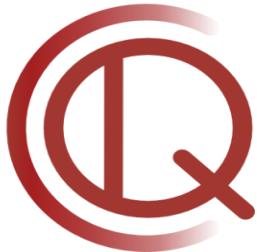


The laboratory to study  
quantum many-body  
dynamics

# Center for Quantum Dynamics



<http://QD-lab.org>

<http://mctdhb.org>

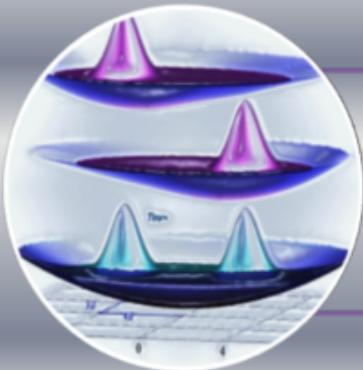
Alexej I. Streltsov

UNIVERSITÄT HEIDELBERG (Germany)

Many-body theory  
of bosons group  
Heidelberg, Germany

## **Talk: MCTDHB theory: predictions and applications**

624. Wilhelm und Else Heraeus-Seminar  
Simulating Quantum Processes and Devices  
Physikzentrum Bad Honnef,  
September 19 - 22, 2016



The laboratory to study  
quantum many-body  
dynamics

<http://qdlab.org>

## **Talk:** MCTDHB theory: predictions and applications

### **Outline:**

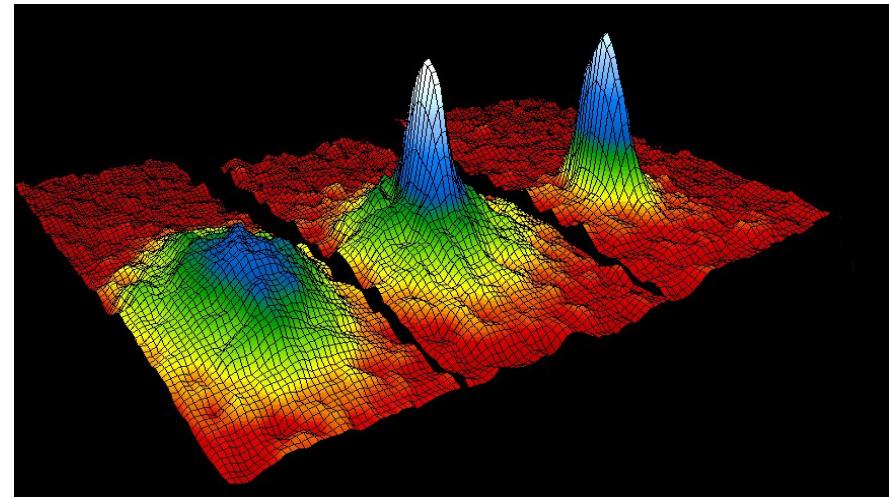
- Introduction to the field of ultracold atoms and molecules
- Idea behind the MCTDHB method and benchmarks
- Applications to BECs with Repulsive, Attractive, Short- and Long-range inter-boson interactions in 1-D-, 2-D-, 3-D...
- Condensation and Fragmentation: How to measure?
- MCTDHB-Laboratory package      <http://qdlab.org>
- Conclusions



The Nobel Prize in Physics 2001 was awarded jointly to Eric A. Cornell, Wolfgang Ketterle and Carl E. Wieman *"for the achievement of Bose-Einstein condensation in dilute gases of alkali atoms, and for early fundamental studies of the properties of the condensates"*

The density of the atomic cloud is shown, with temperature decreasing from left to right. The high peak, the Bose-Einstein condensate, emerges above the other atoms. The picture is from the JILA laboratory.

Bose-Einstein Condensation  
at 400, 200, and 50 nano-Kelvins (<http://www.colorado.edu/physics/2000/index.pl>)



$$\Psi(\mathbf{x}, \mathbf{t}) = \Psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N, \mathbf{t})$$

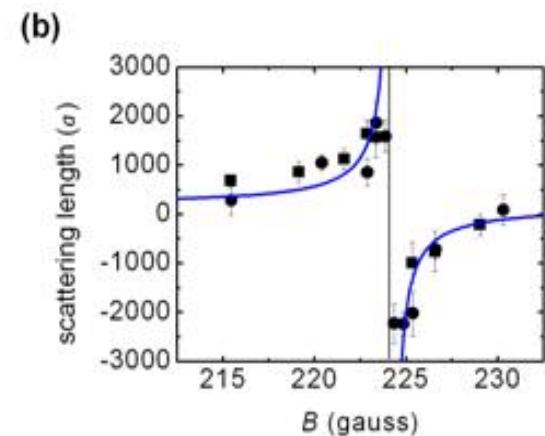
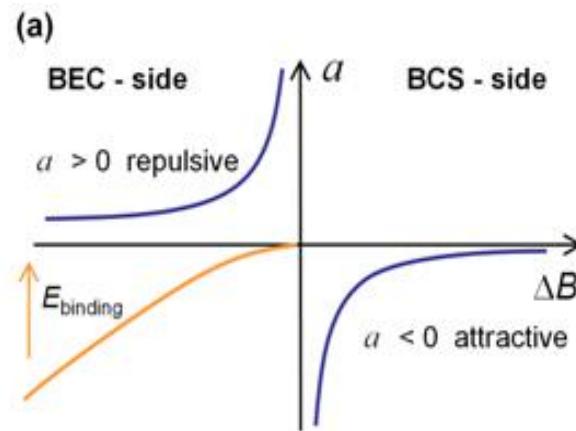
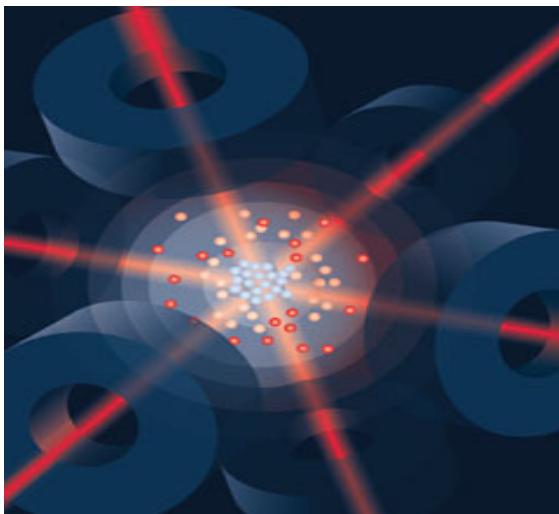
$$\rho(r, r'; \mathbf{t}) = \int \Psi^*(r, r_2, r_3, \dots, r_N; \mathbf{t}) \Psi(r', r_2, r_3, \dots, r_N; \mathbf{t}) dr_2 \dots dr_N = \sum_{k,q} \rho_{kq}(\mathbf{t}) \phi_k^*(r, \mathbf{t}) \phi_q(r', \mathbf{t})$$

The density of the many-particle wave-function is directly available in experiments

# All the terms of the Hamiltonian are under experimental control and can be manipulated

$$\hat{\mathbf{H}} = \sum_{i=1}^N \left( -\frac{1}{2m} \nabla_{\vec{r}_i}^2 + V(\vec{r}_i; \textcolor{red}{t}) \right) + \sum_{i < j} \lambda_0 W(\vec{r}_i, \vec{r}_j; \textcolor{red}{t})$$

BECs of alkaline, alkaline earth, and lanthanoid atoms  
( ${}^7\text{Li}$ ,  ${}^{23}\text{Na}$ ,  ${}^{39}\text{K}$ ,  ${}^{41}\text{K}$ ,  ${}^{85}\text{Rb}$ ,  ${}^{87}\text{Rb}$ ,  ${}^{133}\text{Cs}$ ,  ${}^{52}\text{Cr}$ ,  ${}^{40}\text{Ca}$ ,  ${}^{84}\text{Sr}$ ,  ${}^{86}\text{Sr}$ ,  ${}^{88}\text{Sr}$ ,  ${}^{174}\text{Yb}$ ,  ${}^{164}\text{Dy}$ , and  ${}^{168}\text{Er}$ )



The interatomic interaction can be widely varied with a magnetic Feshbach resonance... (Greiner Lab at Harvard.)

Magneto-optical trap  $\rightarrow \mathbf{V}(r, t)$

**1D-2D-3D: Control on dimensionality by changing the aspect ratio of the trap**

$$\mathbf{V}(x, y, z) = \frac{1}{2} m \omega_x^2 x^2 + \frac{1}{2} m \omega_y^2 y^2 + \frac{1}{2} m \omega_z^2 z^2$$

# Time-Dependent Schrödinger equation governs the physics of trapped ultra-cold atomic clouds

$$i\hbar \frac{\partial}{\partial t} \Psi(\mathbf{x},t) = \hat{\mathbf{H}} \Psi(\mathbf{x},t)$$

$$\hat{\mathbf{H}} = \sum_{i=1}^N \left( -\frac{1}{2m} \nabla_{\vec{r}_i}^2 + V(\vec{r}_i; \mathbf{t}) \right) + \sum_{i < j} \lambda_0 W(\vec{r}_i, \vec{r}_j; \mathbf{t})$$

One has to specify initial condition

$$\Psi(\mathbf{x}, \mathbf{t} = 0) = \Psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N, \mathbf{t} = 0)$$

and propagate  $\Psi(\mathbf{x}, \mathbf{t}) \rightarrow \Psi(\mathbf{x}, \mathbf{t} + \Delta t)$

To solve the Time-Dependent Many-Boson Schrödinger Equation

we apply the Multi Configurational Time Dependnet Hartree (for) Bosons method:

PRL 99, 030402 (2007), PRA 77, 033613 (2008)

It solves TDSE numerically exactly – see for benchmarking PRA 86, 063606 (2012)

<http://QDlab.org>

**Condensation:** O. Penrose and L. Onsager (1956)

**Fragmentation:** P. Nozieres and D. Saint James (1982)

$$\hat{\mathbf{H}} = \sum_{i=1}^N \left( -\frac{1}{2m} \nabla_{\vec{r}_i}^2 + V(\vec{r}_i; \textcolor{red}{t}) \right) + \sum_{i < j} \lambda_0 W(\vec{r}_i, \vec{r}_j; \textcolor{red}{t})$$

$$\rho(r, r'; \textcolor{red}{t}) = \int \Psi^*(r, r_2, \dots, r_N; \textcolor{red}{t}) \Psi(r', r_2, \dots, r_N; \textcolor{red}{t}) dr_2 \dots dr_N = \sum \rho_{kq}(\textcolor{red}{t}) \phi_k^*(r', \textcolor{red}{t}) \phi_q(r, \textcolor{red}{t})$$

$\xrightarrow{\text{Diagonalization}}$   $= \sum_i n_i \phi_i^{NO}(r, \textcolor{red}{t}) \phi_i^{*,NO}(r', \textcolor{red}{t}) = \sum_i n_i \left| \phi_i^{NO}(r = r', \textcolor{red}{t}) \right|^2$

**Natural analysis (eigenvalues and eigenvectors of the RDM):**

$n_i$  – natural occupation numbers  $\phi_i^{\text{NO}}$  – natural orbitals

**Condensation:**  $n_1 \approx N$  is macroscopic occupation Phys. Rev. 104 (1956)

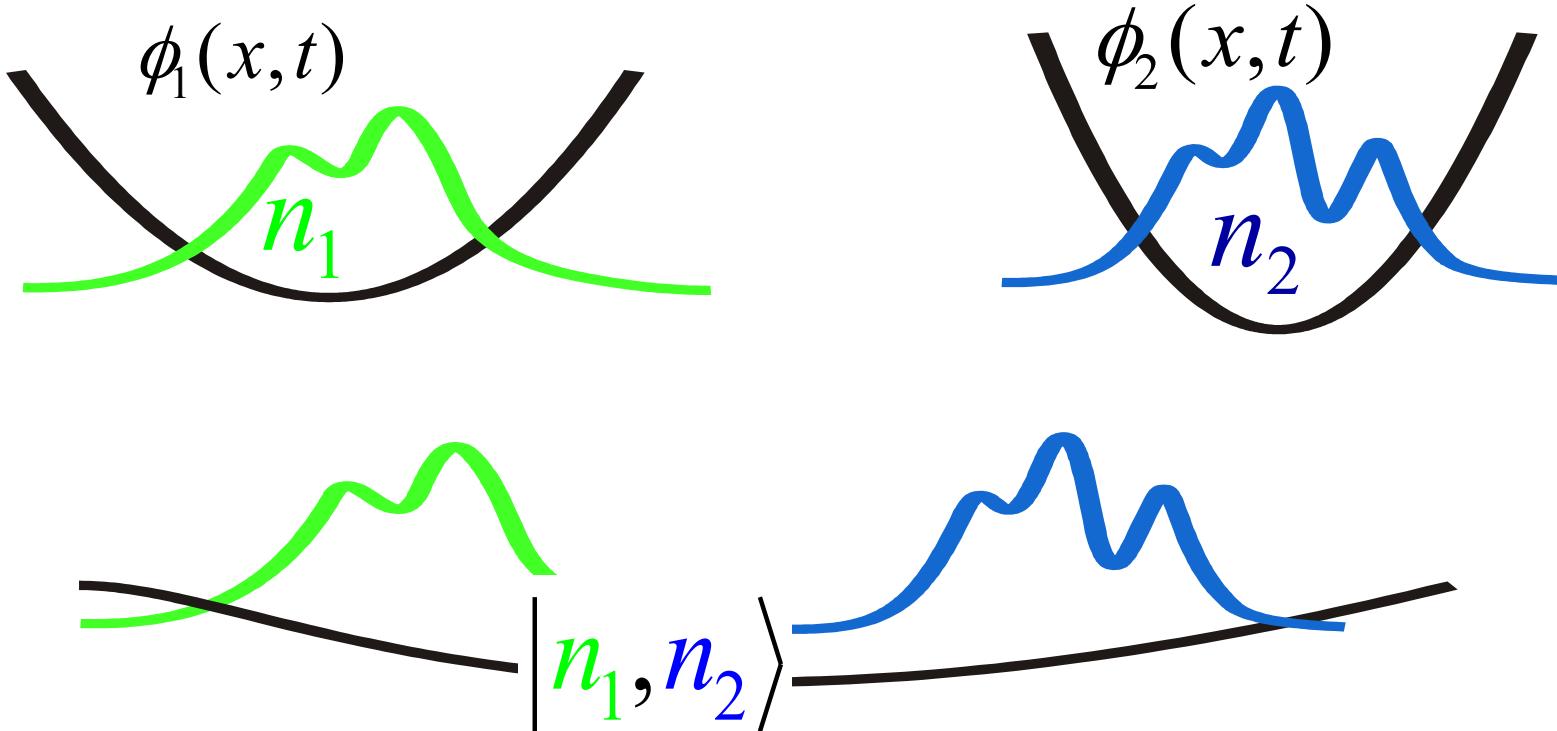
**Fragmentation:** several NO macroscopically occupied J. Phys. France 43, 1133 (1982)

e.g.  $n_1 \approx N/2$   $n_2 \approx N/2$  **2-Fold** fragmentation

# Multi-Configurational Time-Dependent Hartree for Bosons

## MCTDHB: Key idea

PRL 99, 030402 (2007), PRA 77, 033613 (2008)



$$\cdots C_{n_1-1, n_2+1}(t) |n_1-1, n_2+1\rangle + C_{n_1, n_2}(t) |n_1, n_2\rangle + C_{n_1+1, n_2-1}(t) |n_1+1, n_2-1\rangle \cdots$$

