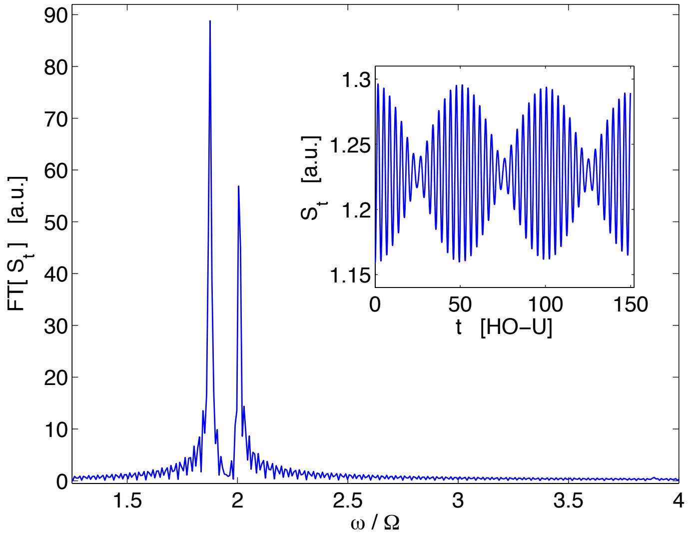
Prototype example and first application of ML-MCTDHB.

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

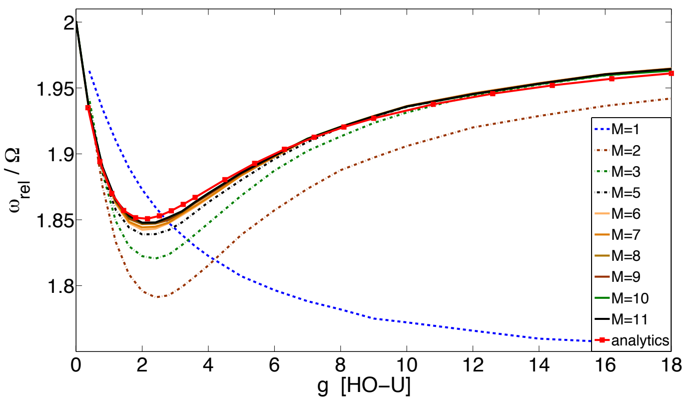
Answer the question:

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

Start with two atoms...



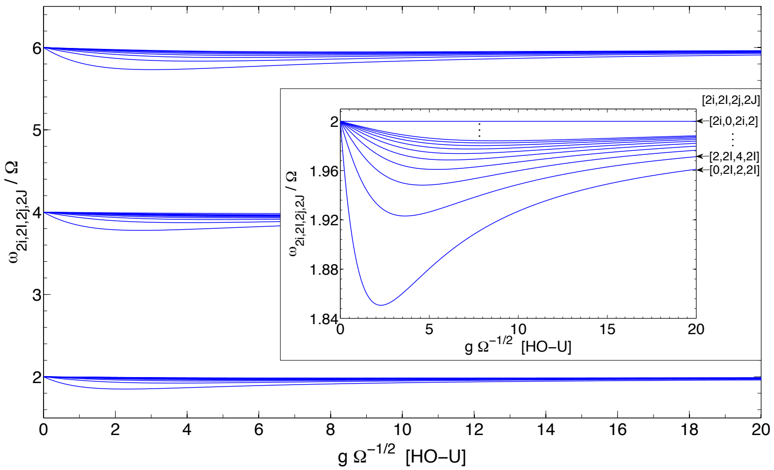
- Beating and breathing dynamics of $< X^2 >$
- Two dominant peaks in a background of frequencies: Relative + CM motion



- Relative motion breathing mode frequency varies with g whereas CM one not.

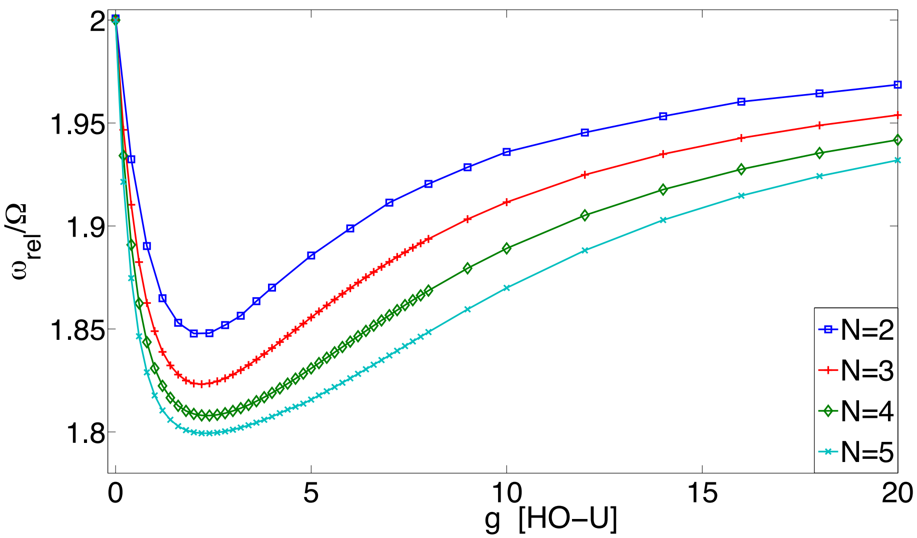
Rich breathing spectrum: Infinite sets of bands around $2n\Omega$ - but strongly suppressed !

A more detailed view...

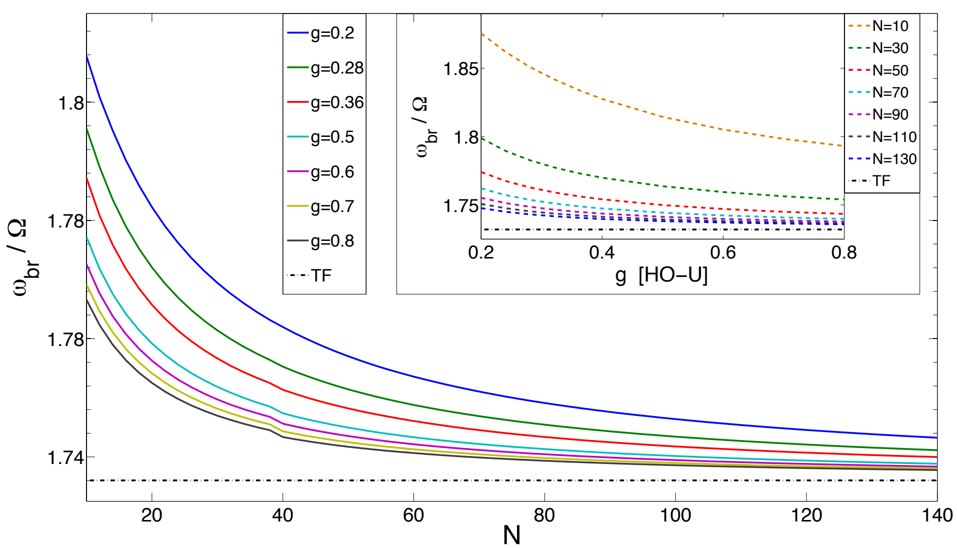


- Full breathing/beating mode spectrum up to 20 quanta at any interaction strength up to $\approx 6\Omega$.
- Inset: detailed view on the lowest band.
- Frequencies: $\omega_{2i,2I,2j,2J}$ which refers to the frequency arising from $\langle\Phi_{2I}\phi_{2i}|\,\hat{X}^2\,|\Phi_{2J}\phi_{2j}\rangle$.

Moving up to 140 atoms...

