Applications of the ML-MCTDHB to the Nonequilibrium Quantum Dynamics of Ultracold Systems

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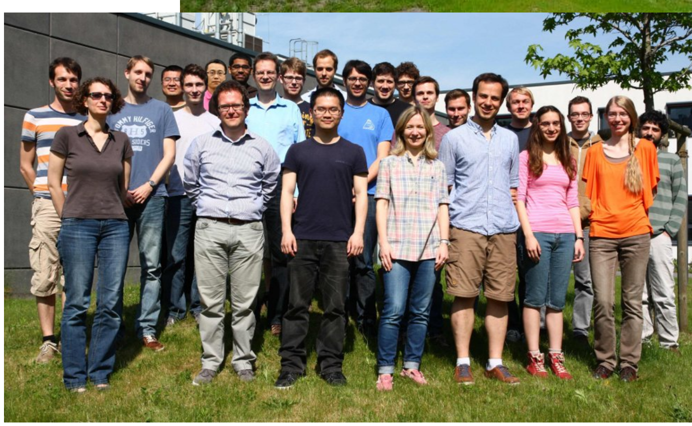
624. WE-Heraeus-Seminar: Simulating Quantum Processes and Devices
Bad Honnef, September 19-22, 2016

The Centre 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)

funded by the SFB 925 ’Light induced dynamics and control of correlated quantum systems’ of the German Science Foundation (DFG).

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.

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, 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

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: A brief account of the methodology and then 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).]

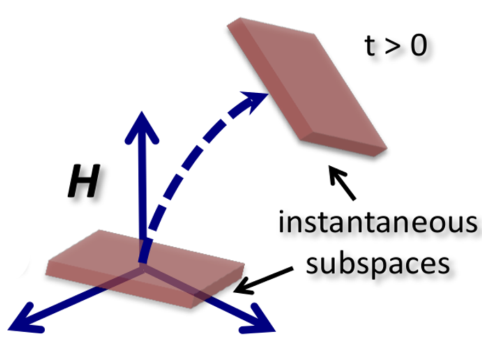
  MCTDH (1990): few distinguishable DOFs, quantum molecular dynamics

  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



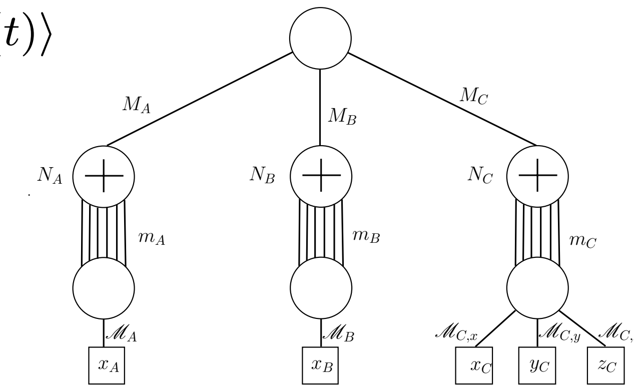
Hierarchy within ML-MCTDHB

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:

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

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

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

$\Rightarrow$ 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 $|\phi^{(\sigma)}_j(t)\rangle$ 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

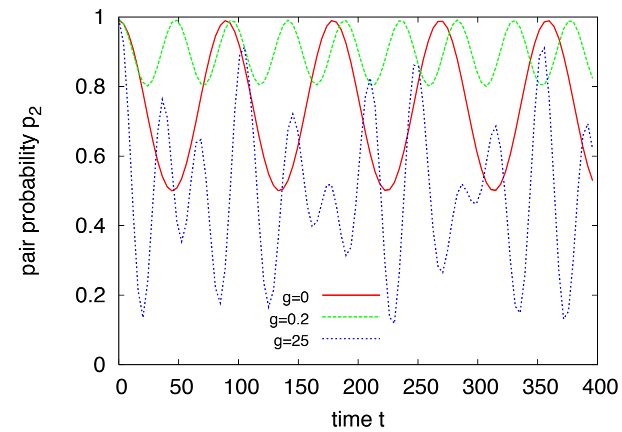
Few-boson systems - Perspectives

- 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.

Few-boson systems: Double Well



- No interactions: Rabi oscillations.
- Weak interactions: Delayed tunneling.
- Intermediate interactions:
  - Tunneling comes almost to a hold in spite of repulsive interactions.
  - Pair tunneling takes over !
- Very strong interactions: Fragmented pair tunneling.

$\triangleright$ $N = 2$ atoms

K. Winkler *et al.*, Nature **441**, 853 (2006); S. Fölling *et al.*, Nature **448**, 1029 (2007)

S. Zöllner, H.D. Meyer and P.S., PRL **100**, 040401 (2008); PRA **78**, 013621 (2008)

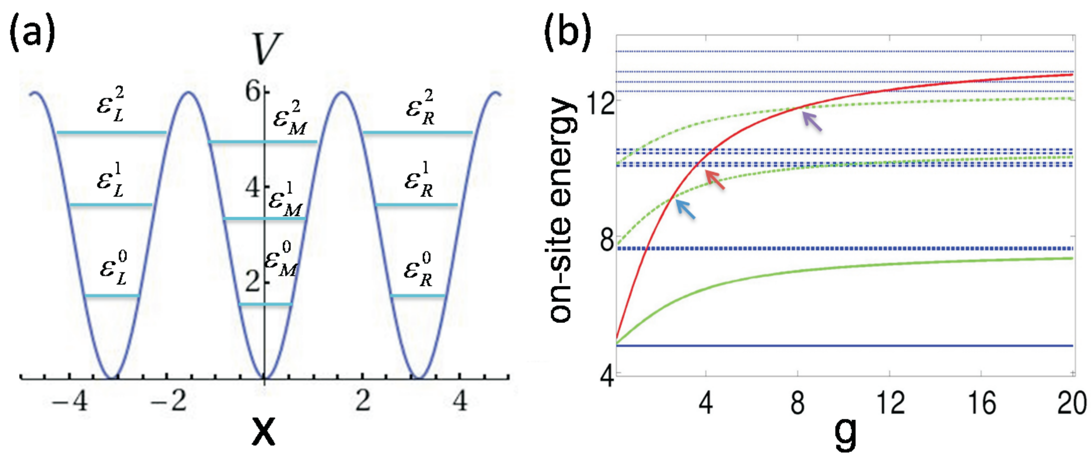
Interband Tunneling: Motivation

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 !

Interband Tunneling: Analysis Tool

- Methodology: Multi-Layer Multi-Configuration Time-Dependent Hartree for Bosons
- Novel number-state representation including interaction effects for analysis

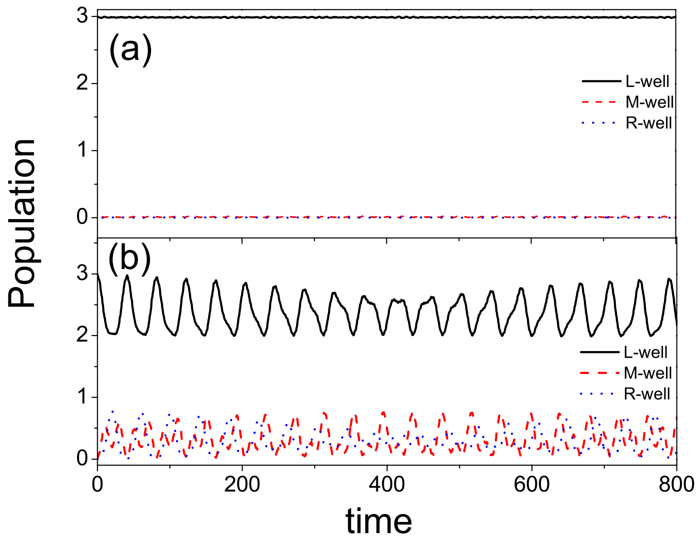


Three bosons: Single, pair and triple modes.