Orbitals  $\phi$ 's and expansion coefficients  $C_{n_1, n_2}$ 's  
are time-dependent, i.e., change during the evolution

# Multiconfigurational Time-Dependent Hartree for Bosons

## MCTDHB: Ideology

PRL 99, 030402 (2007), PRA 77, 033613 (2008)

**MCTDHB(M)** ansatz for the wave-function:  
linear combination of time-dependent permanents

$$\Psi_{MCTDHB(M)} = \sum_{i_1, i_2, \dots, i_M}^{F_N^M} C_{i_1, i_2, \dots, i_M}(t) \Phi_{i_1 i_2 \dots i_M}(x_1, \dots, x_N, t) = \sum_{i_1, i_2, \dots, i_M}^{F_N^M} C_{i_1, i_2, \dots, i_M}(t) |i_1 i_2 i_3 i_4 \dots i_M; \mathbf{t}\rangle$$

Every permanent  $|i_1 i_2 i_3 i_4 \dots i_M; \mathbf{t}\rangle$   
is a symmetrized time-dependent Hartree product

$$\Phi_{i_1 i_2 i_3 i_4 \dots i_M}(x_1, x_2, \dots, x_N, t) = S \underbrace{\phi_1(x_1, t) \dots \phi_1(x_{i_1}, t)}_{i_1} \underbrace{\dots \phi_2(x_{i_1+i_2}, t) \dots \phi_M(x_{N-i_M}, t)}_{i_2} \underbrace{\dots \phi_M(x_N, t)}_{i_M}$$

Limiting one-configurational **MCTDHB(M=1)** case  
gives the famous Gross-Pitaevskii mean-field theory

$$\Psi_{GP \equiv MCTDHB(1)} = \phi(x_1, t) \phi(x_2, t) \phi(x_3, t) \dots \phi(x_N, t) \rightarrow |N, 0, 0, \dots, 0; t\rangle$$

# MCTDHB(M=1) is fully equivalent to the famous Gross-Pitaevskii equation

$$\begin{cases} \mathbf{H}(t)\mathbf{C}(t) = i \frac{\partial \mathbf{C}}{\partial t} \\ i\hat{\mathbf{P}} \left| \frac{\partial \phi_j}{\partial t} \right\rangle = \hat{\mathbf{P}} \left[ \hat{h} \left| \phi_j \right\rangle + \sum_{k,s,q,l=1}^M \left\{ \rho(t) \right\}_{jk}^{-1} \rho_{ksql} \hat{W}_{sl} \left| \phi_q \right\rangle \right], \\ \hat{\mathbf{P}} = 1 - \sum_{j'=1}^M \left| \phi_{j'} \right\rangle \left\langle \phi_{j'} \right| \end{cases}$$

Gross-Pitaevskii mean-field theory  
Aka NLSE

$$\left( -\frac{1}{2m} \frac{\partial^2}{\partial x^2} + \lambda_0(N-1) |\phi(x,t)|^2 \right) \phi(x,t) = i \frac{\partial \phi(x,t)}{\partial t}$$

$$\begin{bmatrix} C_{N,0,0,L,0} \\ \dots \\ C_{0,0,L,N} \end{bmatrix} \rightarrow \begin{bmatrix} \rho_{kq} = \langle \Psi | b_k^\dagger b_q | \Psi \rangle \\ \rho_{ksql} = \langle \Psi | b_k^\dagger b_s^\dagger b_l b_q | \Psi \rangle \end{bmatrix}$$

$$\langle \Psi | b_k^\dagger b_k^\dagger b_k b_k | \Psi \rangle = \sum_{i_1, L, i_M} C_{i_1, L, i_M}^* C_{i_1, L, i_M} n_k (n_k - 1)$$

$$\begin{bmatrix} \phi_1 \\ \dots \\ \phi_M \end{bmatrix} \rightarrow \begin{bmatrix} h_{kq} = \int \phi_k^*(r, \textcolor{red}{t}) \hat{h}(r, t) \phi_q(r, \textcolor{red}{t}) dr \\ W_{ksql} = \int \phi_k^*(r, \textcolor{red}{t}) \phi_s^*(r', \textcolor{red}{t}) \hat{W}(r, r') \phi_q(r, \textcolor{red}{t}) \phi_l(r, \textcolor{red}{t}) dr dr' \end{bmatrix}$$

$$\Rightarrow \sum_{q=1} \left[ \rho_{kq} \hat{h} + \sum_{s,l=1} \rho_{ksql} \hat{W}_{sl} \right] \left| \phi_q \right\rangle; \quad \hat{W}_{sl} = \int \phi_s^*(r', \textcolor{red}{t}) \hat{W}(r, r') \phi_l(r, \textcolor{red}{t}) dr'$$

# Multi-Configurational Time-Dependent Hartree for Bosons, Fermions and Mixtures

$$\Psi(x_1, x_2, \dots, x_N, t) = \sum_{i_1, i_2, i_3, i_M}^{F_N^M} C_{i_1, i_2, i_3, i_M}(t) \Phi_{i_1 i_2 i_3 i_4 \dots i_M}(x_1, x_2, \dots, x_N, t)$$

e.g. Bosons:

$$\Phi_{i_1 i_2 i_3 i_4 \dots i_M}(x_1, x_2, \dots, x_N, t) = \underbrace{\varphi_1(x_1, t) \cdots \varphi_1(x_{i_1}, t)}_{i_1} \cdots \underbrace{\varphi_M(x_{N-i_M}, t) \cdots \varphi_M(x_N, t)}_{i_M}$$

- ✓ **time-dependent** orbitals are determined variationally!  
This reduces the number of functions needed substantially
- ✓ expressions derived are for general two-, three-... many-body interactions

**MCTDHB:**

A.I. Streltsov, O.E. Alon, and L.S. Cederbaum, Phys. Rev. Lett. **99**, 030402 (2007)

O.E. Alon, A.I. Streltsov, and L.S. Cederbaum, Phys. Rev. A **77**, 033613 (2008)

J. Zanghellini, M. Kitzler, C. Fabian, T. Brabec, and A. Scrinzi, Laser Phys. **13**, 1064 (2003)

T. Kato and H. Kono, Chem. Phys. Lett. **392**, 533 (2004)

M. Nest, T. Klamroth, and P. Saalfrank, J. Chem. Phys. **122**, 124102 (2005)

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O.E. Alon, A.I. Streltsov, and L.S. Cederbaum, Phys. Rev. A **76**, 062501 (2007)

O.E. Alon, A.I. Streltsov, and L.S. Cederbaum, Phys. Rev. A **79**, 022503 (2008)

O.E. Alon, A.I. Streltsov, L.S. Cederbaum, K. Sakmann, A.U.J. Lode, J. Grond, Chem. Phys. **401**, 2 (2012)

J. Grond, A.I. Streltsov, L.S. Cederbaum, and O.E. Alon, Phys. Rev. A **86**, 063607 (2012),

O.E. Alon, A.I. Streltsov, L.S. Cederbaum, J. Chem. Phys. **140**, 034108 (2014)

**MCTDHF:**

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T. Kato and H. Kono, Chem. Phys. Lett. **392**, 533 (2004)

M. Nest, T. Klamroth, and P. Saalfrank, J. Chem. Phys. **122**, 124102 (2005)

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O.E. Alon, A.I. Streltsov, and L.S. Cederbaum, Phys. Rev. A **79**, 022503 (2008)

O.E. Alon, A.I. Streltsov, L.S. Cederbaum, K. Sakmann, A.U.J. Lode, J. Grond, Chem. Phys. **401**, 2 (2012)

J. Grond, A.I. Streltsov, L.S. Cederbaum, and O.E. Alon, Phys. Rev. A **86**, 063607 (2012),

O.E. Alon, A.I. Streltsov, L.S. Cederbaum, J. Chem. Phys. **140**, 034108 (2014)

**MCTDH-XY:**

**MCTDH-conversion:**

**Recursive formulation:**

**Linear Response:**

# Benchmarks: PRA 86, 063606 (2012)

## **MCTDHB vs. Exact Results**

### **Harmonic Interaction Model (HIM)**

HIM is exactly solvable in *any* D dimensions

$$\hat{H} = \sum_{i=1}^N \left( -\frac{1}{2} \partial_{\vec{r}_i}^2 + \frac{1}{2} \varpi^2 \vec{r}_i^2 \right) + \sum_{i \neq j} K_0 (\vec{r}_i - \vec{r}_j)^2$$

by transformation to the center-of-mass and relative coordinates:

$$\vec{q}_i = \frac{1}{\sqrt{j(j+1)}} \sum_{i=1}^j (\vec{r}_{j+1} - \vec{r}_i), \quad j = 1, \dots, N-1; \quad \vec{q}_N = \frac{1}{\sqrt{N}} \sum_{i=1}^N \vec{r}_i \quad \delta_N = \sqrt{\varpi^2 + 2N K_0}$$

$$\hat{H} = \sum_{i=1}^{N-1} \left( -\frac{1}{2} \partial_{\vec{q}_i}^2 + \frac{1}{2} \delta_N^2 \vec{q}_i^2 \right) - \frac{1}{2} \partial_{\vec{q}_N}^2 + \frac{1}{2} \varpi^2 \vec{q}_N^2$$

$$E_{exact}^{Ground State} = \frac{D}{2} (N-1) \delta_N + \frac{D}{2} \varpi$$

# Benchmarks - Static: PRA 86, 063606 (2012)

***MCTDHB vs. Exact Results. Exact HIM Results***

**HIM Ground State – enormous relevance of the self-consistency**

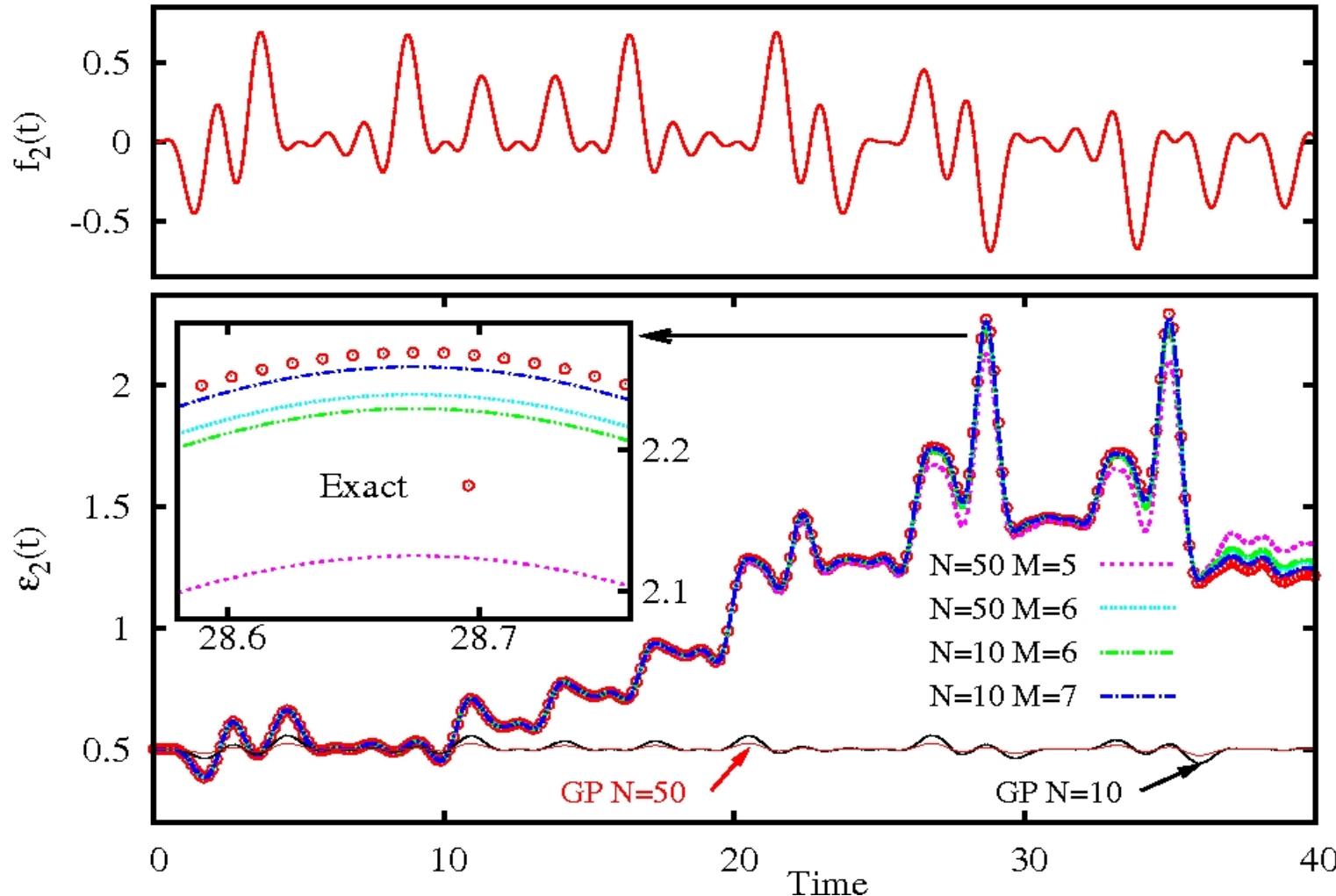
M	N=10	N=100	N=1000
1	7.071067811865483	70.71067811865483	707.1067811865483
2	7.038769026303168	70.68016951747168	707.0764334257315
3	7.038350652406389	70.68012541218675	707.0764289871865
4	7.038348424909910	70.68012539174549	
5	7.038348415349058	70.68012539173762	
6	7.038348415311494		
7	7.038348415311018		
$E_{\text{exact}}$	7.038348415311011	70.68012539173752	707.0764289869851