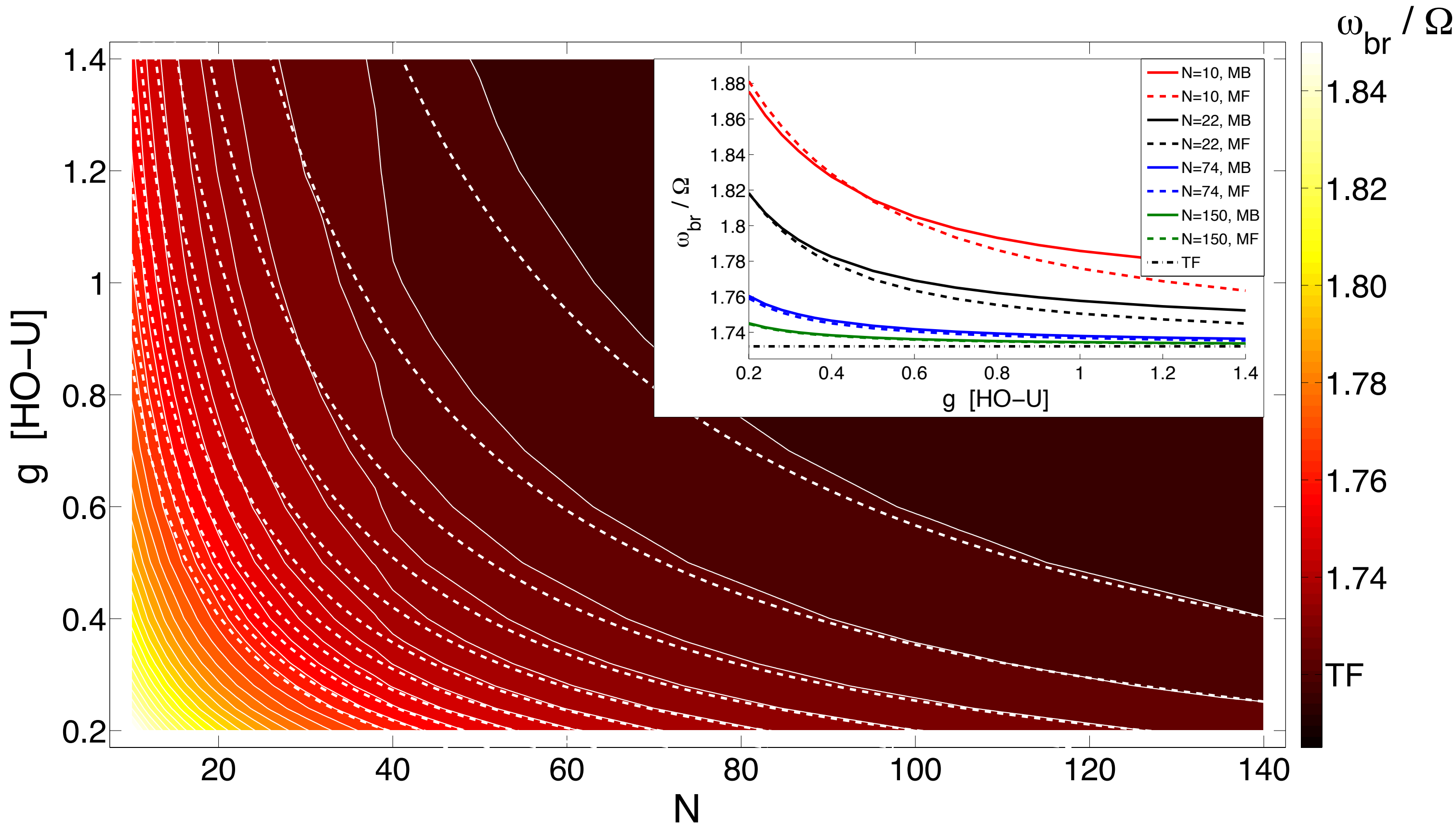


- CM breathing mode becomes strongly suppressed
- Breathing of the relative motion becomes dominant !



- 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)

5. 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.

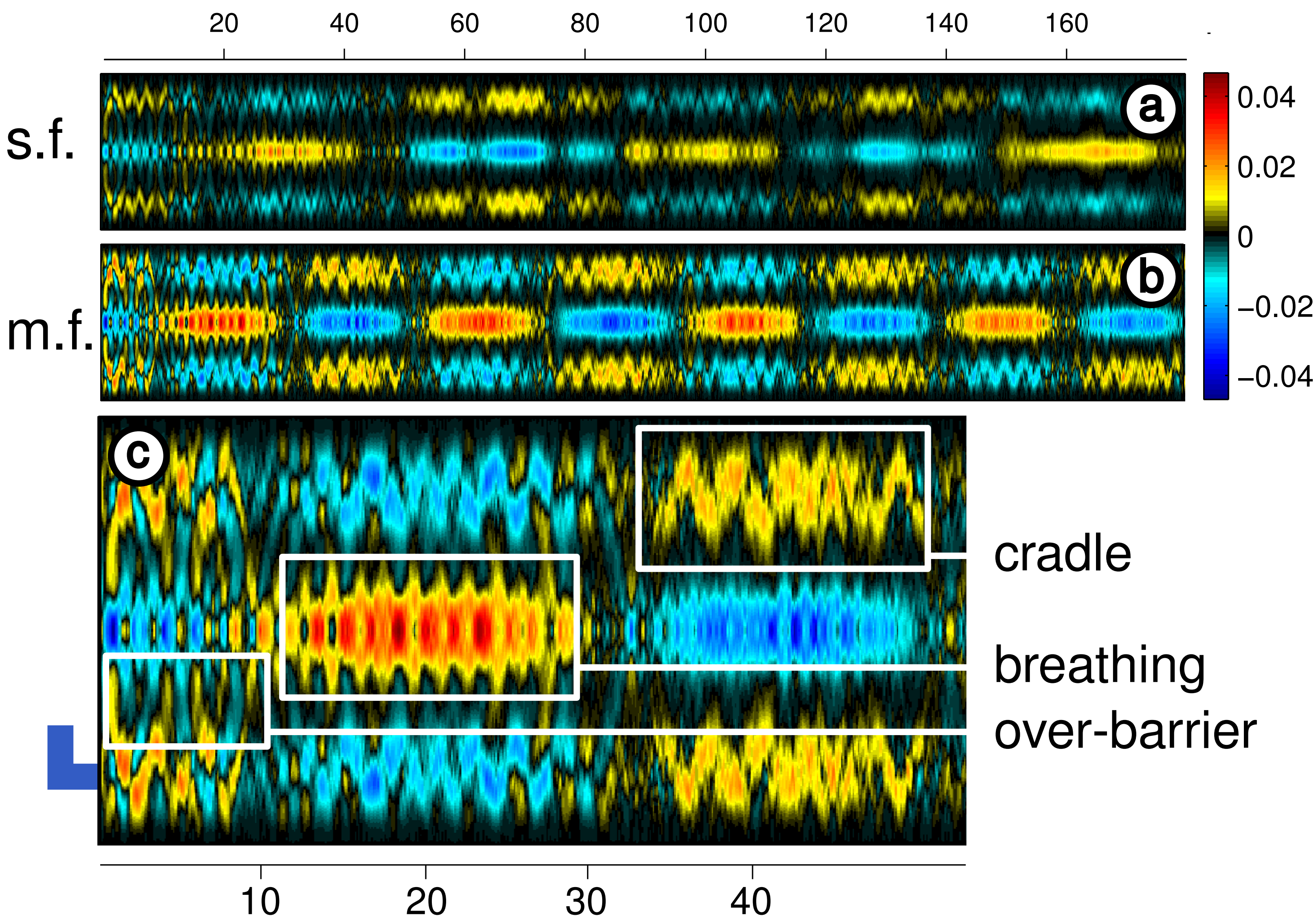
Resonance phenomena: Coupling of density-wave and cradle modes leads to a corresponding beating phenomenon !

$\Rightarrow$ 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.

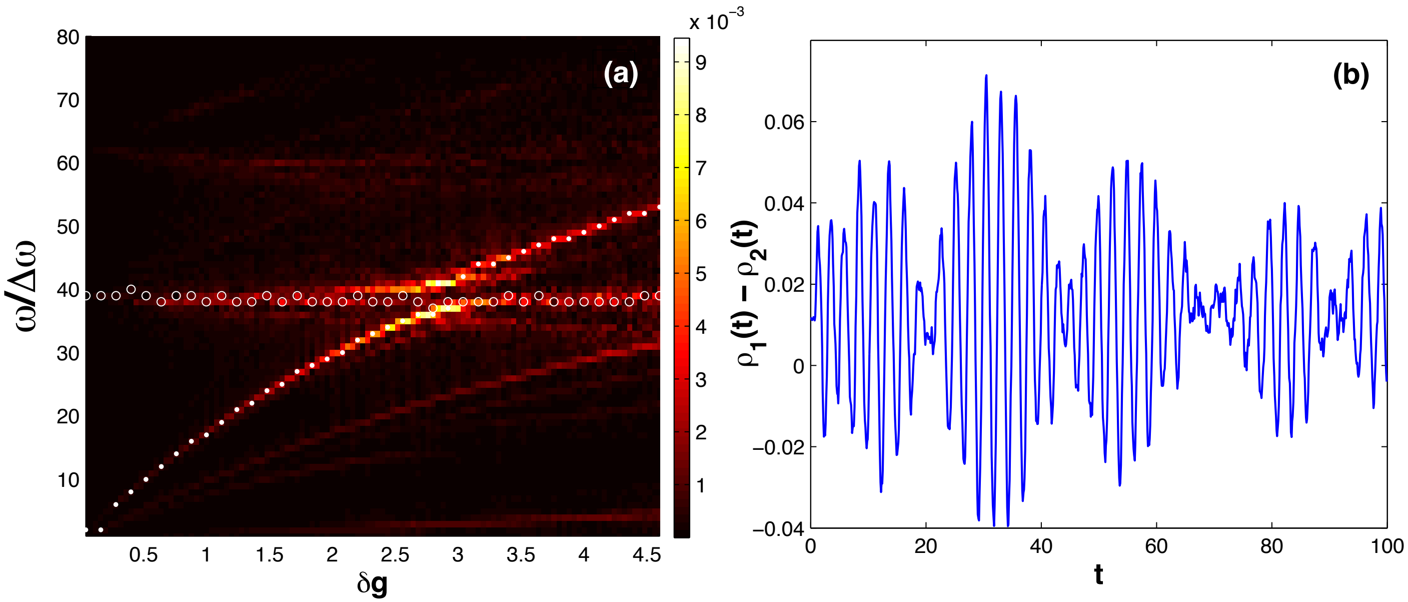


Density waves and their tunneling.