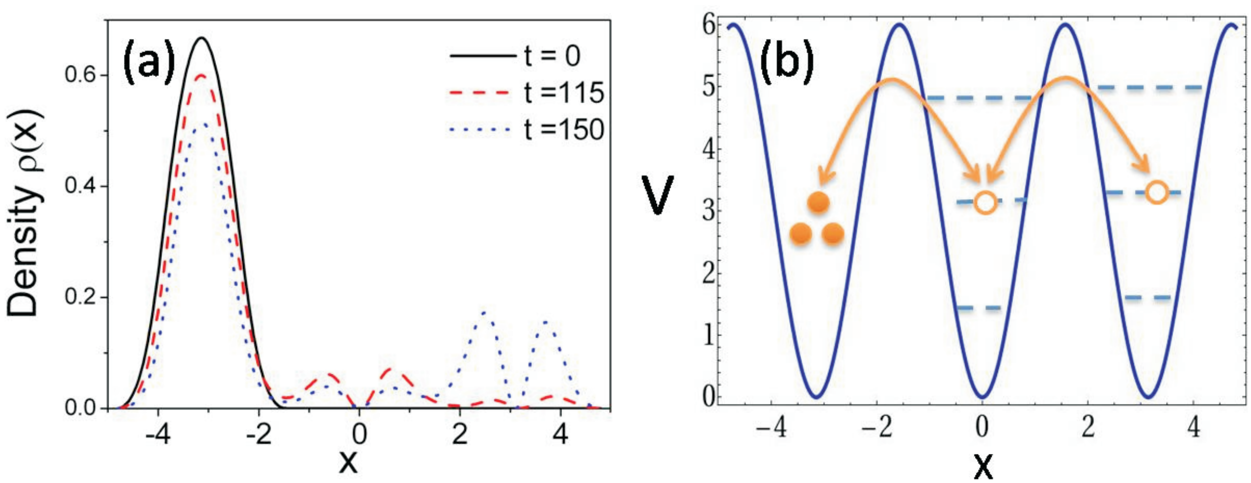
Interband Tunneling: Single boson tunneling

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

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



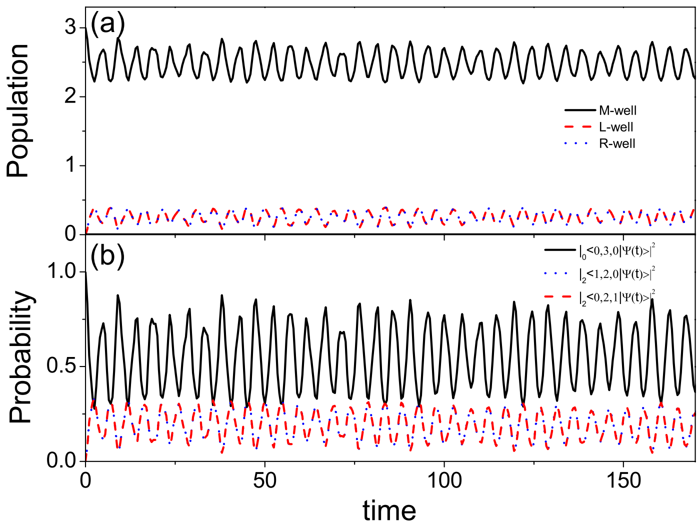
Single boson tunneling to middle and right well via $|3,0,0\rangle_0 \Leftrightarrow |2,1,0\rangle_1 \Leftrightarrow |2,0,1\rangle_1$ i.e. via first-excited states !



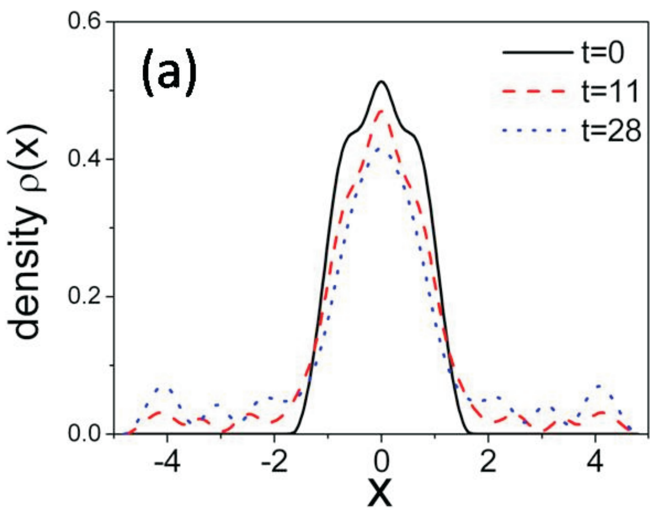
Interbanding Tunneling: Single boson tunneling

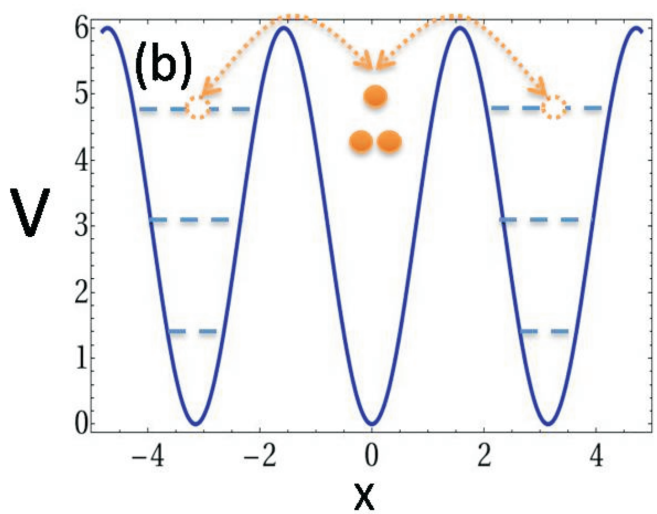
Three bosons initially in the middle well: $\Psi \approx |0,3,0\rangle_0$

(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 !