# Benchmarks-Dynamics: PRA 86, 063606 (2012)

**MCTDHB vs. Exact Results**

Driven Time-dependent HIM

Driven by  $f_2(t) = \sin(t)\cos(2t)\sin(0.5t)\sin(0.4t)$ ,  $N=10$ ,  $N=50$ ,  $K_0 = 0.5$



# Fragmentation phenomena with MCTDHB

## Heidelberg:

**Ramp-up a barrier:** PRL 99, 030402 (2007)

**Interference:** PRL 98, 110405 (2007)

**Fragmentons:** PRL 100, 130401 (2008)

**CATons:** Formation PRA 80, 043616 (2009); Efficient generation JPB, 42 091004 (2009)

**Fragmentation in 3D:** PRL 100, 040402 (2008); PRA 82, 033613 (2010)

**BJJs:** Exact dynamics of Josephson junctions: PRL 103, 220601 (2009); PRA 82, 013620 (2010)

**Bright solions:** Swift loss of coherence: PRL 106, 240401 (2011)

**How bosons tunnel to open space:** Proc. Natl. Acad. Sci. 109, 13521 (2012)

**Finite- and long-range 1-2-3D:** PRA 88, 041602(R) (2014); PRA 87, 033631 (2013), PRA 89, 061602(R) (2014)

**Tunneling in 2D:** PRA 90, 043620 (2014), PRA 92, 043627 (2014)

## Graz/Vienna Heidelberg-Hamburg-Ulm:

**Optimal control of number squeezing:** PRA 79, 021603 (2009), PRA 80, 053625 (2009)

**Optimal control CRAB-MCTDHB:** PRA 92, 062110 (2015)

**Interferometry:** NJP 12, 065036 (2010), PRA 84, 023619 (2011)

## Vienna II:

**Wave Chaos and depletion:** PRA 86, 013630 (2012), J. Phys.: Conf. Ser. 488 012032 (2014)

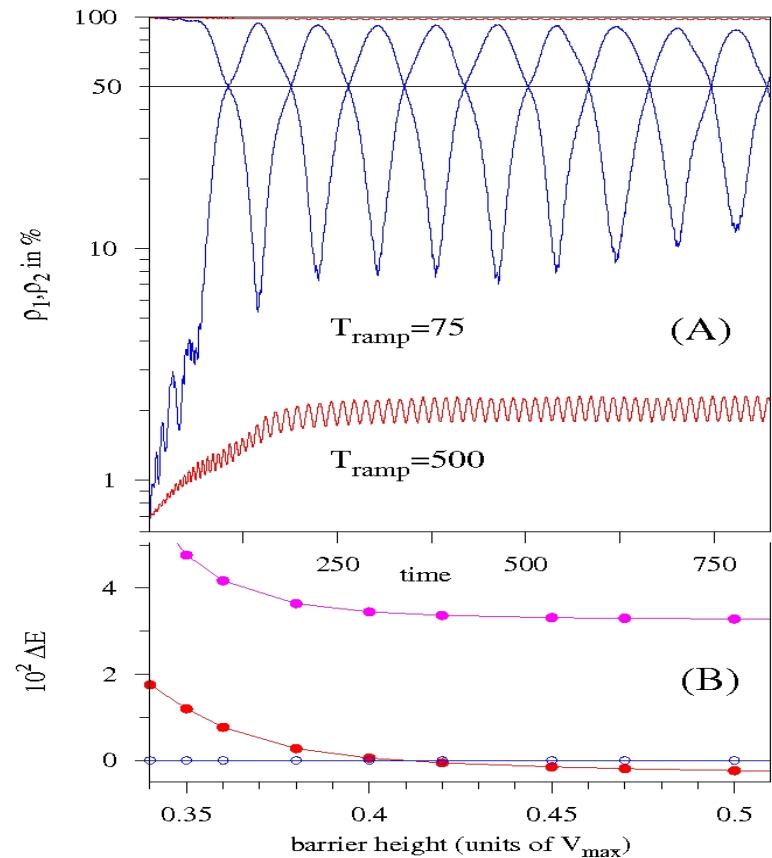
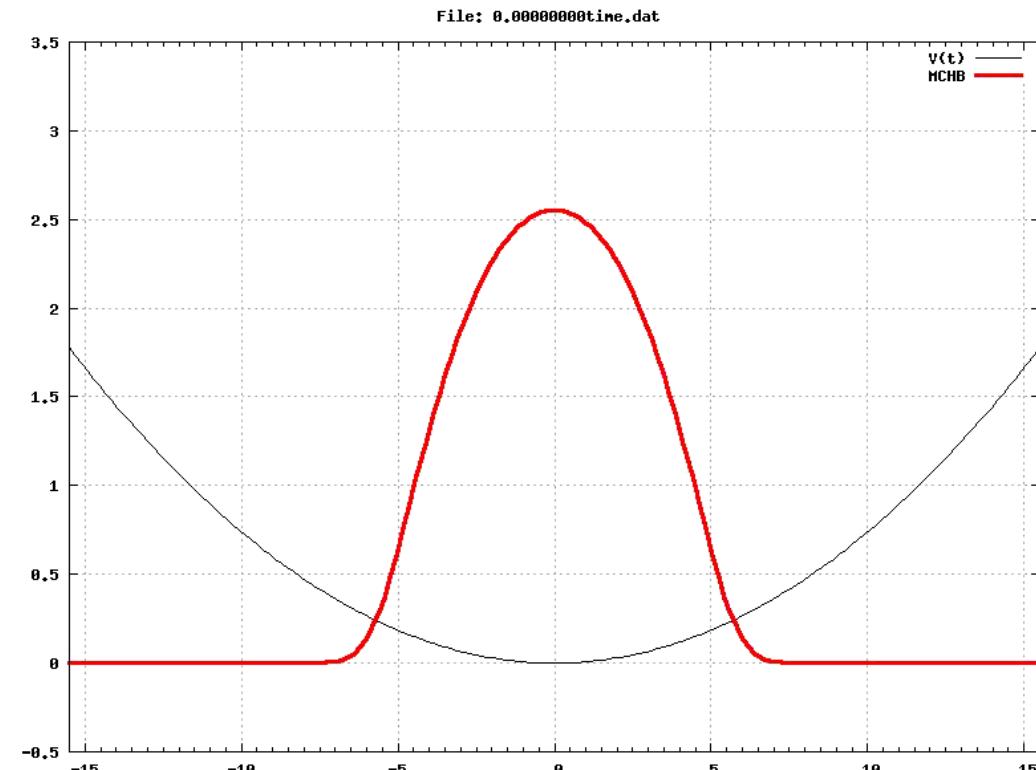
**Just/recently started:** Aarhus, Berkeley, Barcelona, Basel, Cambridge, Dubna, Haifa,  
Hamburg, Hannover, Kaiserslautern, São Paulo, Stanford, Ulm, ...

**want to join?**

<http://MCTDHB.org> <http://qdlab.org>

# Fragmentation phenomena with MCTDHB

**Repulsive BECs** - is split onto two by ramping-up a Gaussian time-dependent barrier **PRL 99, 030402 (2007)**

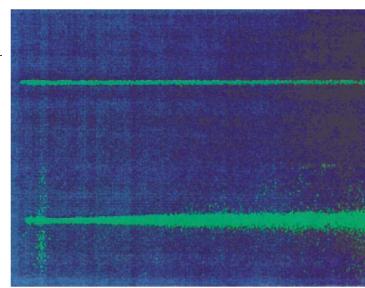


**(i) Adiabatic regime** initial condensed ground-state evolves towards the ground two-fold fragmented eigenstate of the final trap

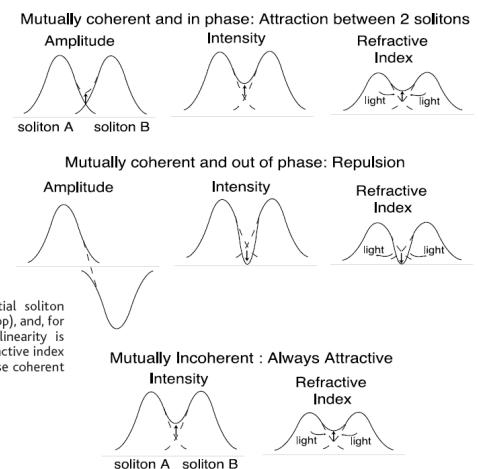
**(ii) Inverse regime** time-dependent state stays condensed during all the evolution and thereby evolves to a non-ground many-body eigenstate

# Optical Spatial Solitons and Their Interactions: Universality and Diversity

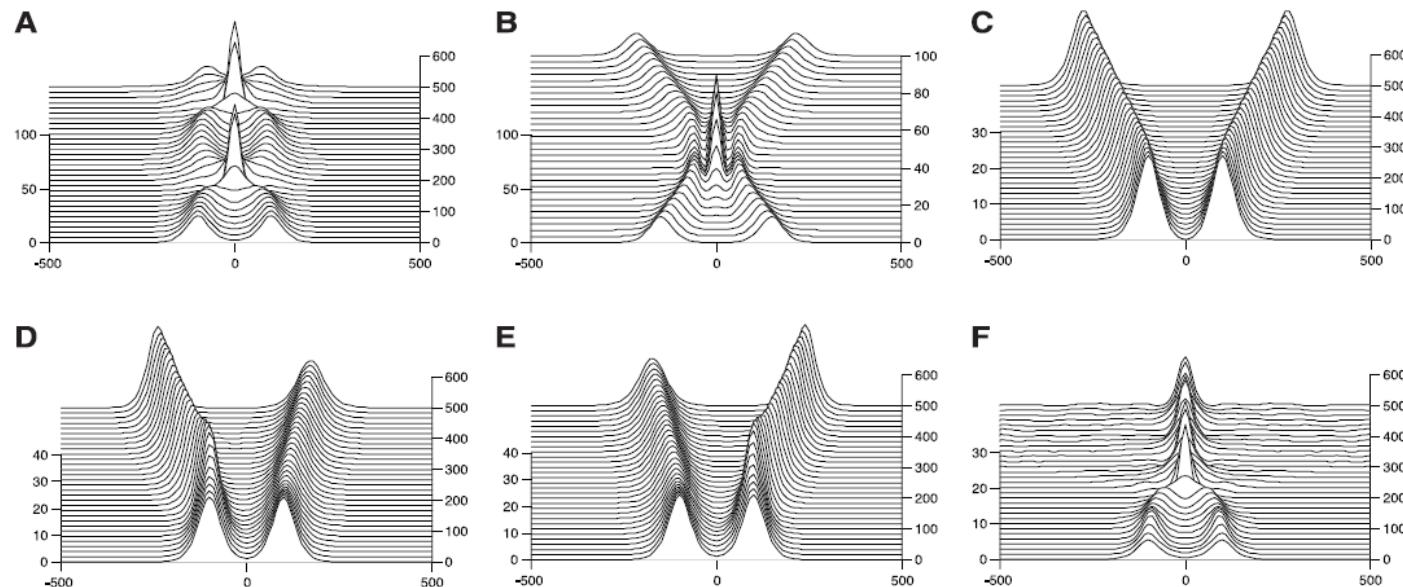
George I. Stegeman<sup>1</sup> and Mordechai Segev<sup>2,3</sup>



**Fig. 2 (above).** A top view photograph of a 10- $\mu\text{m}$ -wide spatial soliton propagating in a strontium barium niobate photorefractive crystal (top), and, for comparison, the same beam diffracting naturally when the nonlinearity is "turned off" (bottom). (23) **Fig. 3 (right).** Schematic of the refractive index spatial distribution for a collision between in-phase and out-of-phase coherent spatial solitons.



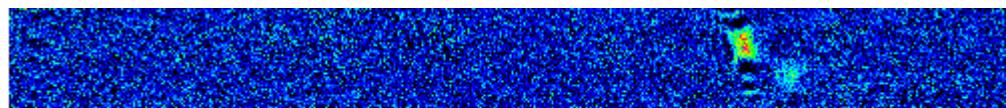
**Fig. 4.** Beam evolution calculations of the interactions between two solitons for the following cases: (A) Parallel input trajectories, in-phase Kerr solitons; (B) converging input trajectories, in-phase Kerr solitons; (C) parallel input trajectories, out-of-phase Kerr solitons; (D) parallel input trajectories,  $\pi/2$  relative phase between Kerr solitons; (E) parallel input trajectories,  $3\pi/2$  relative phase between Kerr solitons; and (F) fusion of two solitons input on parallel trajectories in saturating nonlinear media for "small" input separations.



# Formation of a Matter-Wave Bright Soliton

L. Khaykovich,<sup>1</sup> F. Schreck,<sup>1</sup> G. Ferrari,<sup>1,2</sup> T. Bourdel,<sup>1</sup>  
J. Cubizolles,<sup>1</sup> L. D. Carr,<sup>1</sup> Y. Castin,<sup>1</sup> C. Salomon<sup>1\*</sup>

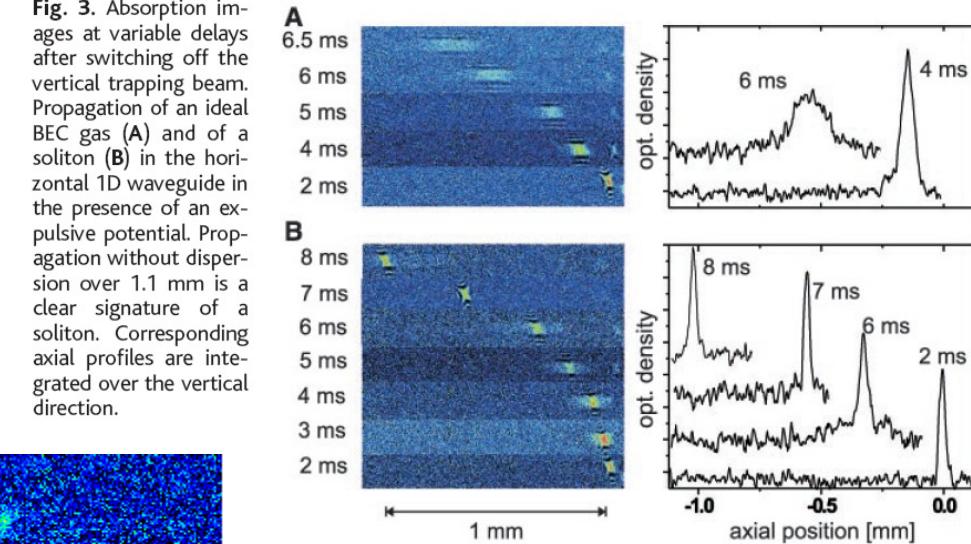
We report the production of matter-wave solitons in an ultracold lithium-7 gas. The effective interaction between atoms in a Bose-Einstein condensate is tuned with a Feshbach resonance from repulsive to attractive before release in a one-dimensional optical waveguide. Propagation of the soliton without dispersion over a macroscopic distance of 1.1 millimeter is observed. A simple theoretical model explains the stability region of the soliton. These matter-wave solitons open possibilities for future applications in coherent atom optics, atom interferometry, and atom transport.