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)

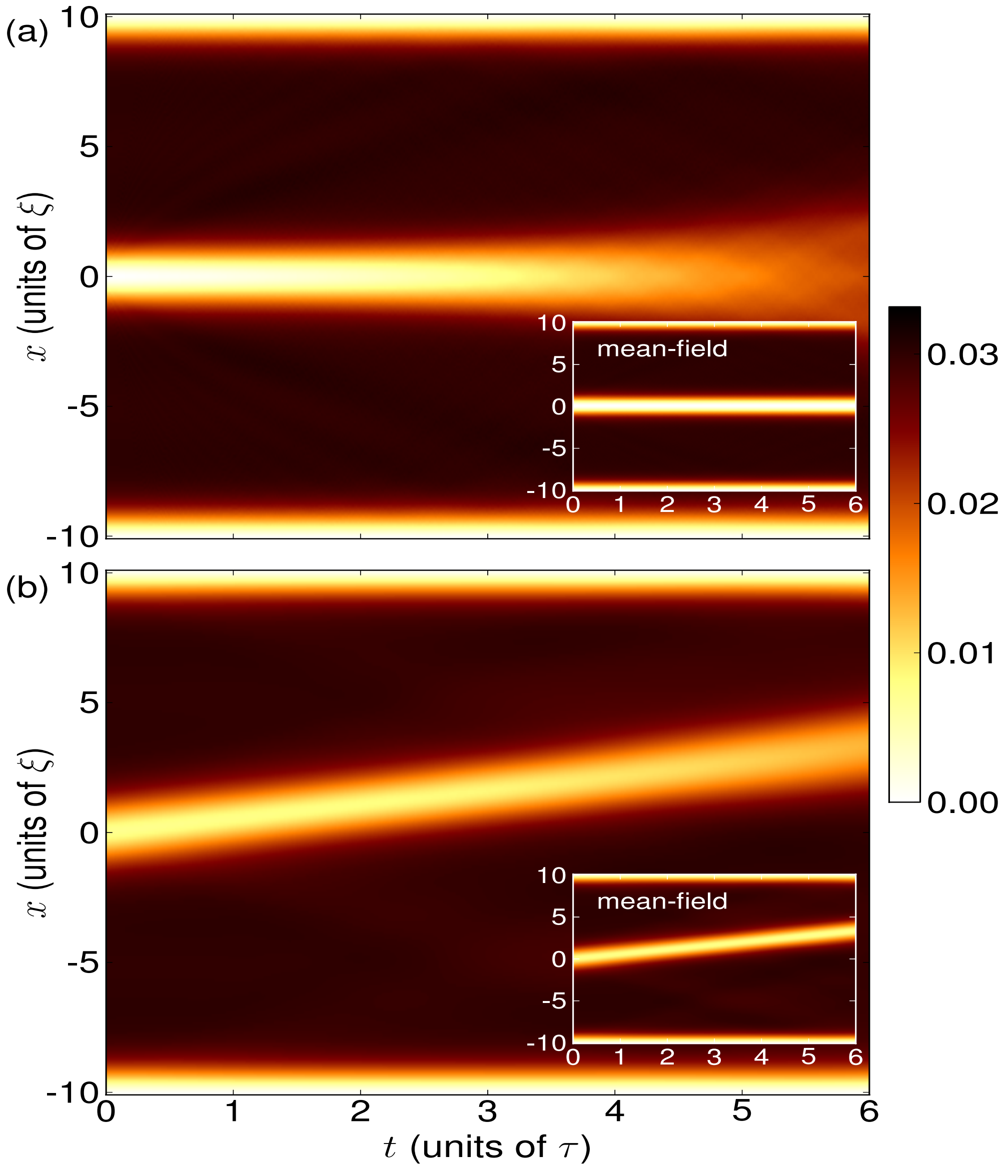
6. Many-body processes in black and grey matter-wave solitons

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.

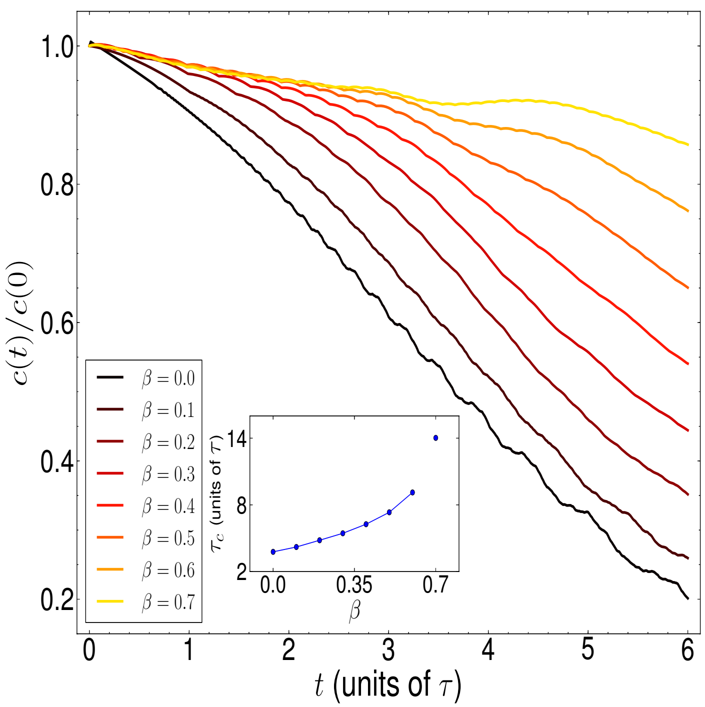
  CARR ET AL, PRL 103, 140403 (2009); PRA 80, 053612 (2009); PRA 63, 051601 (2001); RUOSTEKOSKI ET AL, PRL 104, 194192 (2010)

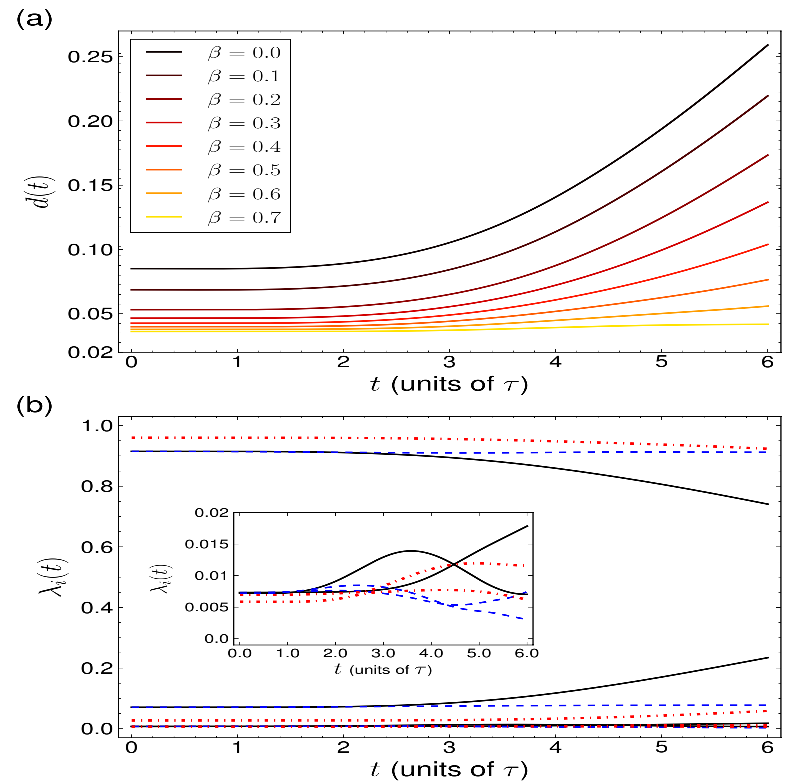
Density dynamics



- 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

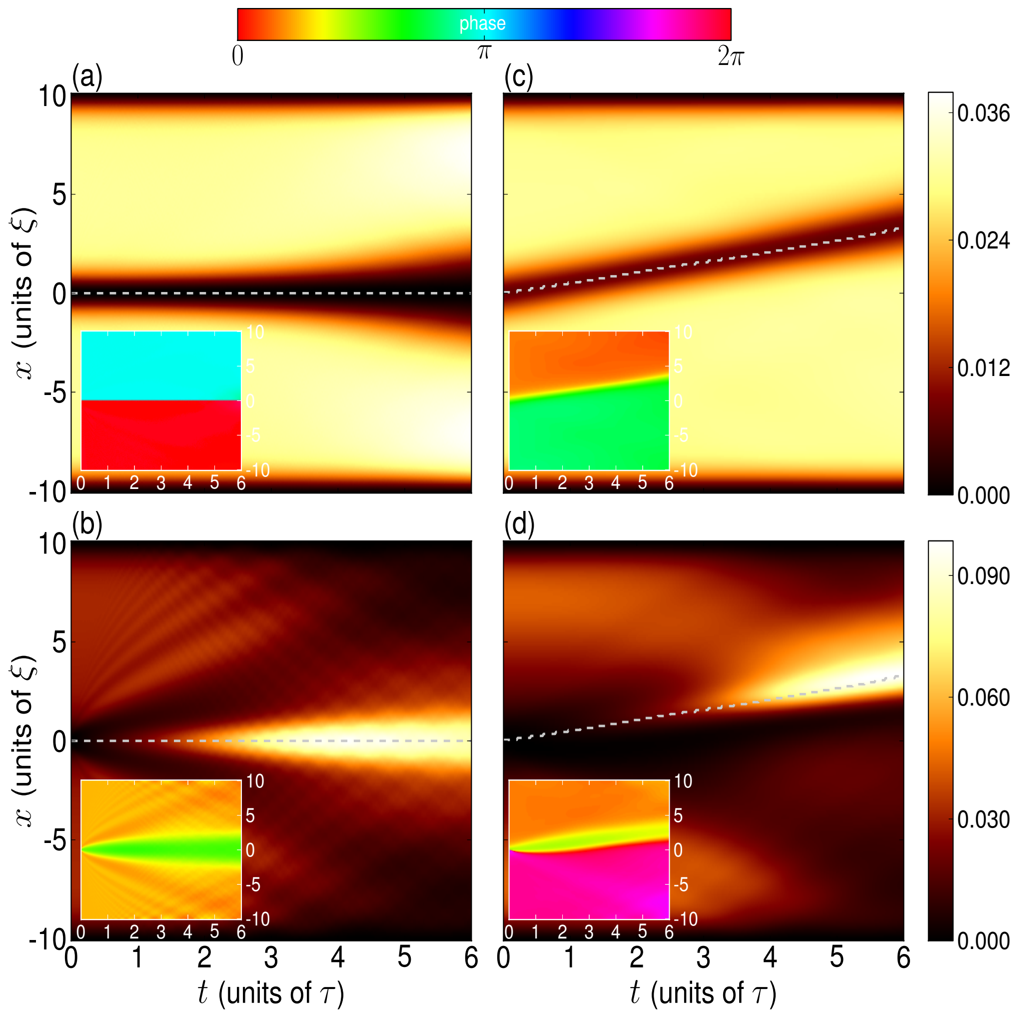




- Relative contrast $c(t)/c(0)$ of dark solitons for various $\beta = \frac{u}{s}$ $\left(c(t) = \frac{\max \rho_1(x,0) - \rho_1(x_t^s,t)}{\max \rho_1(x,0) + \rho_1(x_t^s,t)}\right)$