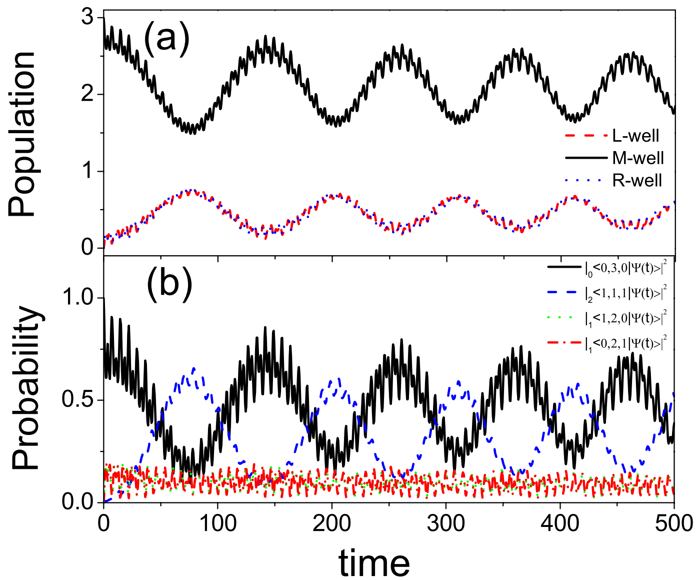




Interband Tunneling: Two boson tunneling

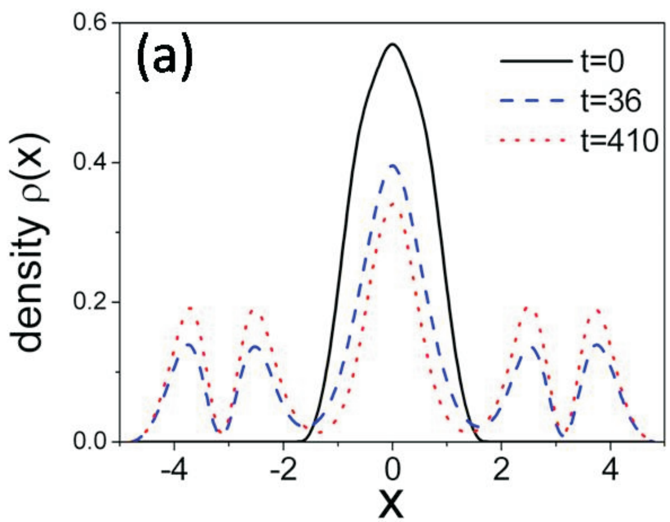
Three bosons initially in the middle well: $\Psi \approx |0,3,0\rangle_0$

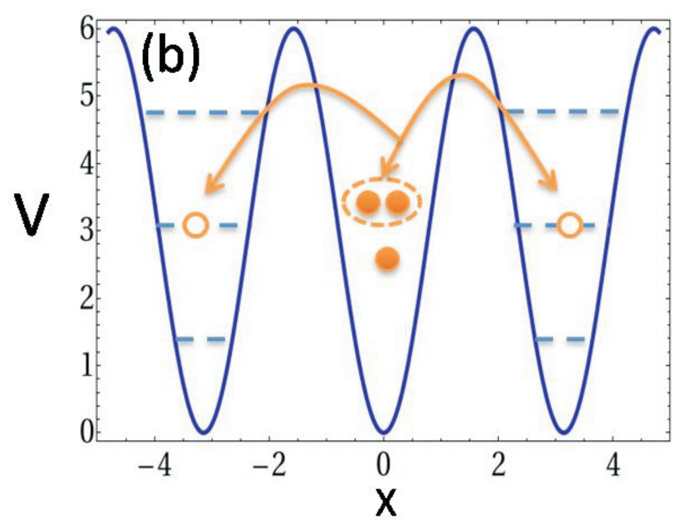
(a) $g = 5.8$



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. 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.

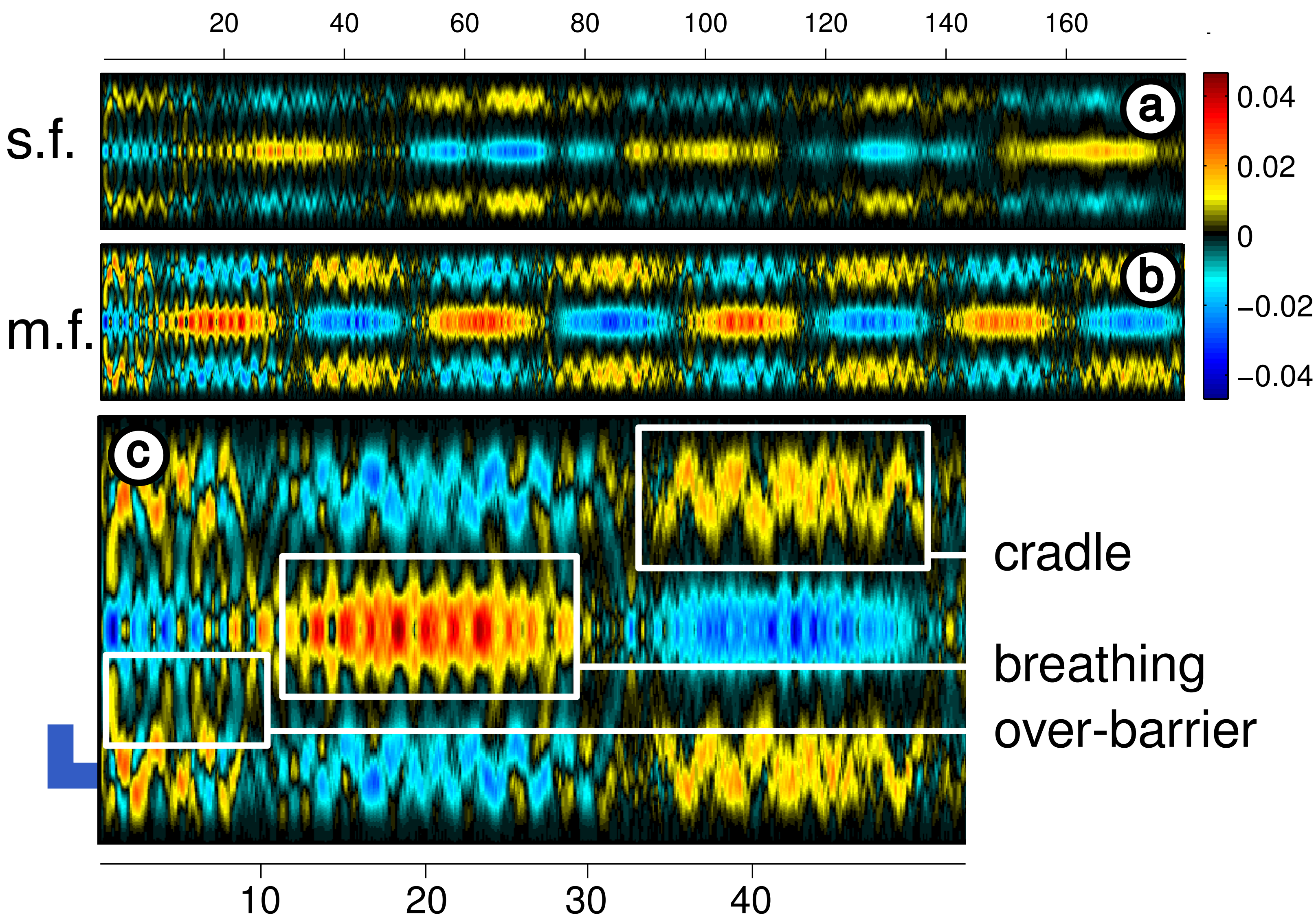
Resonance phenomena: Coupling of density-wave and cradle modes leads to a corresponding beating phenomenon !

$\Rightarrow$ 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.