Absorption images at variable delays (2–8 ms) after switching off the vertical beam  
Propagation of a soliton in the horizontal 1D guide in presence of an expulsive potential

1292

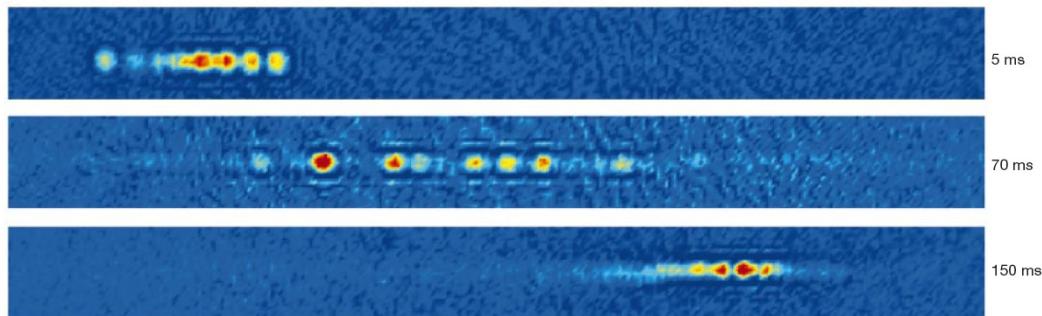
17 MAY 2002 VOL 296 SCIENCE www.sciencemag.org



## Formation and propagation of matter-wave soliton trains

Kevin E. Strecker\*, Guthrie B. Partridge\*, Andrew G. Truscott\*,† & Randall G. Hulet\*

\* Department of Physics and Astronomy and Rice Quantum Institute, Rice University, Houston, Texas 77251, USA



**Figure 4** Repulsive interactions between solitons. The three images show a soliton train near the two turning points and near the centre of oscillation. The spacing between solitons is compressed at the turning points, and spread out at the centre of the oscillation. A simple model based on strong, short-range, repulsive forces between nearest-neighbour solitons indicates that the separation between solitons oscillates at approximately twice the trap frequency, in agreement with observations. The number of

solitons varies from image to image because of shot to shot experimental variations, and because of a very slow loss of soliton signal with time. As the axial length of a soliton is expected to vary as  $1/N$  (ref. 11), solitons with small numbers of atoms produce particularly weak absorption signals, scaling as  $N^2$ . Trains with missing solitons are frequently observed, but it is not clear whether this is because of a slow loss of atoms, or because of sudden loss of an individual soliton.

## Formation of Bright Matter-Wave Solitons during the Collapse of Attractive Bose-Einstein Condensates

Simon L. Cornish,<sup>1,\*</sup> Sarah T. Thompson,<sup>2</sup> and Carl E. Wieman<sup>2</sup>

PRL 112, 060401 (2014)

PHYSICAL REVIEW LETTERS

week ending  
14 FEBRUARY 2014

## Evaporative Production of Bright Atomic Solitons

P. Medley, M. A. Minar, N. C. Cizek, D. Berryrieser, and M. A. Kasevich<sup>\*</sup>  
*Department of Physics, Stanford University, Stanford, California 94305-4060, USA*  
 (Received 19 December 2012; published 14 February 2014)

We describe a method of producing bright atomic solitons of  $^7\text{Li}$  through efficient radio frequency evaporation in a combined magnetic and optical trap. Solitons released in a magnetic waveguide propagate without dispersion, with lifetimes limited by two-body dipolar relaxation. We show how the method can be used to deterministically produce pairs of solitons.

DOI: 10.1103/PhysRevLett.112.060401

PACS numbers: 03.75.Lm, 67.85.-d

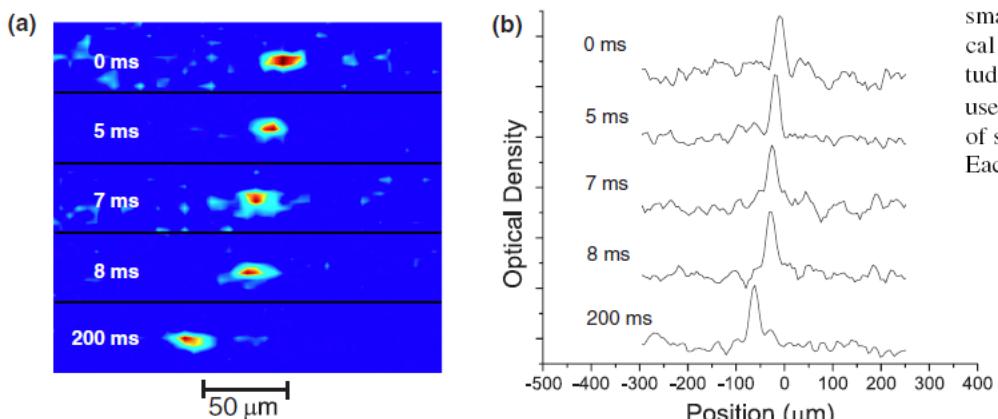


FIG. 2 (color online). (a) Absorption images and (b) axial profiles of solitons after various 1D times of flight in an expulsive waveguide, with curvature at the center of  $|\omega| = 2\pi \times 20$  Hz for all but the 200 ms time of flight experiment, which had  $|\omega| = 2\pi \times 5$  Hz. Each picture is an average of 3 shots.

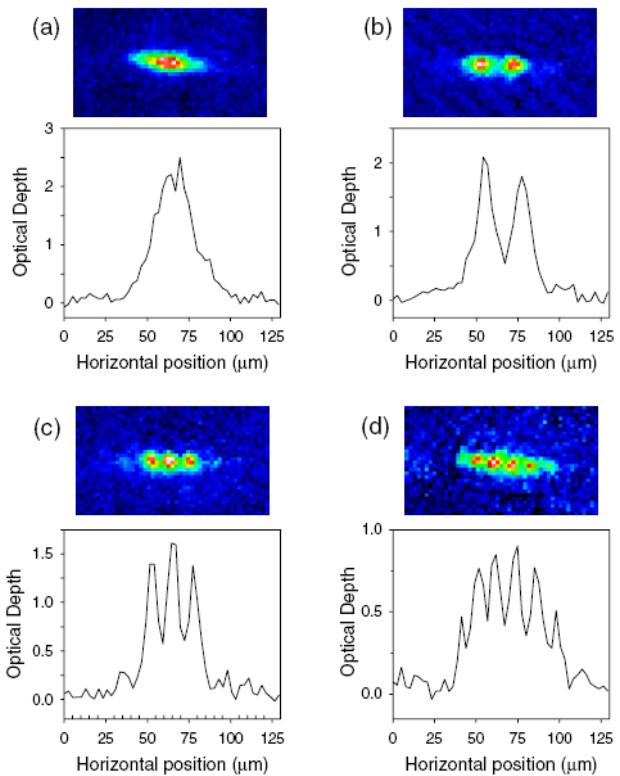
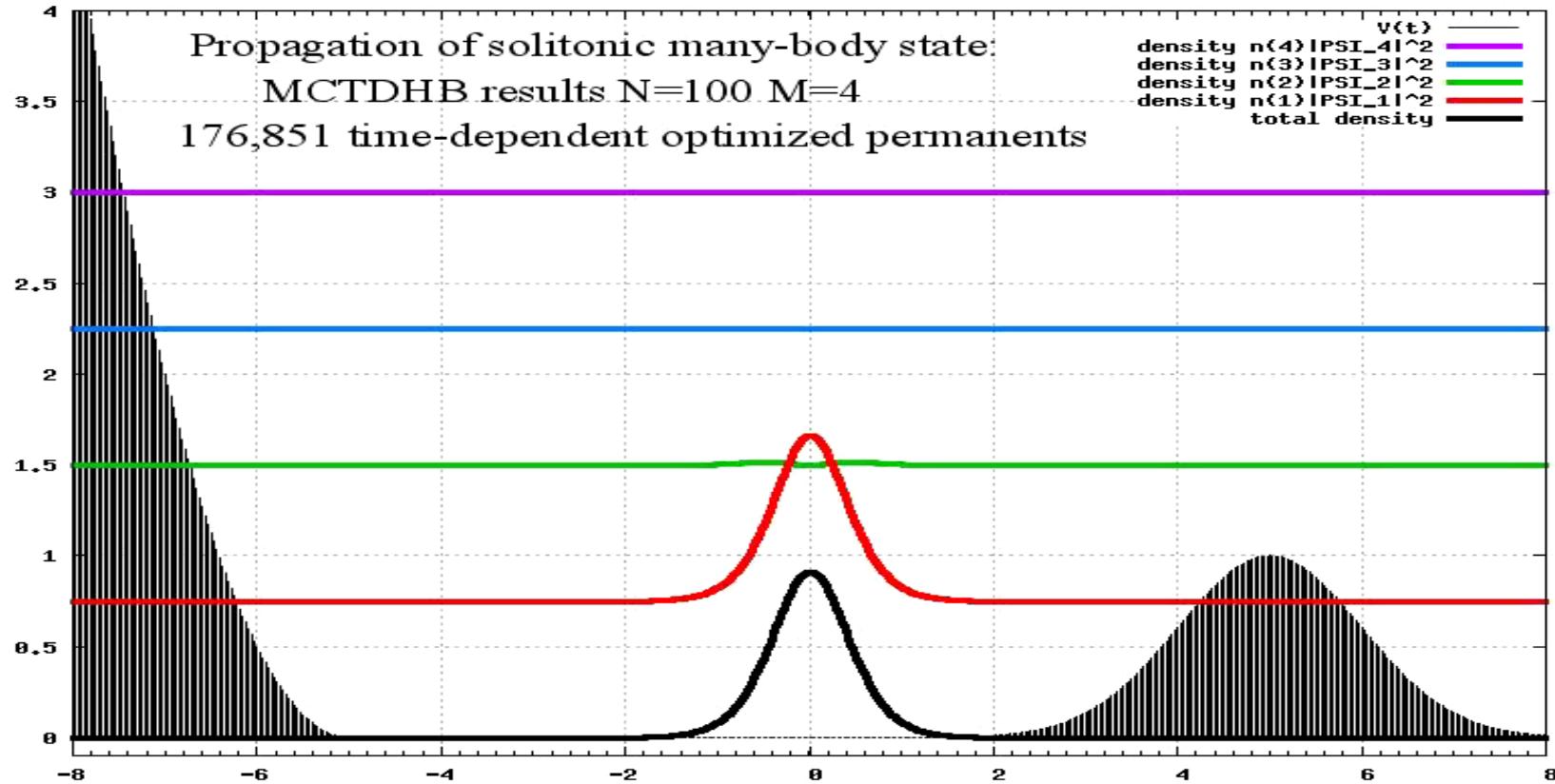


FIG. 3 (color online). Images and cross sections of remnant condensates. (a) When the magnitude of  $a_{\text{collapse}}$  is sufficiently small a single remnant condensate containing less than the critical number is observed to survive the collapse. When the magnitude of  $a_{\text{collapse}}$  is larger and/or larger initial condensates are used, the remnant condensate is observed to split into a number of solitons determined by the conditions of the collapse (b)–(d). Each image is  $77 \times 129 \mu\text{m}$ .

# Dynamically stable, localized quantum many-body Soliton exists at the many-body level

$$\rho(r, r'; \textcolor{red}{t}) = \int \Psi^*(r, r_2, \dots, r_N; \textcolor{red}{t}) \Psi(r', r_2, \dots, r_N; \textcolor{red}{t}) dr_2 \dots dr_N = \sum_{k,q} \rho_{kq}(\textcolor{red}{t}) \phi_k^*(r, \textcolor{red}{t}) \phi_q(r', \textcolor{red}{t}) = \sum_i n_i |\phi_i^{NO}(r = r', \textcolor{red}{t})|^2$$



Initial wave-packet: location at  $x=0$ , velocity  $\vec{v} = -1.0$   
Left: wall  $(x+5)^2/2$  Right: barrier  $\text{Exp}(-(x-5)^2/2)$

# Surprises in Attractive 1D (**Beyond GP**)

Technion/Zagreb/Beer Sheva

H. Buljan, M. Segev, and A. Vardi PRL 95, 180401 (2005)

Paris

Ch. Weiss and Y. Castin PRL 102, 010403 (2009)