- 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

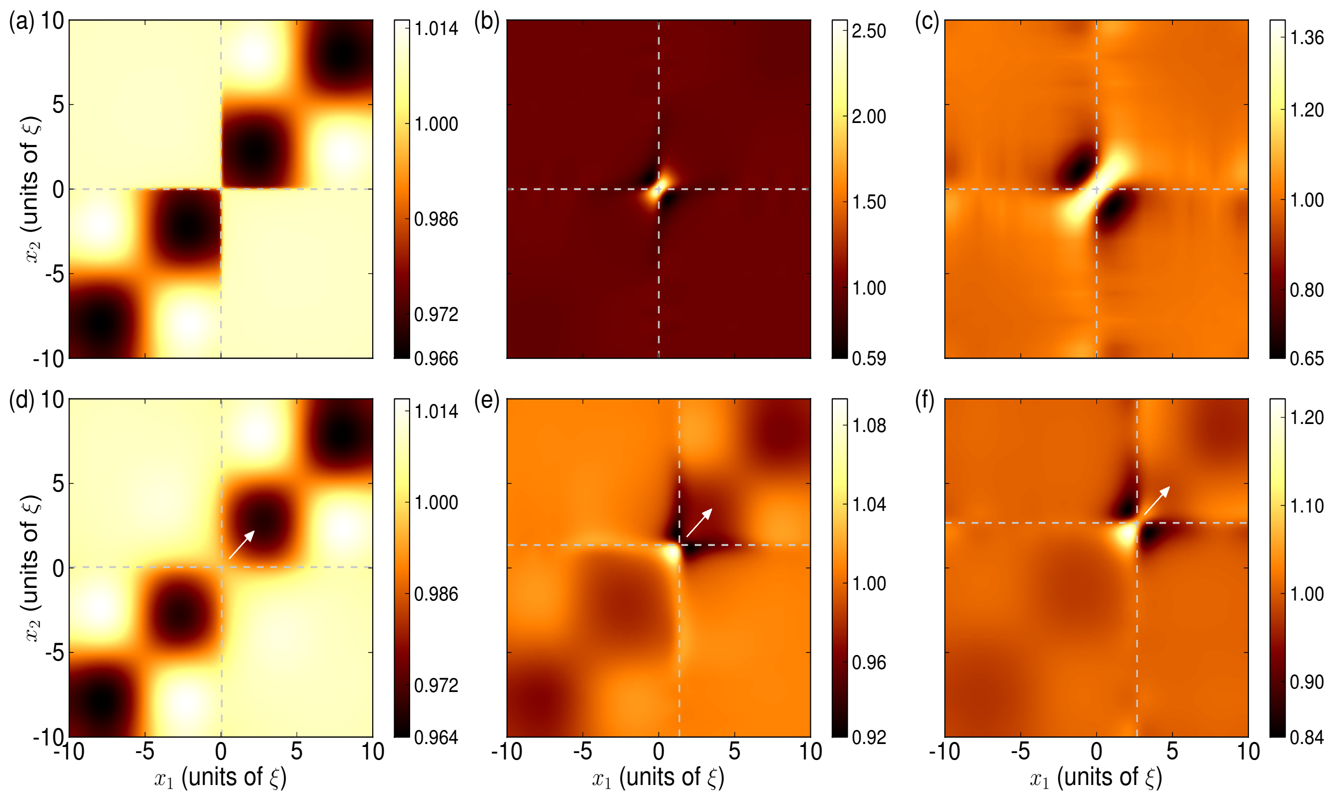


- Density and phase (inset) evolution of the dominant and second dominant natural orbital. (a,b) black soliton (c,d) grey soliton $\beta = 0.5$.

Localized two-body correlations

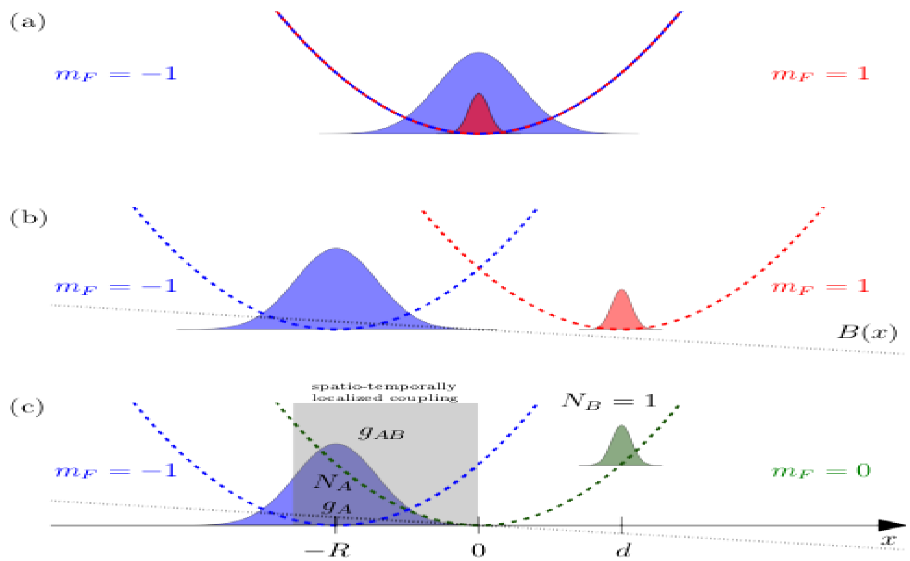
- Two-body correlation function $g_2(x_1, x_2; t)$ for a black soliton (first row) and a grey soliton $\beta = 0.5$ (second) at times $t = 0.0$ (first column), $t = 2.5\tau$ (second) and $t = 5\tau$ (third).

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



7. Correlated dynamics of a single atom coupling to an ensemble

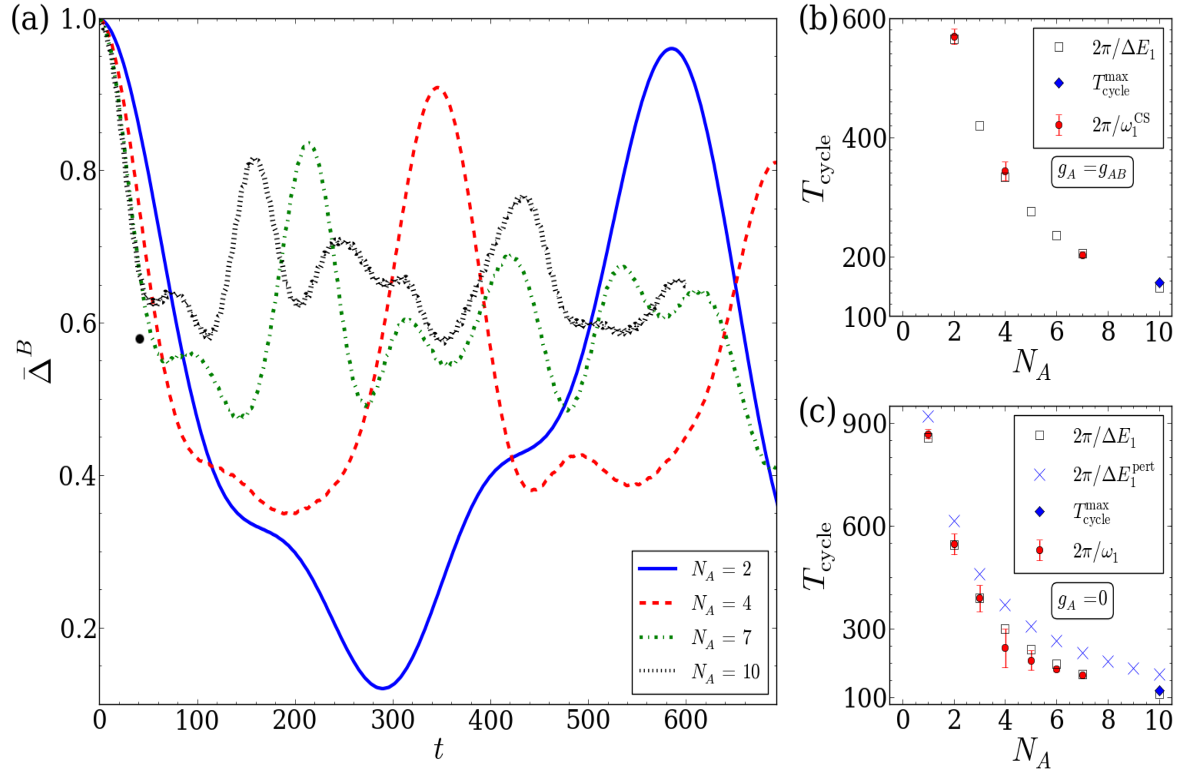
Setup and preparation



- Bipartite system: impurity atom plus ensemble of e.g. bosons of different $m_F = \pm 1$ trapped in optical dipole trap
- Application of external magnetic field gradient separates species
- Initialization in a displaced ground ie. coherent state via RF pulse to $m_F = 0$ for impurity atom.
- $\Rightarrow$ Single atom collisionally coupled to an atomic reservoir: Energy and correlation transfer - entanglement evolution.