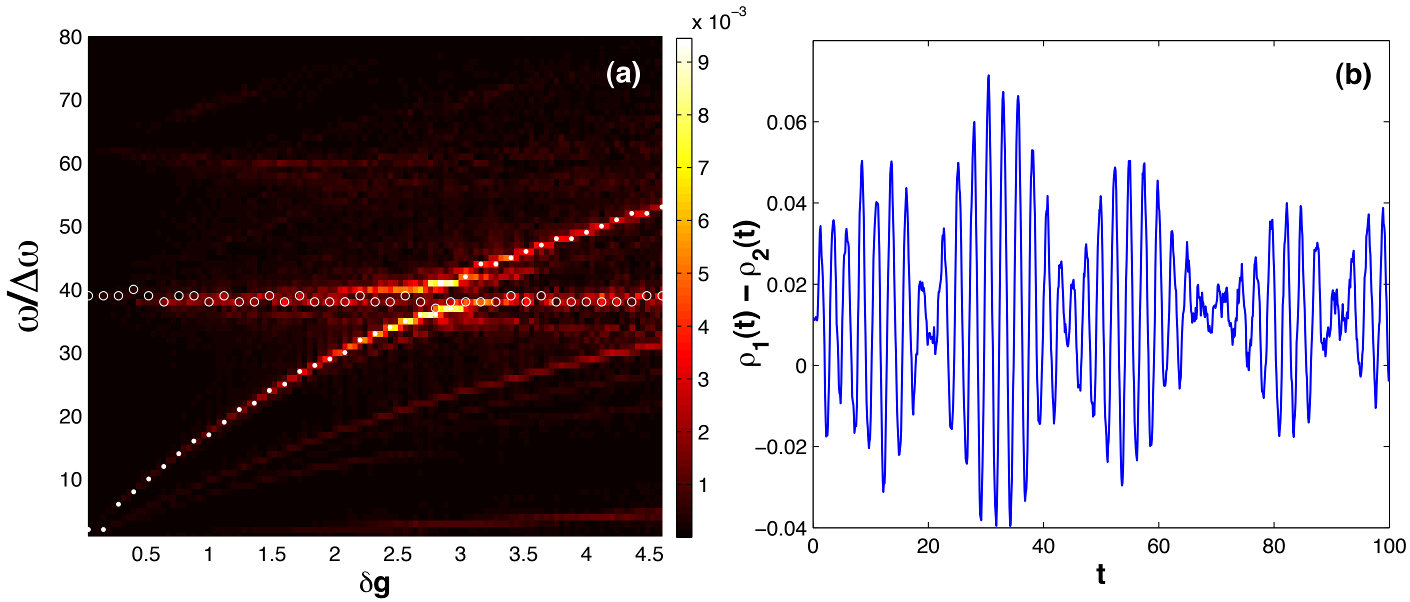


Density waves and their tunneling.

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)

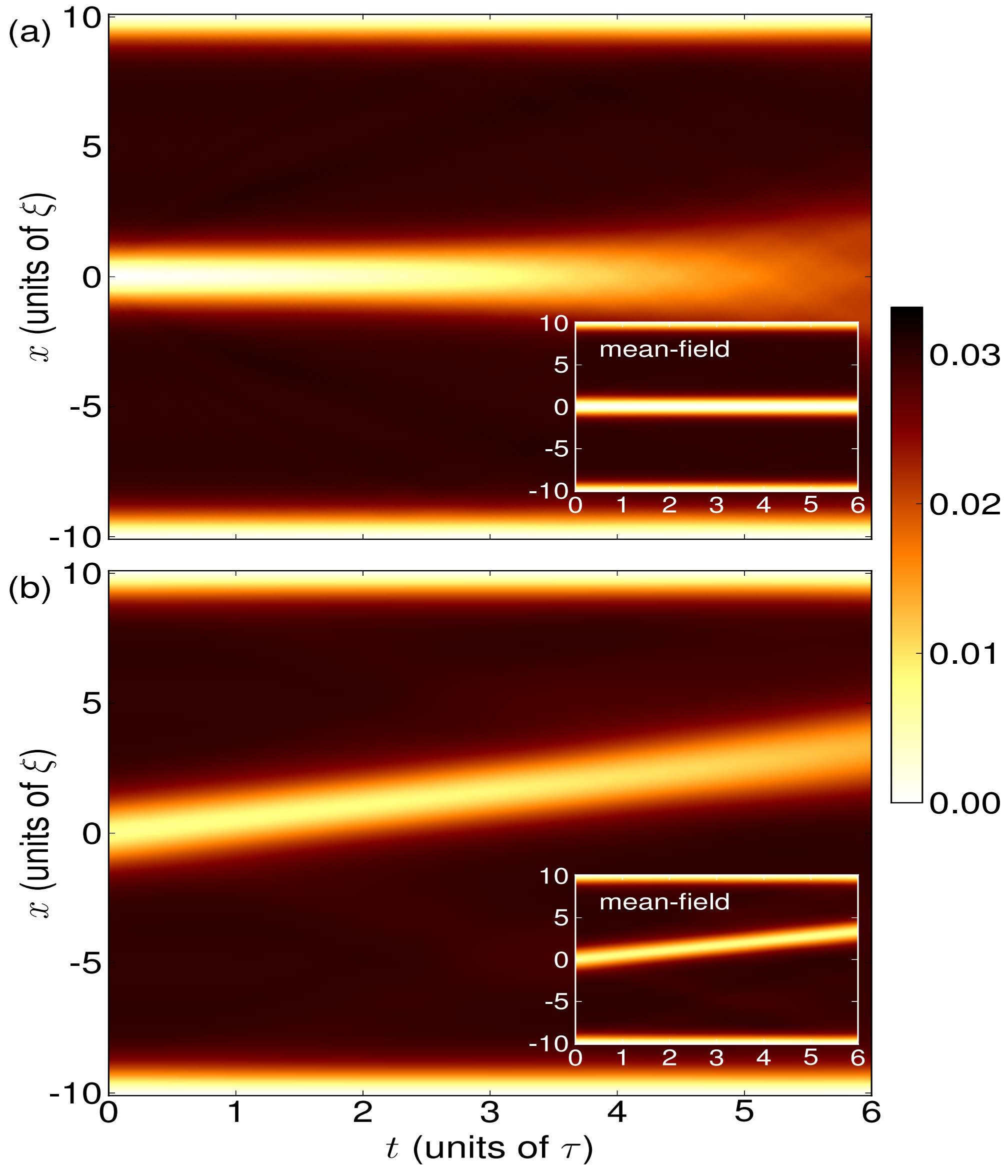
5. Many-body processes in black and grey matter-wave solitons

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.