Heidelberg

**Fragmentons:** PRL 100, 130401 (2008)

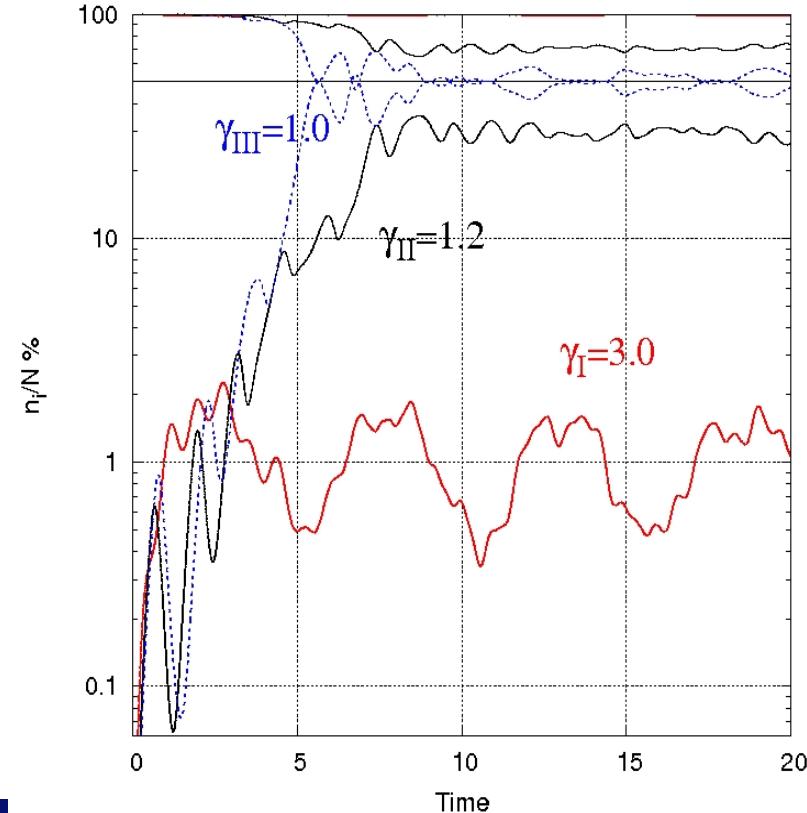
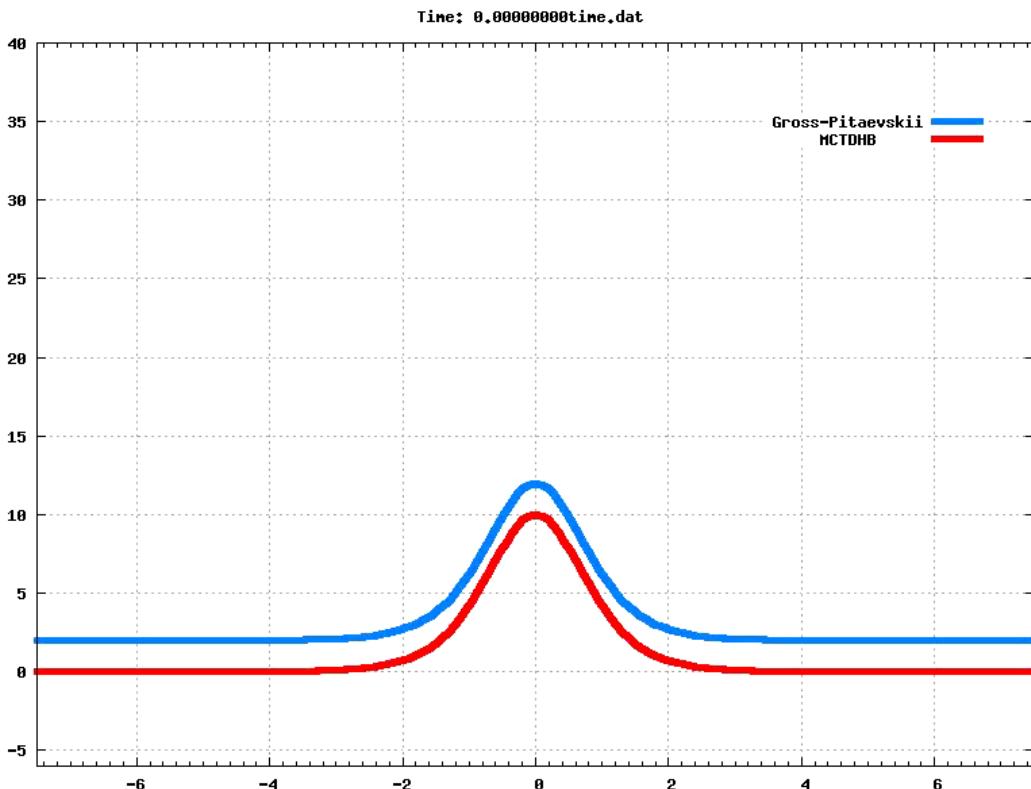
**Catons:** Formation PRA 80, 043616 (2009)

Efficient generation JPB 42, 091004 (2009)

**Death of soliton trains:** PRL 106, 240401 (2011)

# Fragmentation phenomena with the MCTDHB

**Attractive BECs – The initially coherent wave-packet can dynamically dissociate PRL 100, 130401 (2008)**  
into two parts when its energy exceeds a threshold value - formation of Fragmentons



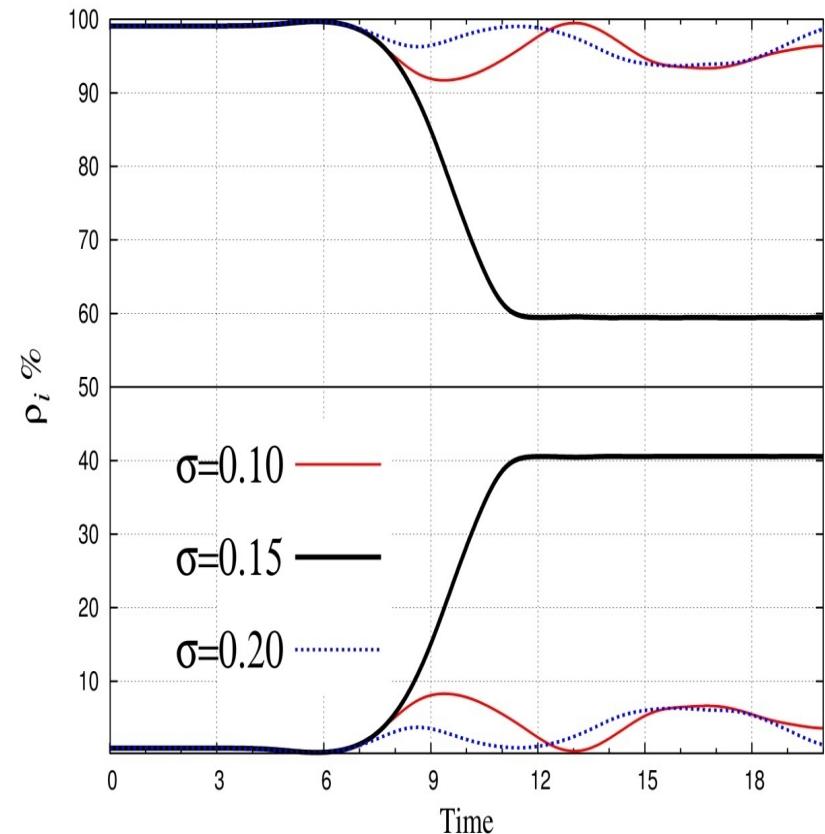
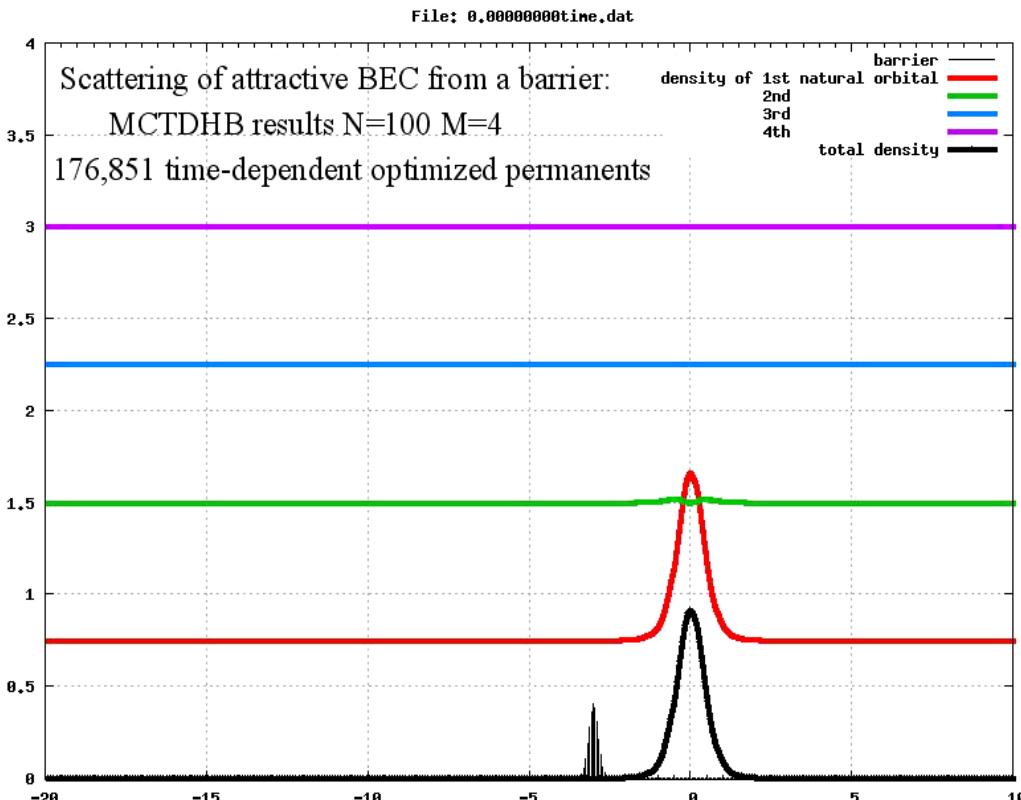
- ✓ The time-dependent GP theory applied to the same initial state does not show up the splitting  
the split object fragmenton possesses remarkable properties:  
(1)two-fold fragmented, (2) propagates almost without dispersion (3) delocalized NO

# Fragmentation phenomena with *the MCTDHB*

**Attractive BECs** – Attractive BEC is scattered from the barrier

PRA 80, 043616 (2009)

(Formation of time-dependent Schrödinger cat-like state – **CATon** )



Efficient generation of Schrödinger cats

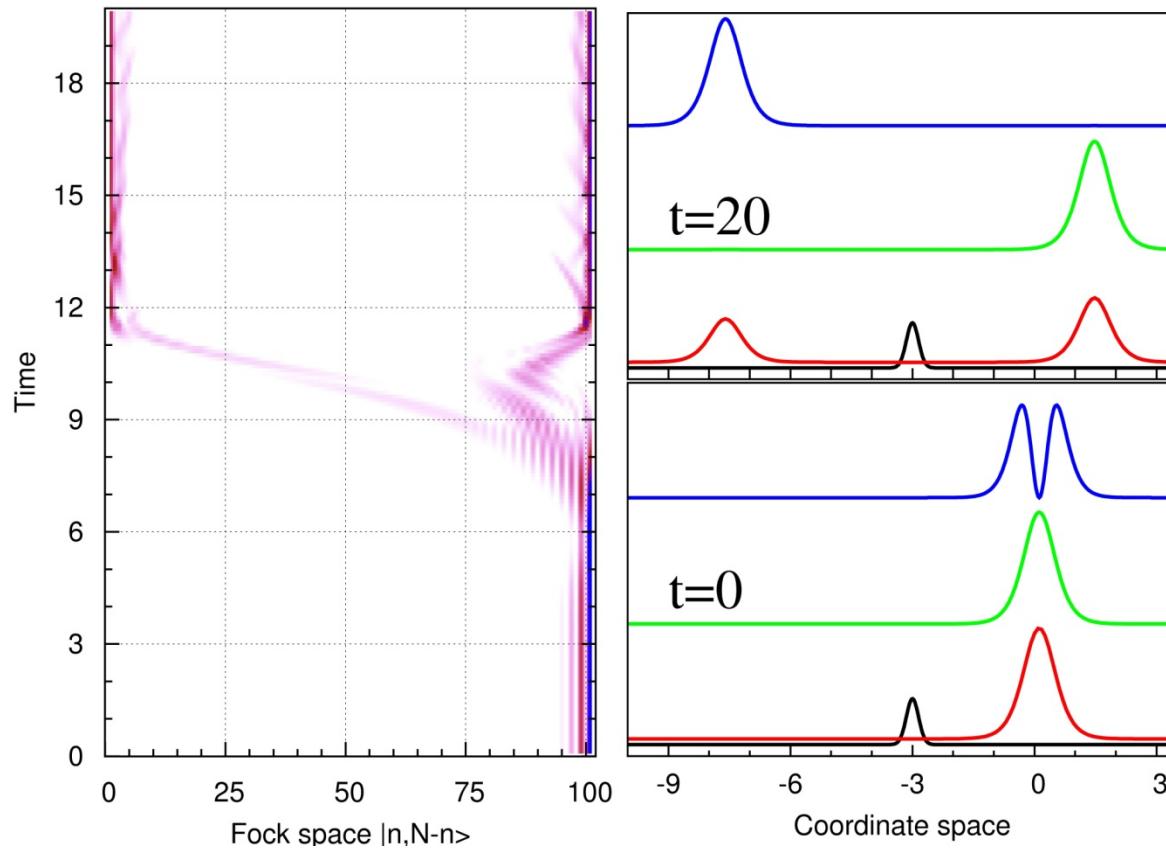
JPB 42, 091004 (2009)

Attractive BEC is threaded by a potential barrier

<http://QDlab.org>

# Analysis of split case (proof that the split object is a Schrödinger cat state)

Fock space is spanned by:  $|N,0\rangle, |N-1,1\rangle, \dots, |1,N-1\rangle, |0,N\rangle$  configurations



**t=20:**

mainly  $|N,0\rangle$  and  $|0,N\rangle$  contribute, respective orbitals are localized at **left (blue)** and **right (green)**