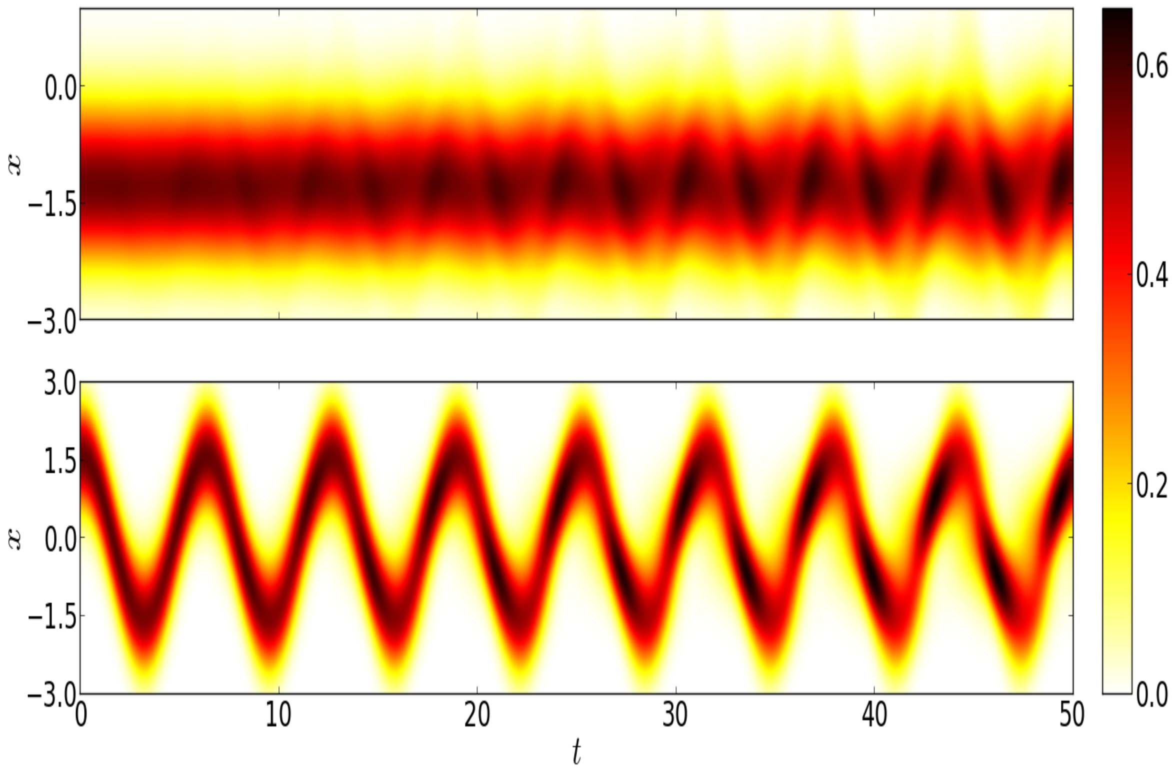
J. KNÖRZER, S. KRÖNKE AND P.S., NJP 17, 053001 (2015)

Energy transfer



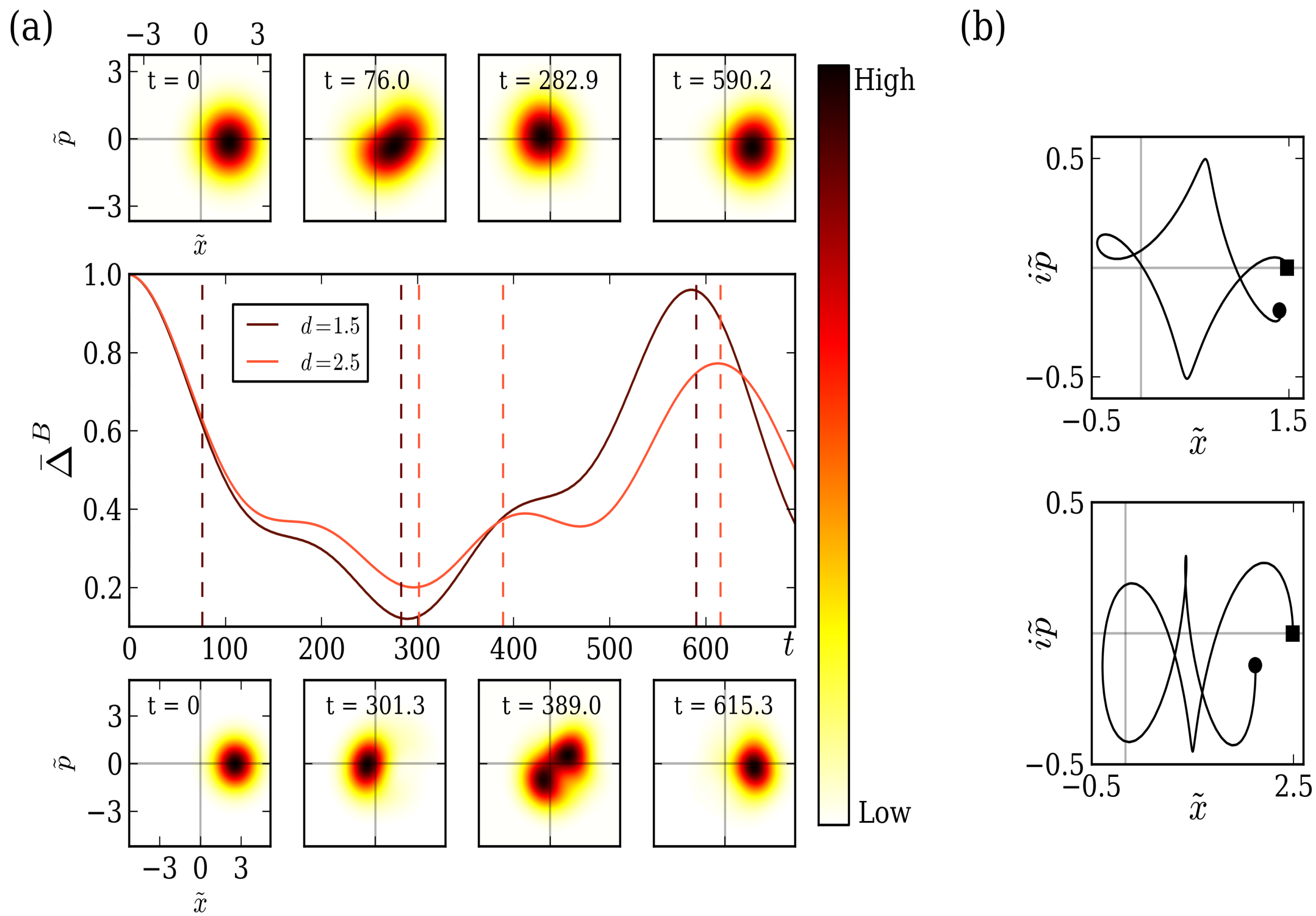
- Spatiotemporally localized inter-species coupling: Focus on long-time behaviour over many cycles.
- Energy transfer cycles with varying particle number of the ensemble