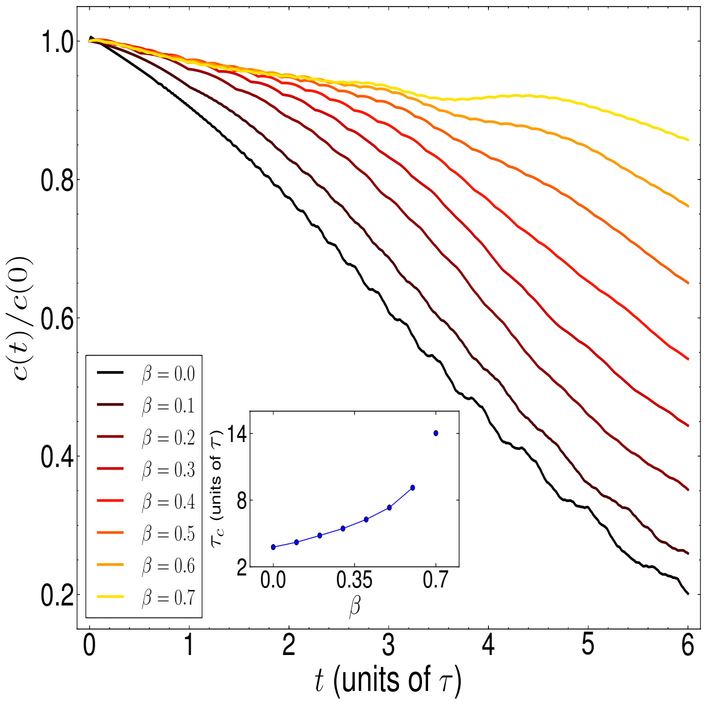
  CARR ET AL, PRL 103, 140403 (2009); PRA 80, 053612 (2009); PRA 63, 051601 (2001); RUOSTEKOSKI ET AL, PRL 104, 194192 (2010)

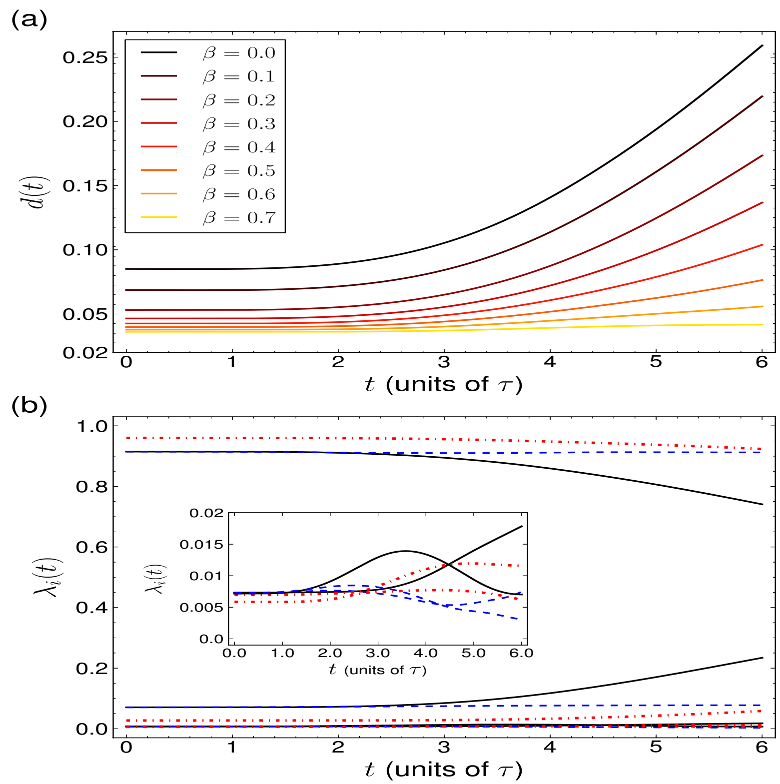
Density dynamics



- 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

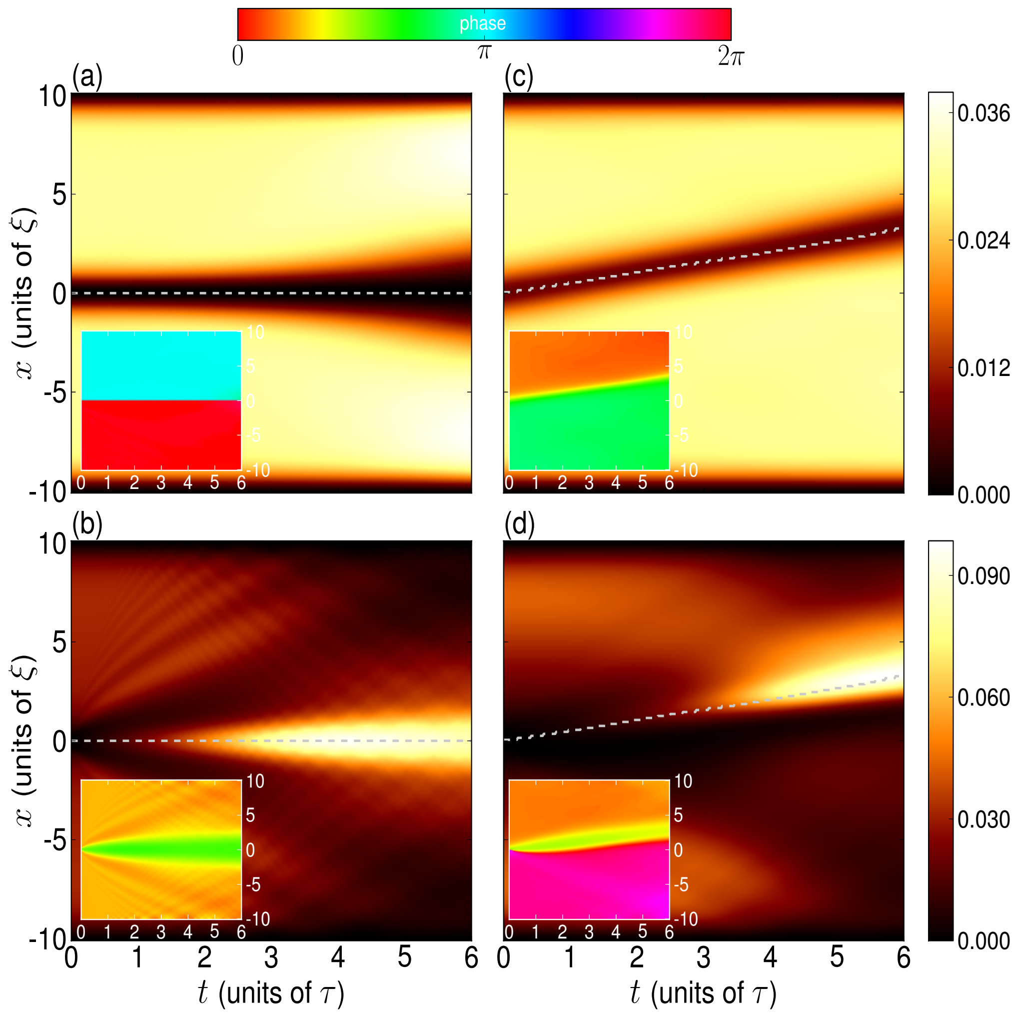




- Relative contrast $c(t)/c(0)$ of dark solitons for various $\beta = \frac{u}{s}$ ($c(t) = \frac{\max \rho_1(x,0) - \rho_1(x_t^s,t)}{\max \rho_1(x,0) + \rho_1(x_t^s,t)}$)