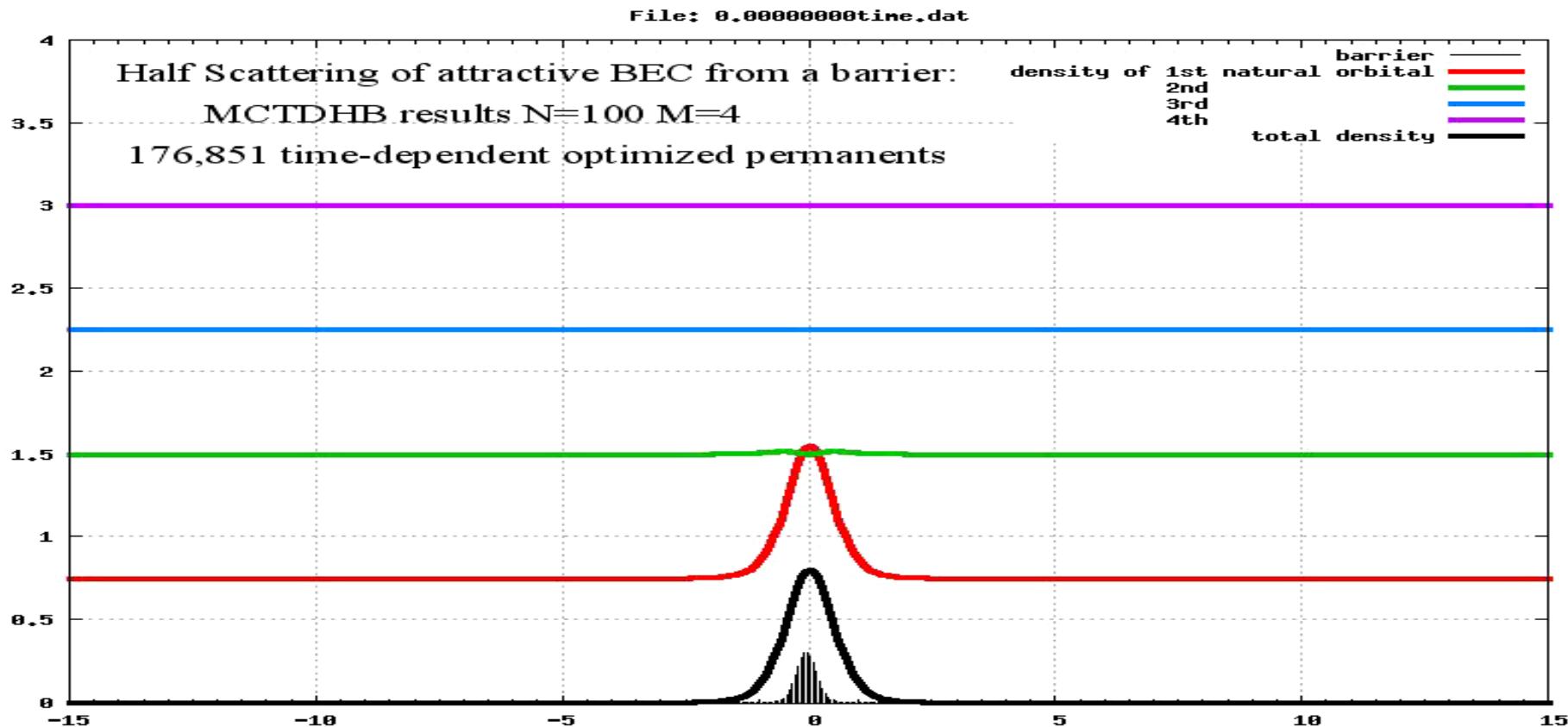
**t=0:**

mainly  $|0,N\rangle$  contribute

We call the **Schrödinger cat** state propagating without dispersion and being of fragmented nature **CATon**

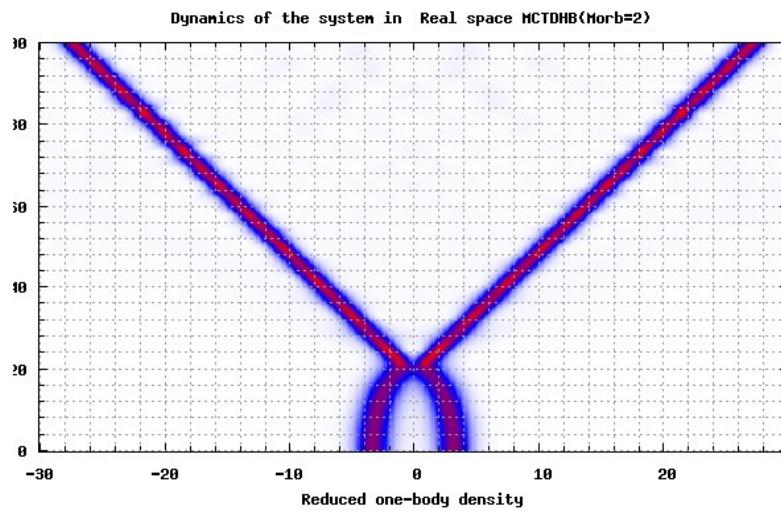
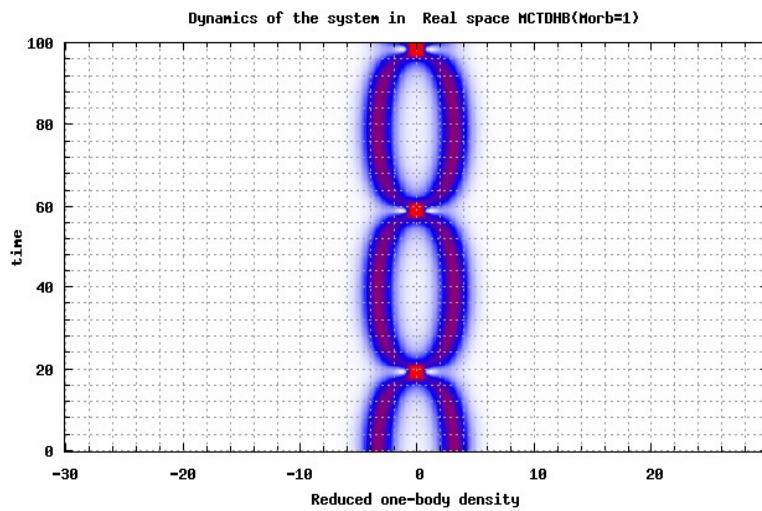
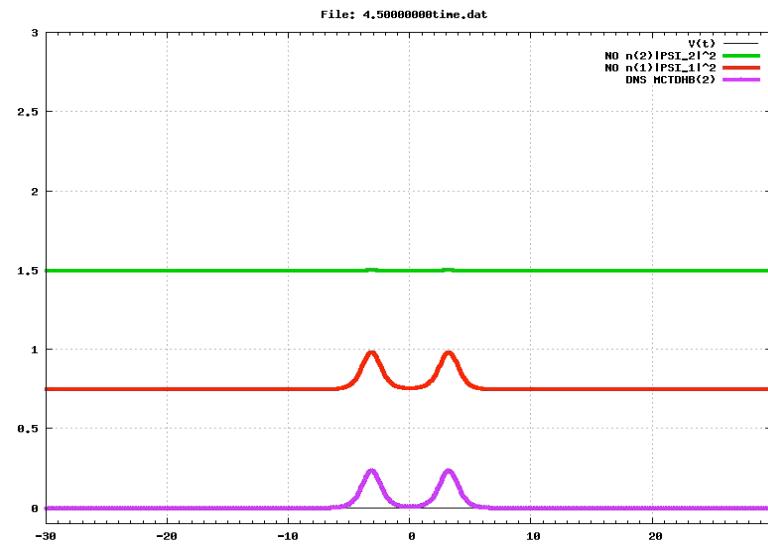
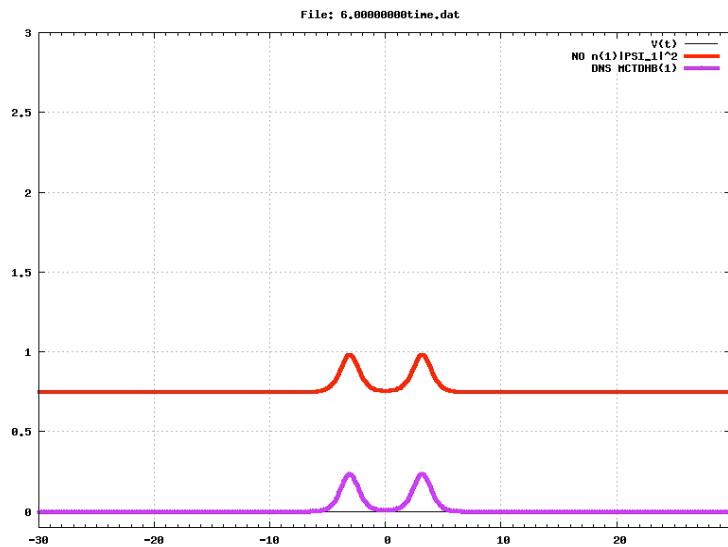
# MCTDHB: Efficient generation of Schrödinger cats : Attractive BEC is threaded by a potential barrier JPB, 42 091004 (2009)

$$\rho(r, r'; \textcolor{red}{t}) = \int \Psi^*(r, r_2, \dots, r_N; \textcolor{red}{t}) \Psi(r', r_2, \dots, r_N; \textcolor{red}{t}) dr_2 \dots dr_N = \sum_{k,q} \rho_{kq}(\textcolor{red}{t}) \phi_k^*(r, \textcolor{red}{t}) \phi_q(r', \textcolor{red}{t}) = \sum_i n_i |\phi_i^{NO}(r = r', \textcolor{red}{t})|^2$$



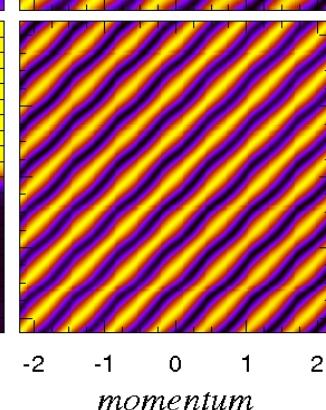
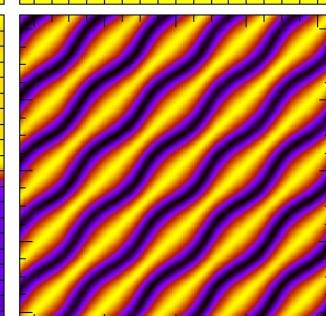
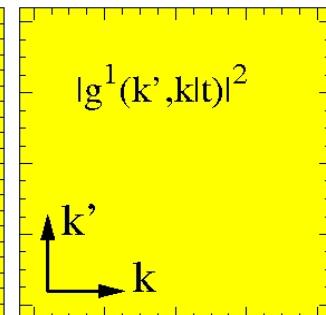
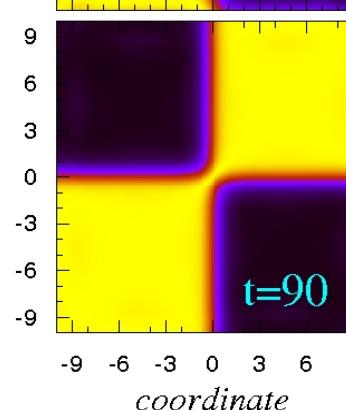
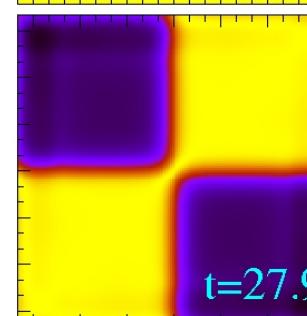
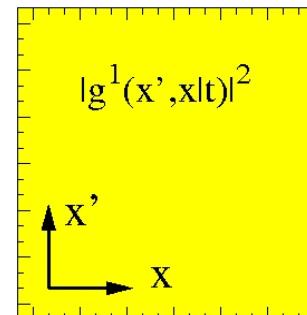
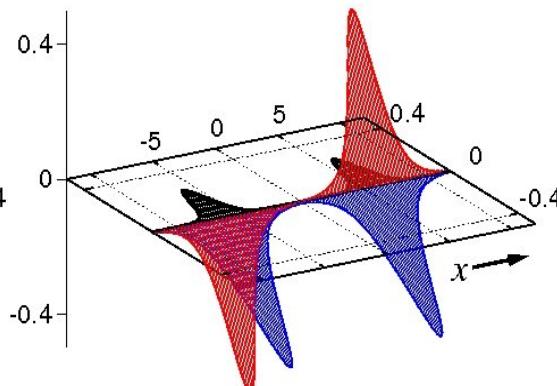
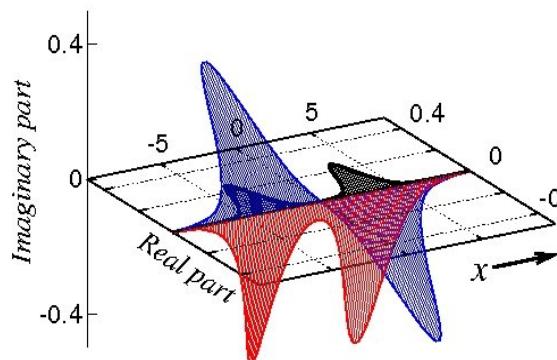
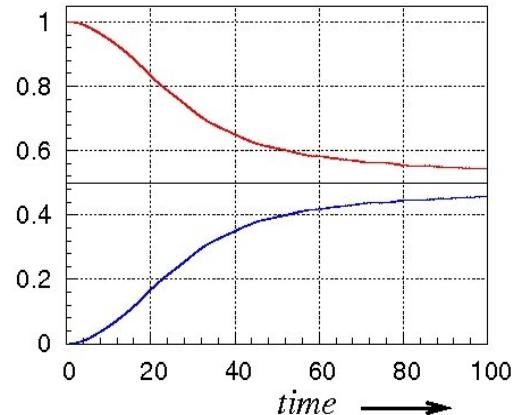
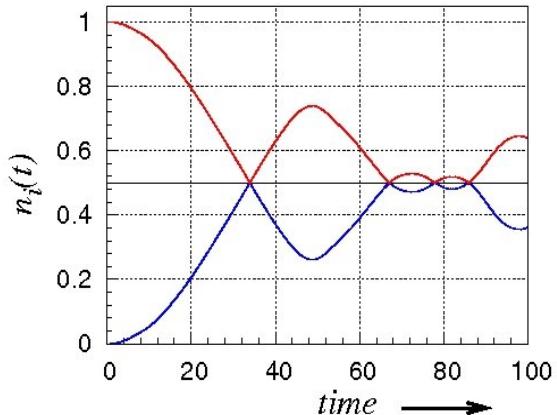
The time-dependent **Schrödinger cat** state – **CATon** is formed