One-body densities



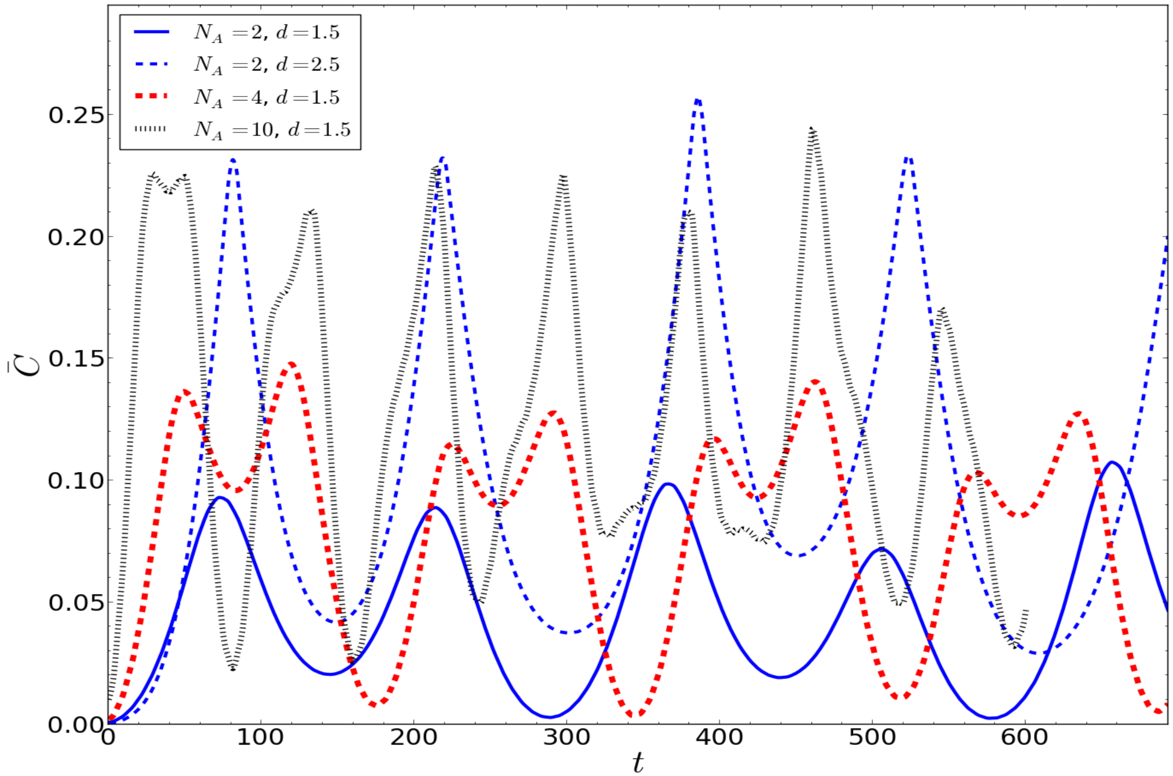
- Time-evolution of densities for the two species (ensemble-top, impurity-bottom) for first eight impurity oscillations.
- Impurity atom initiates oscillatory density modulations in ensemble atoms.
- Backaction on impurity atom.

Coherence analysis



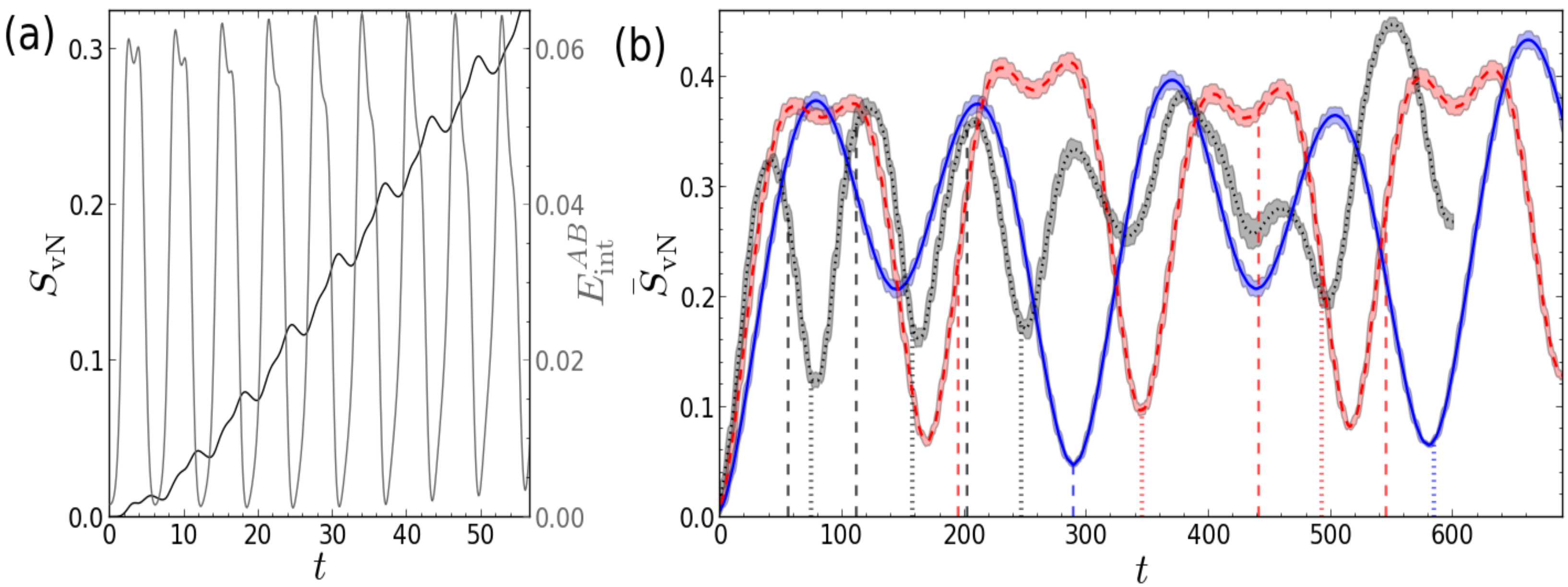
Time-evolution of normalized excess energy Δ_t^B with Husimi distribution $Q_t^B(z, z^*) = \frac{1}{\pi}\langle z|\hat{\rho}_t^B|z\rangle\,, \quad z \in \mathbb{C}$ of reduced density $\hat{\rho}_t^B$ at certain time instants.

Coherence measure



Distance (operator norm) to closest coherent state, as a function of time for different atom numbers in the ensemble.

Correlation analysis



- (a) Short-time evolution of the von Neumann entanglement entropy $S_{\mathrm{vN}}(t)$ and inter-species interaction energy $E_{\mathrm{int}}^{AB}(t) = \langle \hat{H}_{AB} \rangle_t$.
- (b) Long-time evolution of $\bar{S}_{\mathrm{vN}}(t)$. for $N_A = 2$ (blue solid line), $N_A = 4$ (red, dashed) and $N_A = 10$ (black, dotted).

J. KNÖRZER, S. KRÖNKE AND P.S., NJP 17, 053001 (2015)

8. 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

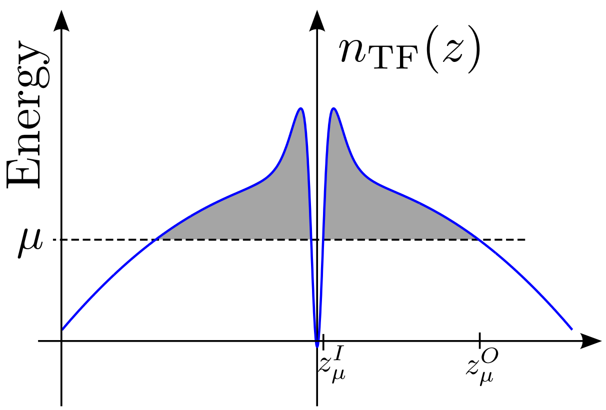
- Atom-ion interaction introduces an additional length scale $R^* = \sqrt{\frac{2C_4\mu}{\hbar^2}}$
- 'Molecular' bound states

- 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: $V(z) = V_0 e^{-\gamma z^2} - \frac{1}{z^4 + \frac{1}{\omega}}$