- 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

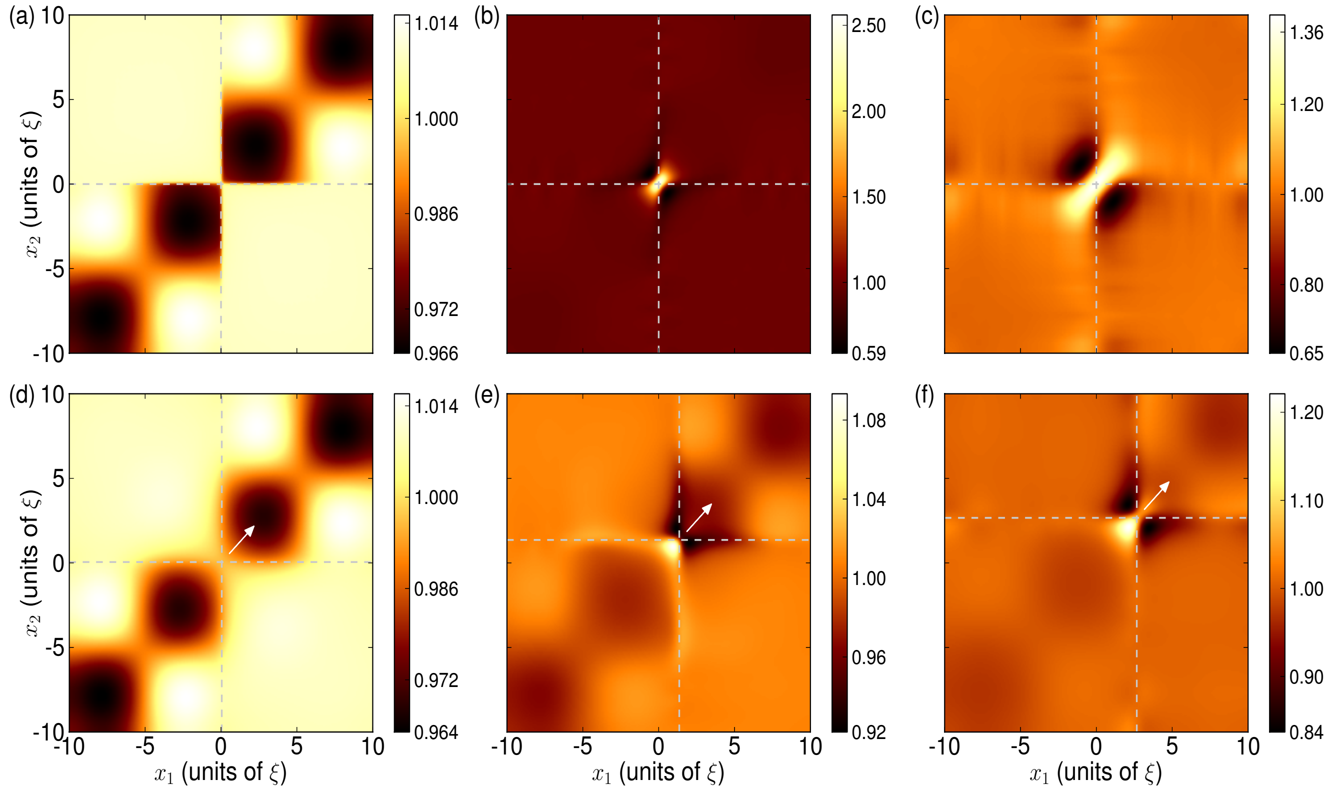


- Density and phase (inset) evolution of the dominant and second dominant natural orbital. (a,b) black soliton (c,d) grey soliton $\beta = 0.5$.

Localized two-body correlations

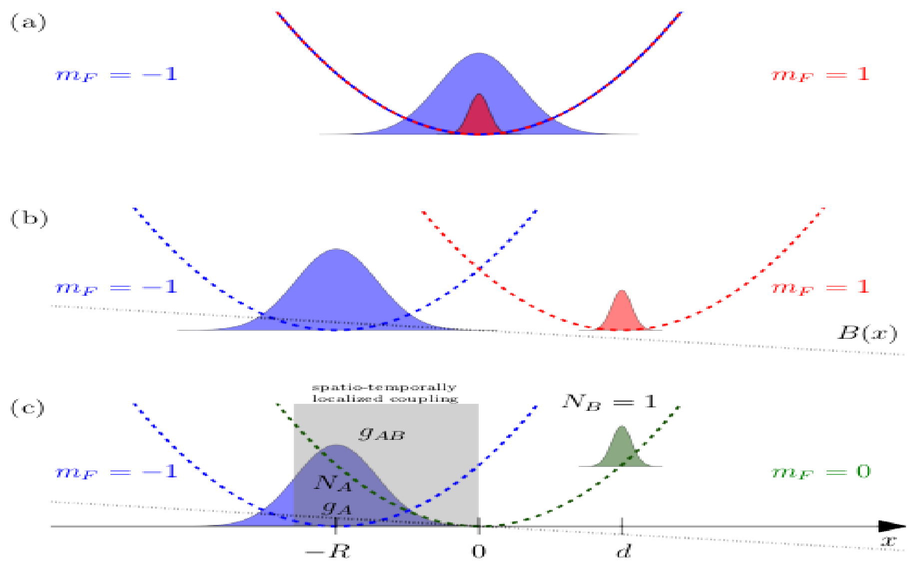
- Two-body correlation function $g_2(x_1, x_2; t)$ for a black soliton (first row) and a grey soliton $\beta = 0.5$ (second) at times $t = 0.0$ (first column), $t = 2.5\tau$ (second) and $t = 5\tau$ (third).

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



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

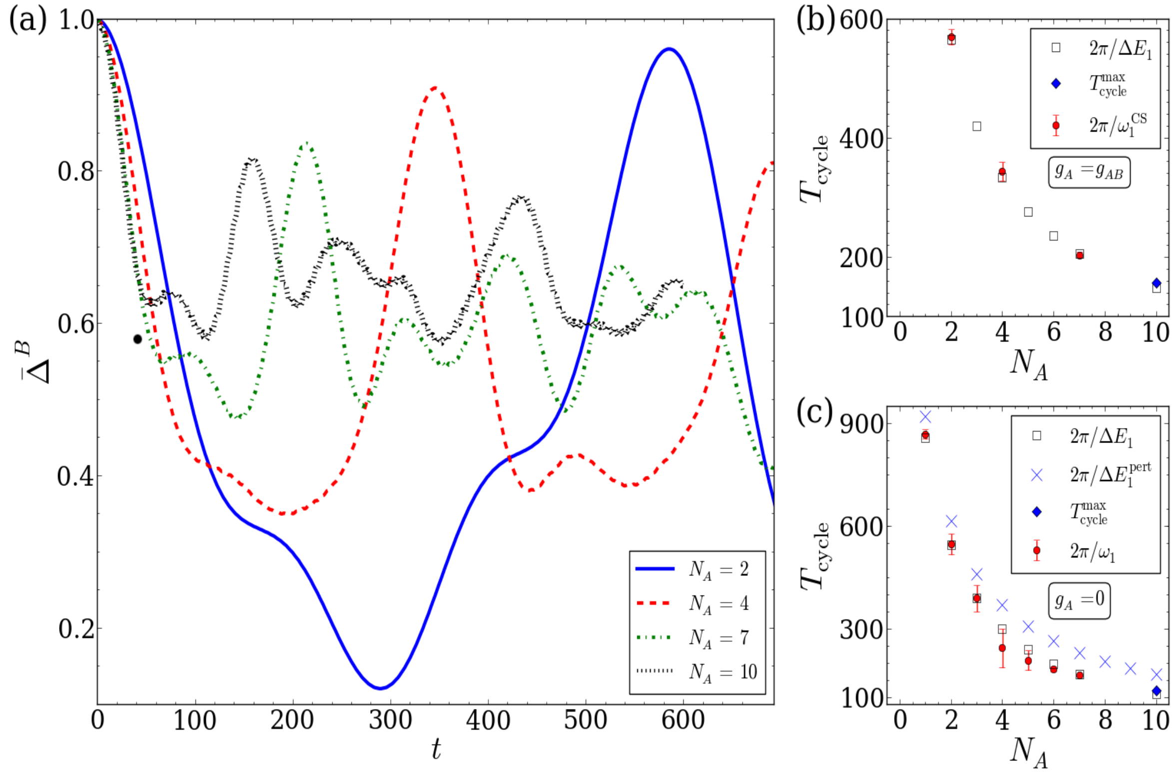
Setup and preparation



- 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.