# Time-evolutions of initially-coherent two-hump in-phase soliton: GP (left) vs. Many-Body (right)



# Fragmentation phenomena with *the MCTDHB*

**Attractive BECs – Fate of bright matter-wave soliton trains in 1D** *PRL 106, 240401 (2011)*  
Swift loss of coherence



***The initially coherent multi-hump  
wave-packets dynamically loose the  
coherence and become fragmented***

<http://QDlab.org>

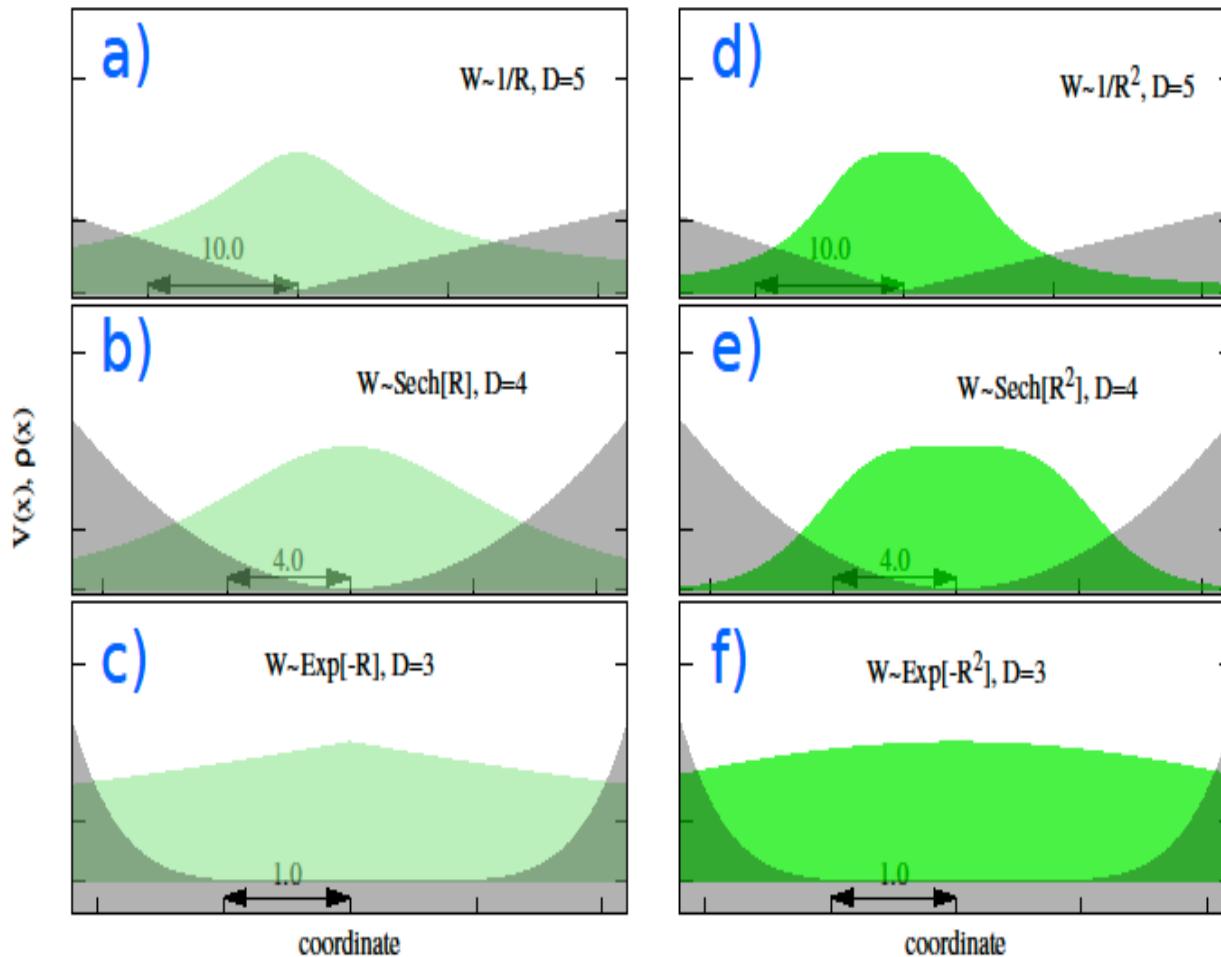
# Conclusions on attractive condensates in 1D

Phys. Rev. A 80, 043616 (2009) arXiv:0812.3573;

J. Phys. B: At. Mol. Opt. Phys. 42 091004 (2009)

- ✓ ***The initially coherent wave-packet threaded by (scattered from) a barrier (can) dynamically dissociate into two parts***
- ✓ ***The time-dependent GP theory applied to similar initial state does not show up the splitting***
- ✓ ***The split object CATon possesses remarkable properties:***
  - (1) *two-fold fragmented, i.e., not coherent*
  - (2) *dynamically stable, i.e., it propagates almost without dispersion*
  - (3) *It is a quantum superposition state – dynamical Schrödinger cat state*

# System of $N=108$ bosons trapped in $V(x)$ and interacting via $\lambda_0 W(x-x')$ Phys. Rev. A 88, 041602(R) (2013)



$$W(R) = 1 / \sqrt{\left(\frac{|x-x'|}{D}\right)^{2n} + 1}$$

$$V(x) = \begin{cases} -x & \text{for } x < 0 \\ 3x/4 & \text{for } x \geq 0 \end{cases}$$

$$W(R) = \text{Sech} \left[ \left( \frac{|x-x'|}{D} \right)^n \right]$$

$$V(x) = \frac{1}{2} x^2$$

$$W(R) = \text{Exp} \left[ -\frac{1}{2} \left( \frac{|x-x'|}{D} \right)^n \right]$$

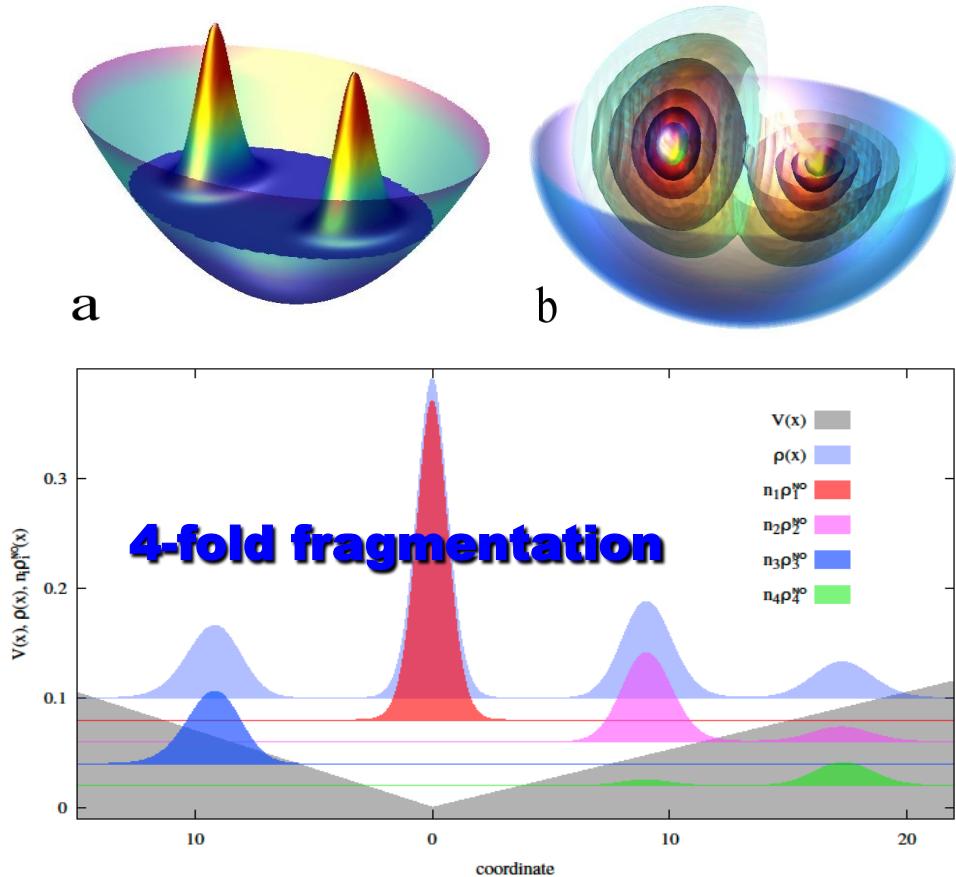
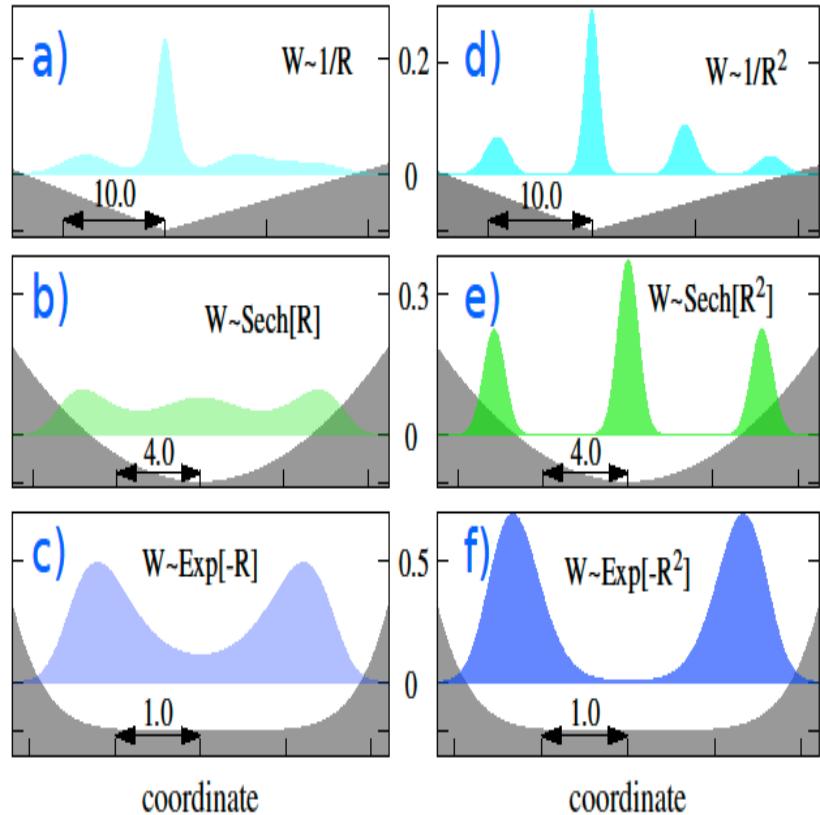
$$V(x) = \frac{1}{2} x^6$$

$W(R)$  depicted on the left and right panels have the same range (width)  $D$ , but tails of the right ones are “shorter”

# Fragmentation phenomena with MCTDHB

**Finite and Long-range interactions – Static properties** Phys. Rev. A 88, 041602(R) (2013)

**Dynamical stability** Phys. Rev. A 89, 061602(R) (2014)



Irrespective to the shapes of inter-particle  $W(R)$  and trapping  $V(r)$  strong inter-particle repulsion leads to formation of multi-hump localized fragmented structures ...

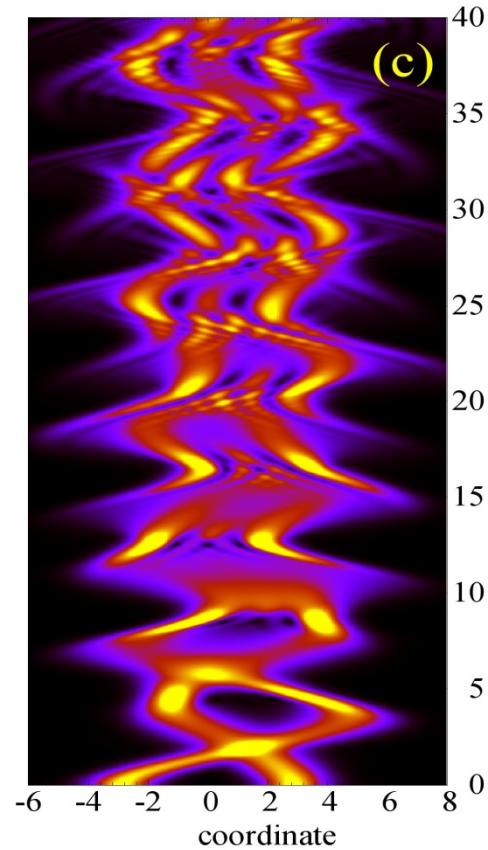
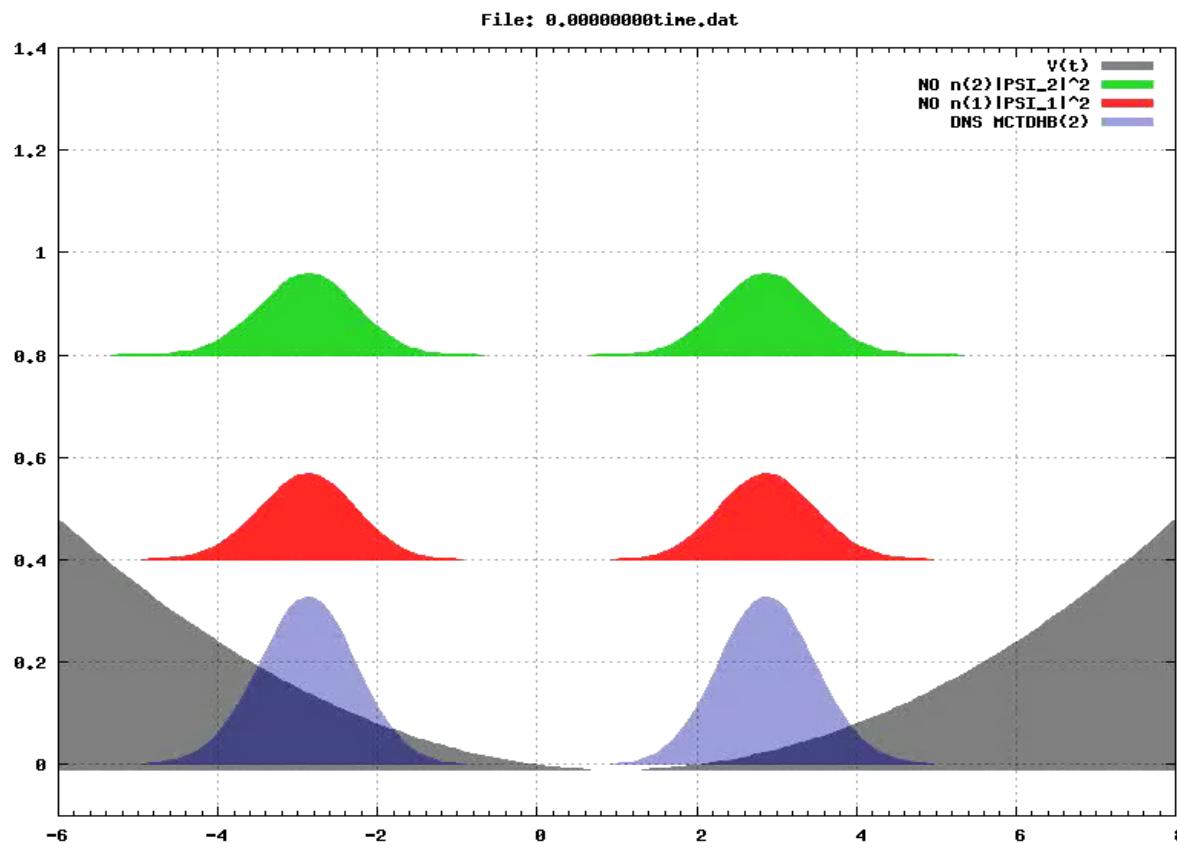
Non-violent regime  $\leftrightarrow$  under-a-barrier AND Violent, explosive regime  $\leftrightarrow$  over-a-barrier dynamics (when the induced barriers are not high enough to keep the sub-clouds apart from each other)