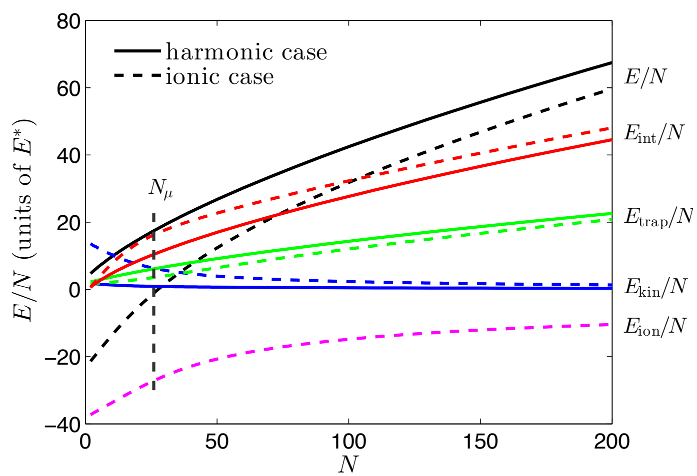
First: Static strongly trapped ion

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

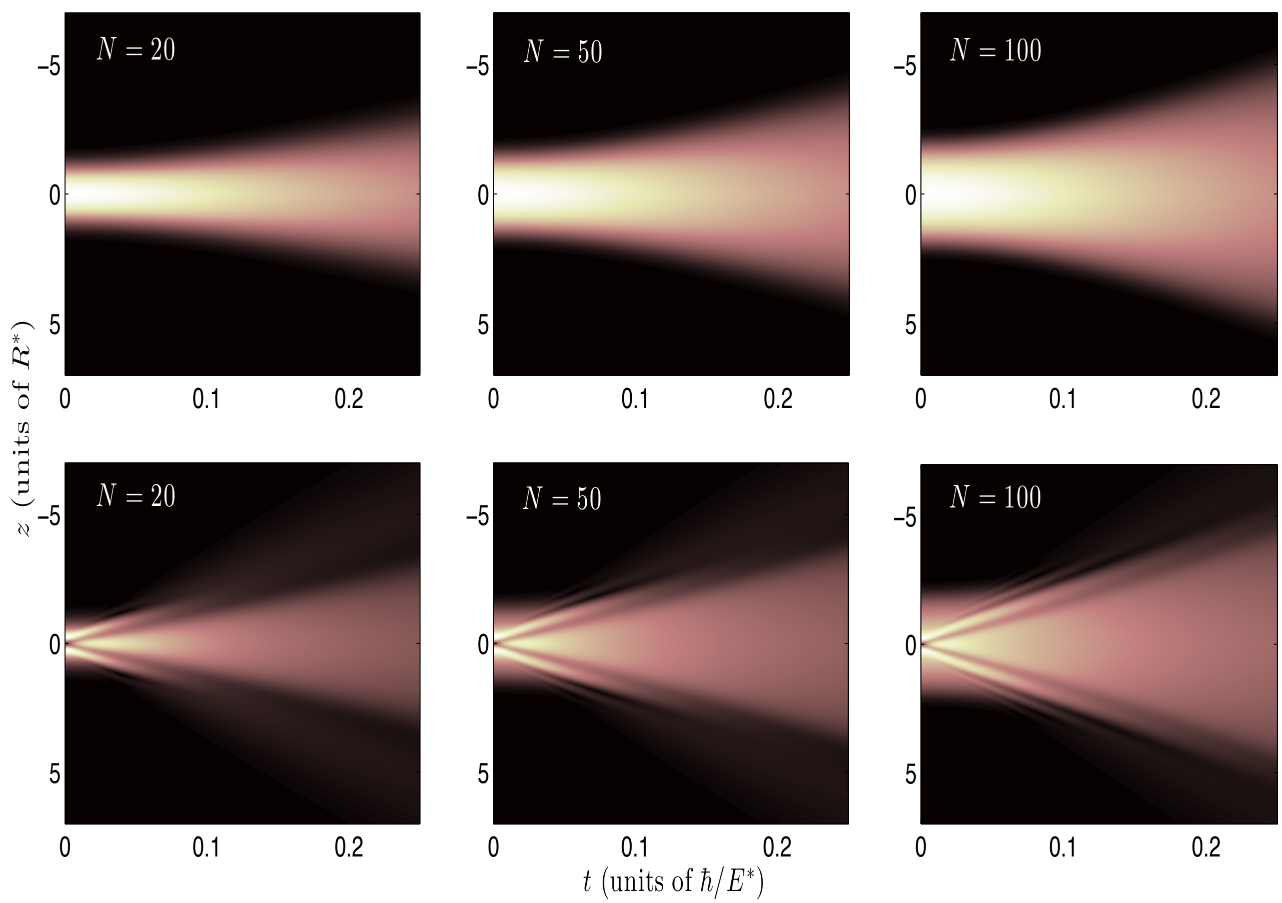
J. Schurer et al, PRA 90, 033601 (2014)



Thomas-Fermi profile



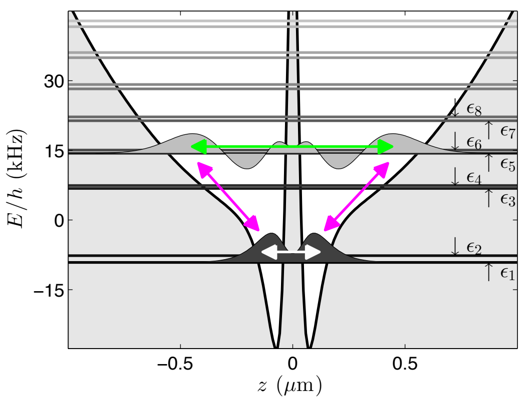
Energetical contributions



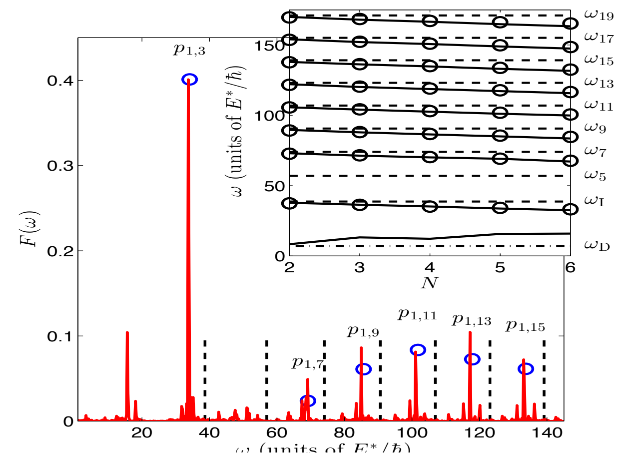
Expansion dynamics of the density

Next: Sudden creation of the ion

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

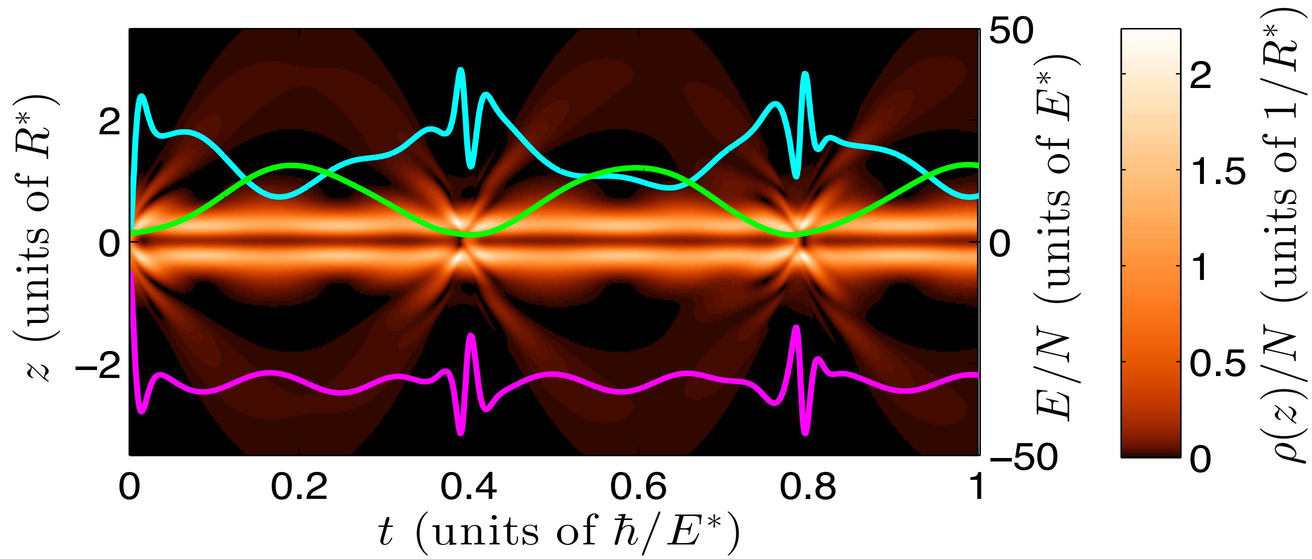


Effective potential, ion-bound and trap states



Excitation spectrum

J. SCHURER ET AL, NJP 17, 083024 (2015)



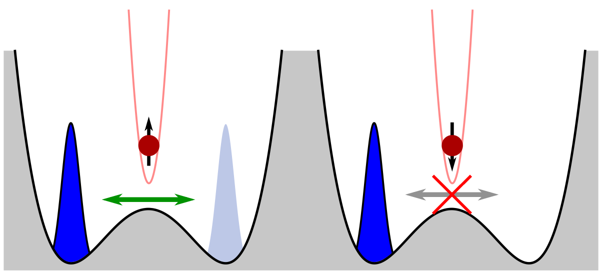
Time evolution of the density and energies per particle

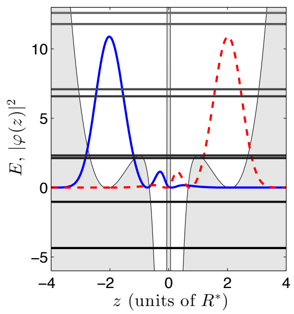
Recent progress: Background

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.

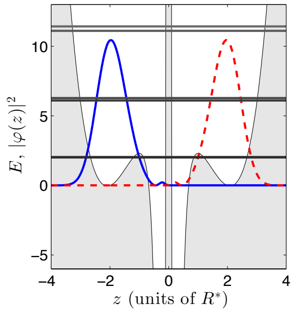
Add an ion: Coupling between the wells can be controlled by the ionic spin state. Ion-bosons entanglement.





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

Unknown impact of many-body correlations on this process !