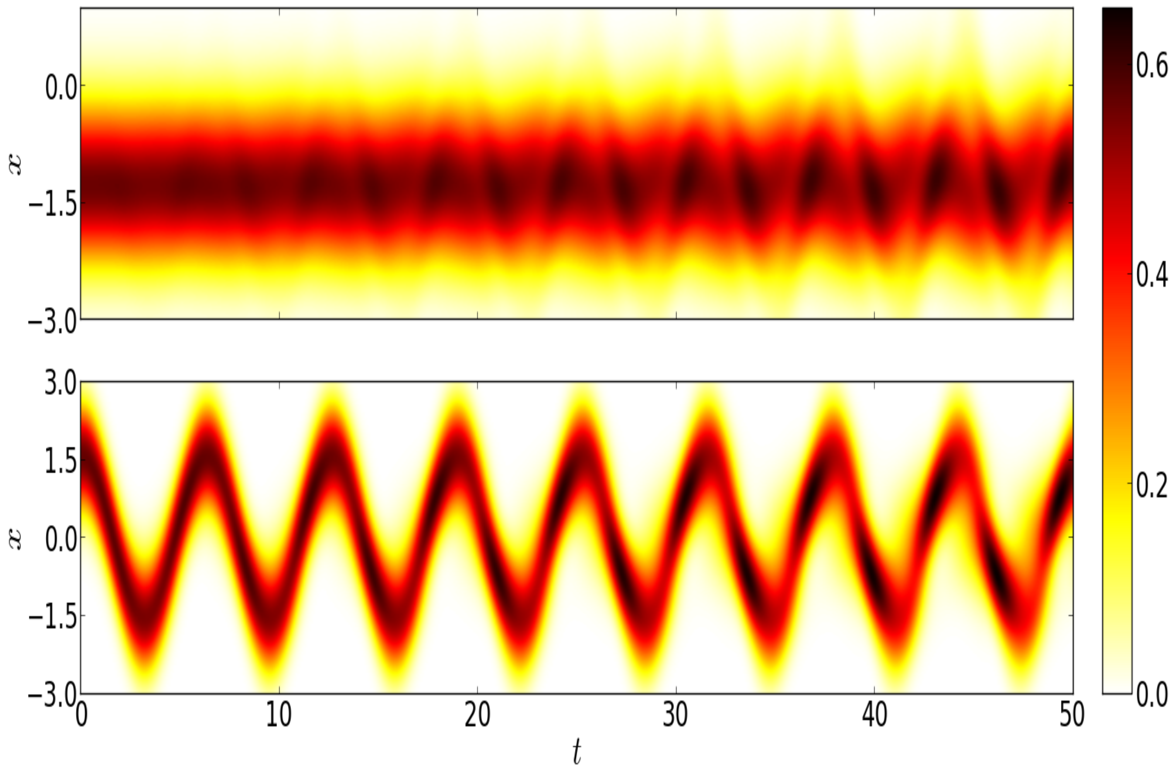
J. Knörzer, S. Krönke and P.S., NJP 17, 053001 (2015)

Energy transfer



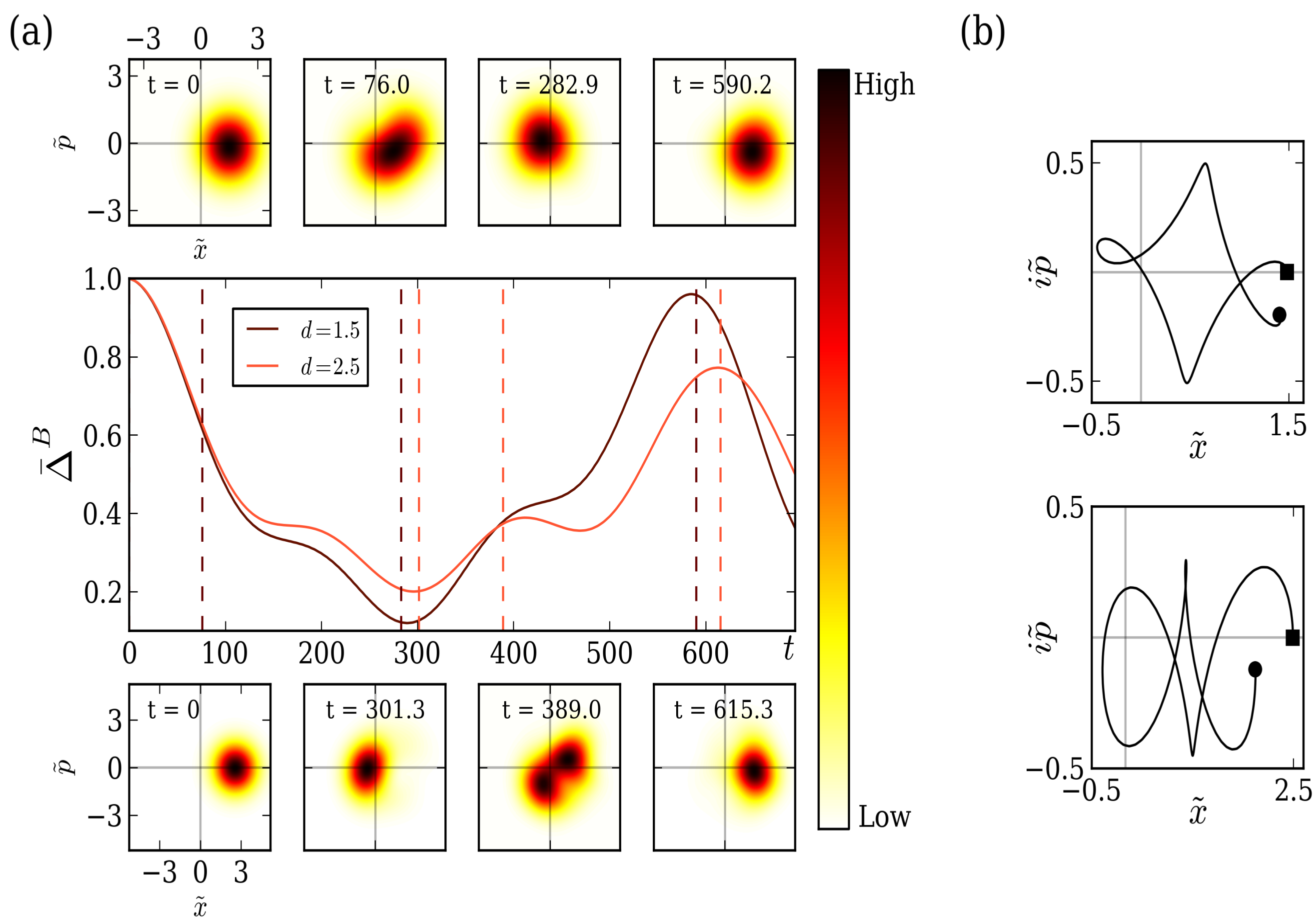
- Spatiotemporally localized inter-species coupling: Focus on long-time behaviour over many cycles.
- Energy transfer cycles with varying particle number of the ensemble