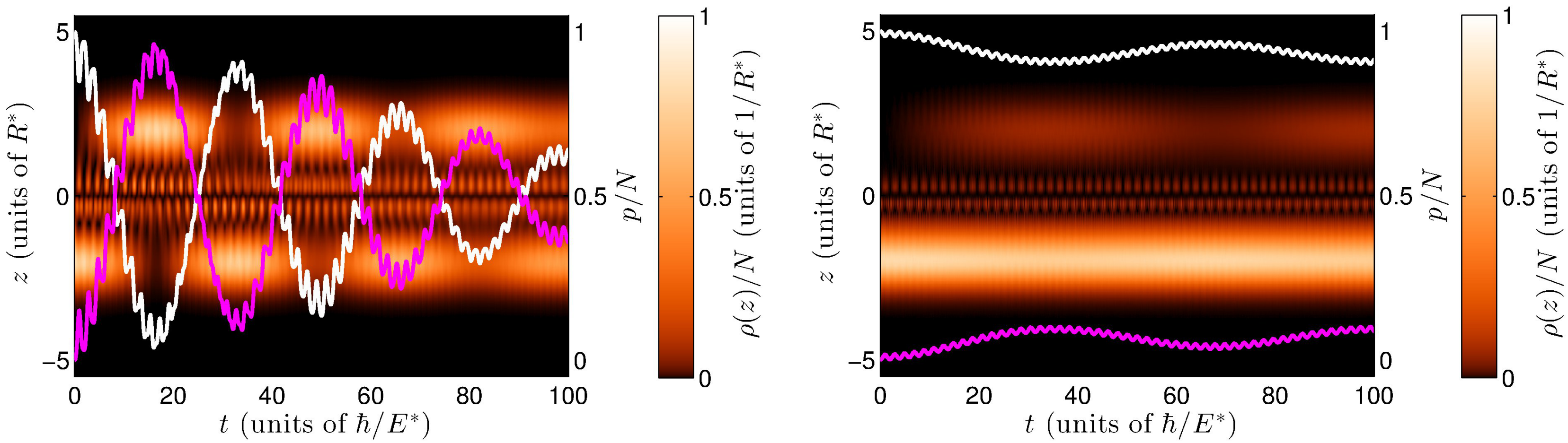


Ion controlled bosonic Josephson junction

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

Tunneling regime
Ion state 1

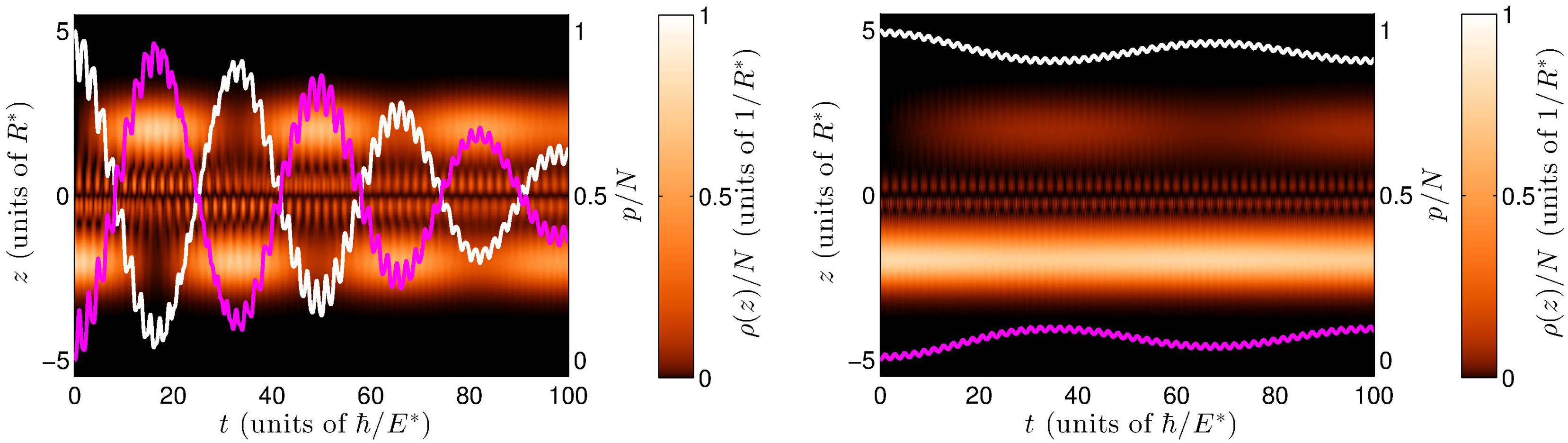
Self-trapping regime
Ion state 2



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

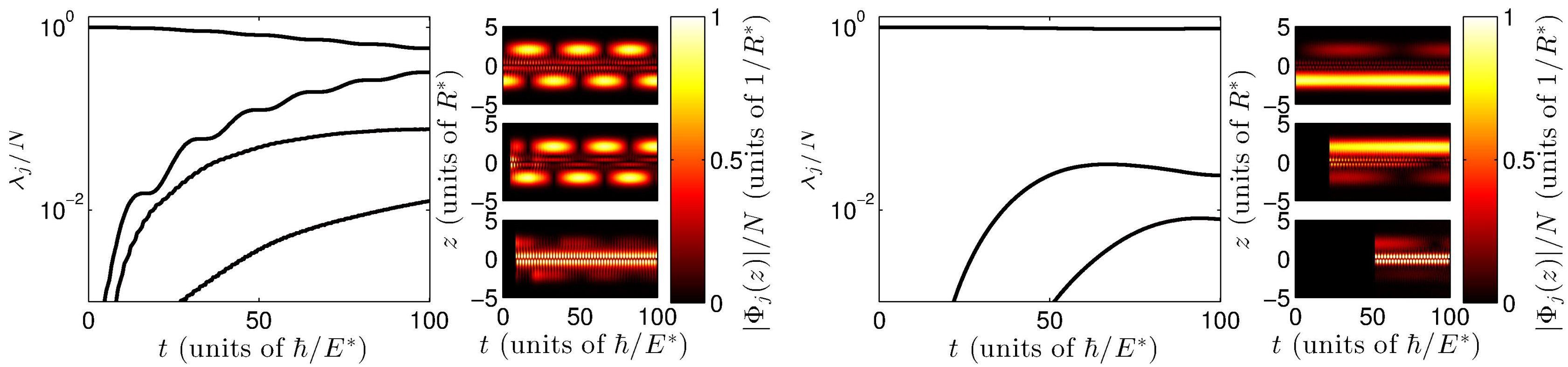


One-body density $\rho(z,t)$ as well as left well p_L and right well p_R occupation

- 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.

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

Tunneling regime   Self-trapping regime



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 !

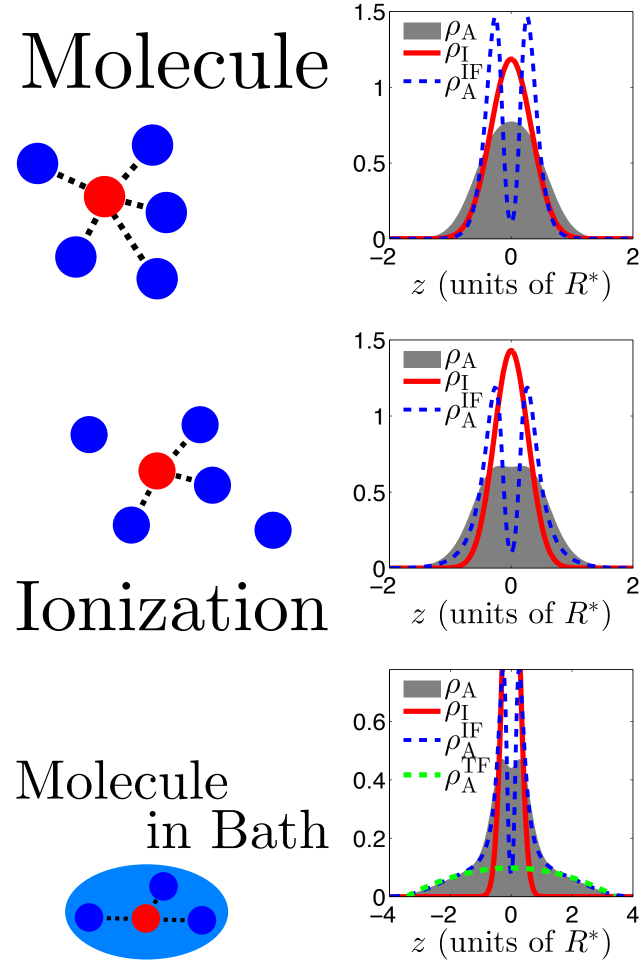
In progress: Mesoscopic charged molecules in a BEC

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



9. Concluding remarks

Conclusions

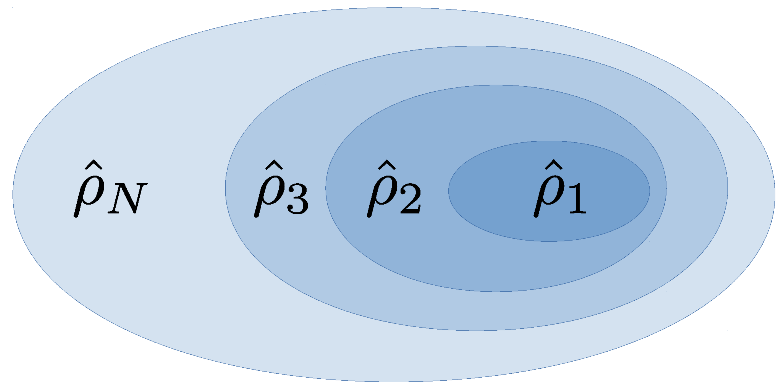
- ML-MCTDHB is a versatile efficient tool for the nonequilibrium dynamics of ultracold bosons.
- Few- to many-body systems can be covered: Shown here for the emergence of collective behaviour.
- Many-mode correlation dynamics: From quench to driving.
- Beyond mean-field effects in nonlinear excitations.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

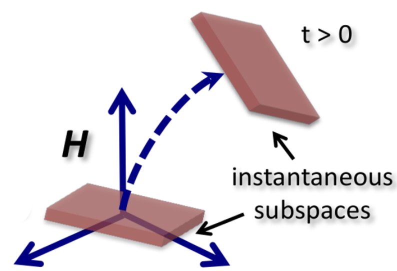
Reduced density-operator propagation: method development

Aim: correlated non-equilibrium quantum dynamics of <u>many</u> ultracold bosonic atoms

Approach:

- focus on dynamics of few-particle reduced density operators $\hat{\rho}_n$
- represent $\hat{\rho}_n$ w.r.t. dynamically optimized basis (MCTDHB theory)
  $\rightarrow$ BBGKY hierarchy for the matrix elements of $\hat{\rho}_n$
  $\rightarrow$ EOM for basis states
- bosonic cumulant expansion for hierarchy truncation





Resulting theory:

- number of atoms becomes a parameter
- dynamically optimized basis
  $\rightarrow$ truncation at high order n

Thank you for your attention !