One-body densities



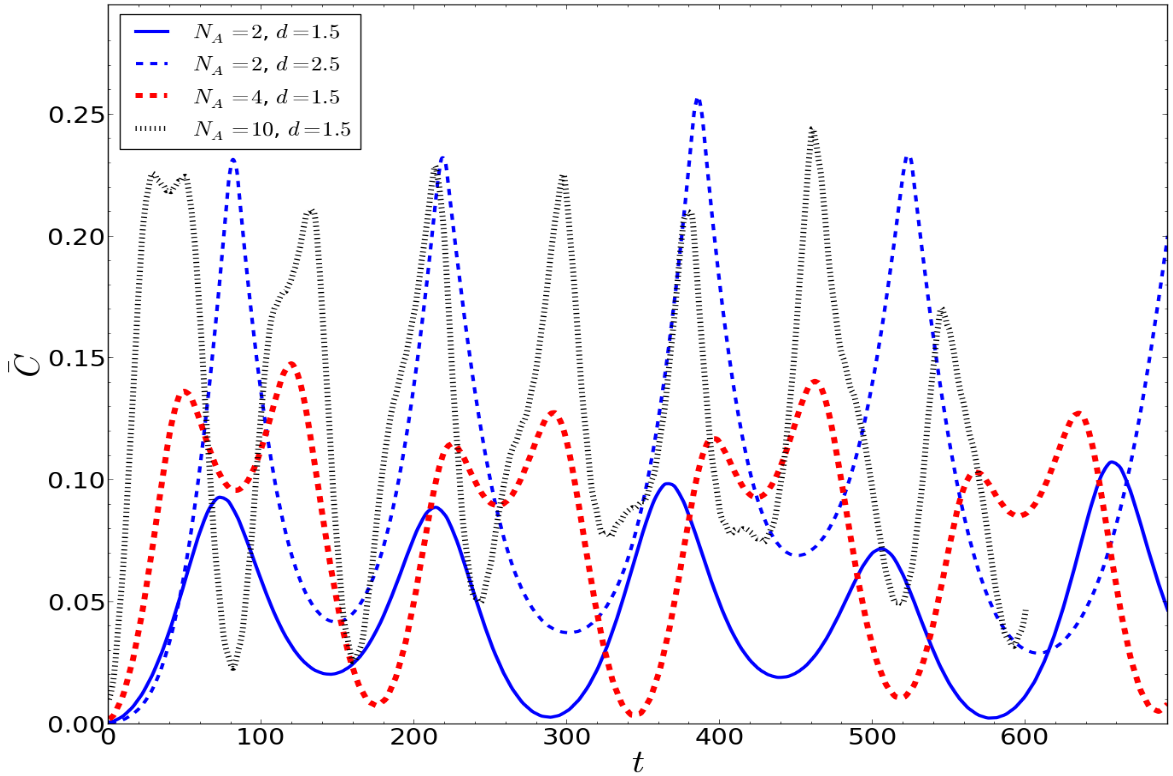
- Time-evolution of densities for the two species (ensemble-top, impurity-bottom) for first eight impurity oscillations.
- Impurity atom initiates oscillatory density modulations in ensemble atoms.
- Backaction on impurity atom.

Coherence analysis



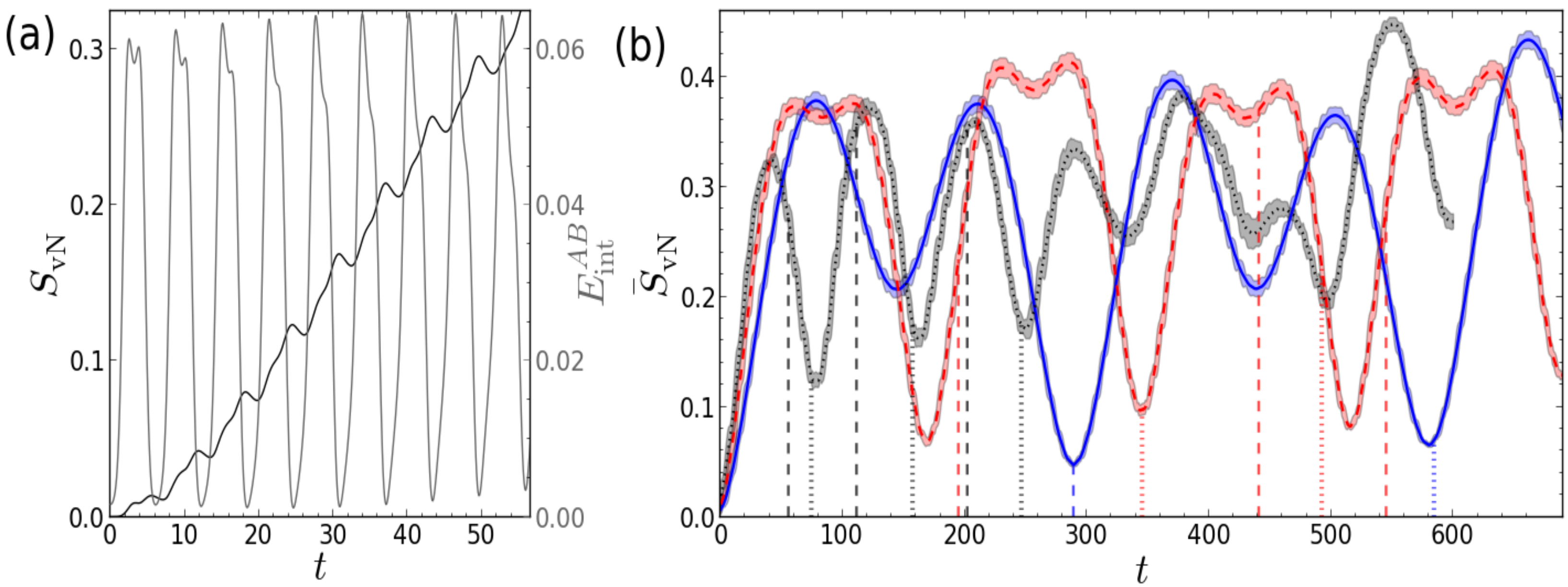
Time-evolution of normalized excess energy Δ_t^B with Husimi distribution $Q_t^B(z, z^*) = \frac{1}{\pi} \langle z | \hat{\rho}_t^B | z \rangle , \quad z \in \mathbb{C}$ of reduced density $\hat{\rho}_t^B$ at certain time instants.

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 $S_{\rm vN}(t)$ and inter-species interaction energy $E_{\rm int}^{AB}(t) = \langle \hat{H}_{AB} \rangle_t$.
- (b) Long-time evolution of $\bar{S}_{\rm vN}(t)$. 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)

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.
- Tunneling mechanisms
- 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 !