# Dynamics N=100: sudden displacement of trap and sudden quench (reduction) of the repulsion

Phys. Rev. A 89, 061602(R) (2014), arXiv:1312.6174

$$V(x) = \frac{1}{2} x^2 \rightarrow V(x - 1)$$

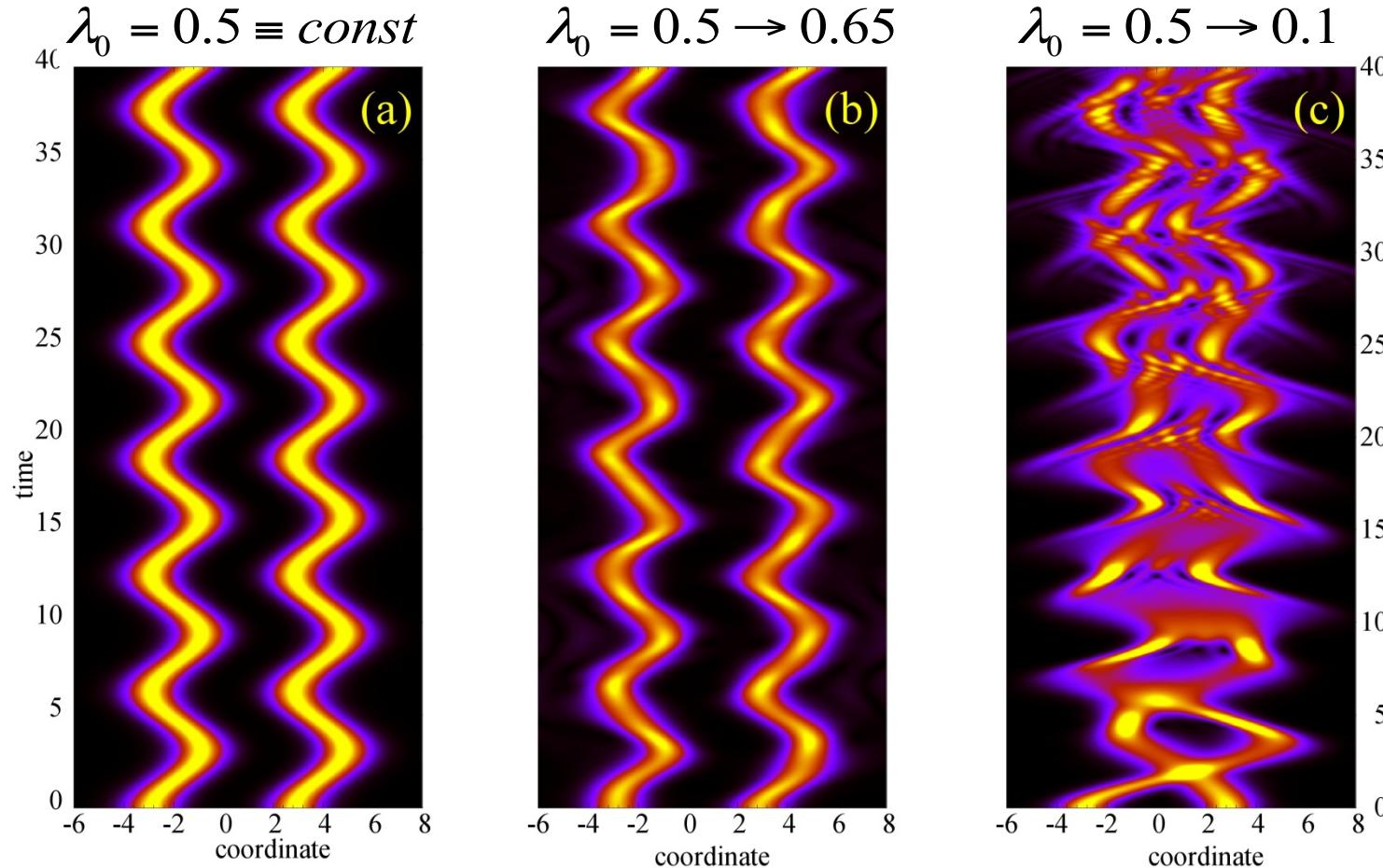
$$\lambda_0 = 0.5 \rightarrow 0.1$$



To visualize wave-packet dynamics we utilize  
Minkovskii-like space-time representation as a 2D plot

# Dynamics N=100: sudden displacement of trap and sudden quench (reduction) of the repulsion

Phys. Rev. A 89, 061602(R) (2014), arXiv:1312.6174



**Message:** Two generic regimes: (i) non-violent (under-a-barrier) and  
(ii) Explosive (over-a-barrier)

# Dynamics N=100: sudden displacement of trap and sudden quenches of the repulsion in 2D

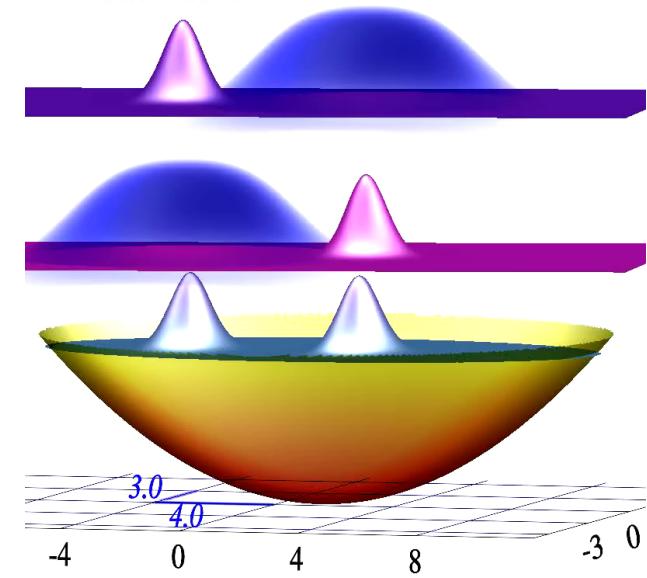
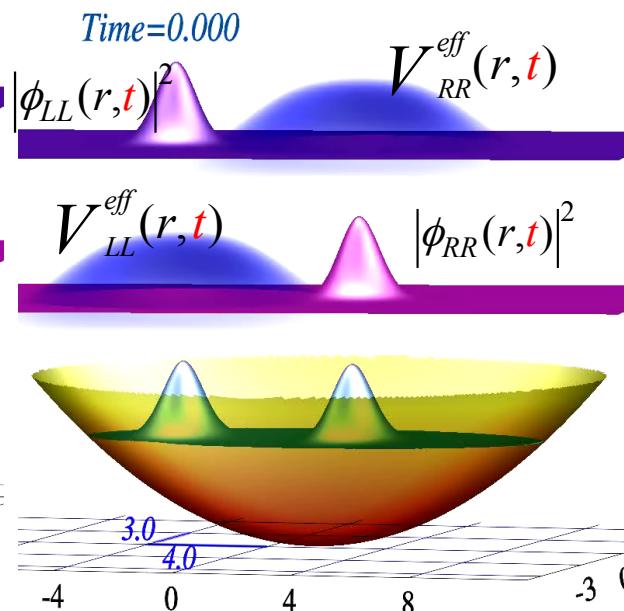
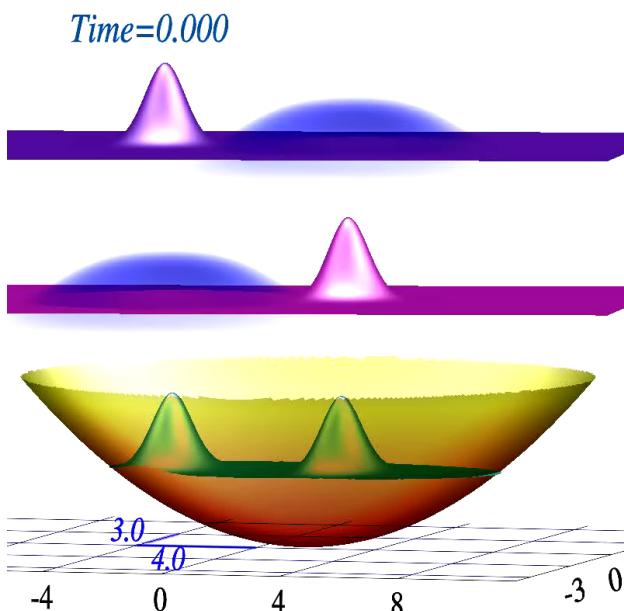
Phys. Rev. A **89**, 061602(R) (2014), arXiv:1312.6174

$$\mathbf{V}(x, y) = \frac{1}{2}x^2 + \frac{3}{2}y^2 \rightarrow \mathbf{V}(x - 1.5, y - 0.5)$$

$$\lambda_0 = 0.5 \rightarrow 0.1$$

$$\lambda_0 = 0.5 \rightarrow 0.7$$

$$\lambda_0 = 0.5 \rightarrow 0.8$$



Two generic regimes: (i) non-violent (under-a-barrier) and  
(ii) Explosive (over-a-barrier)

# Dynamics N=100: sudden displacement of trap and sudden quenches of the repulsion in 3D

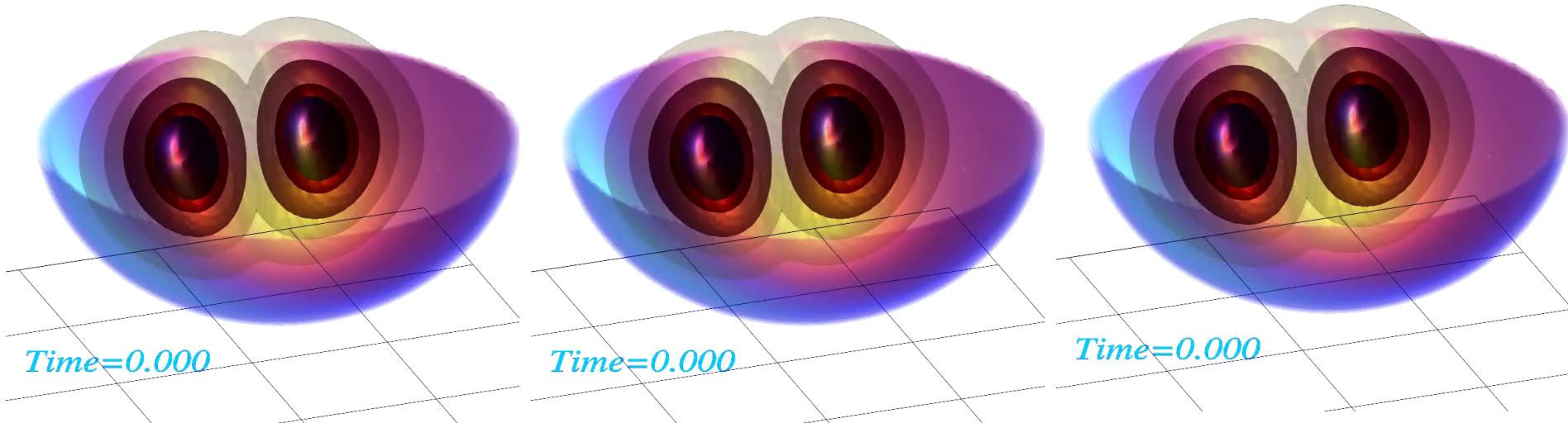
Phys. Rev. A 89, 061602(R) (2014), arXiv:1312.6174

$$\mathbf{V}(x, y, z) = \frac{1}{2}x^2 + \frac{3}{2}y^2 + \frac{3}{2}z^2 \rightarrow \mathbf{V}(x - 1.5, y - 0.5, z - 0.5)$$

$$\lambda_0 = 0.5 \rightarrow 0.1$$

$$\lambda_0 = 0.5 \rightarrow 0.7$$

$$\lambda_0 = 0.5 \rightarrow 0.8$$



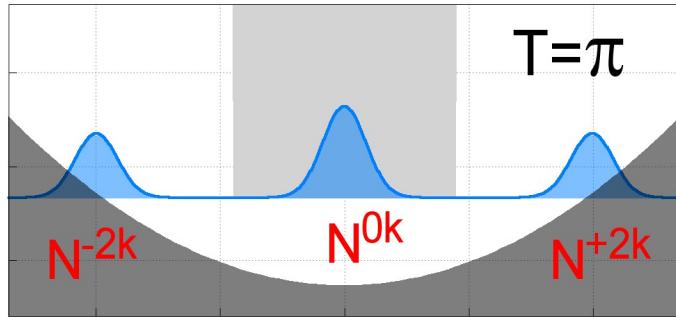
Two generic regimes: (i) non-violent (under-a-barrier) and  
(ii) Explosive (over-a-barrier)

# Fragmentation phenomenon in BECs

Repulsive, attractive, short-, finite- and long-range interactions

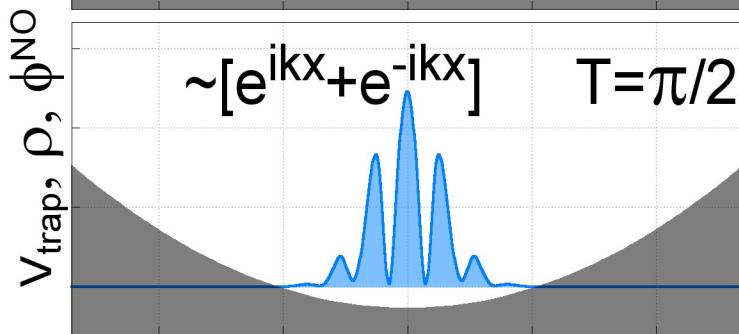
Static and highly-non-equilibrium dynamics, 2- 3- 4- fold fragmentation

**How to measure natural occupations?** With Interferometric Protocol!

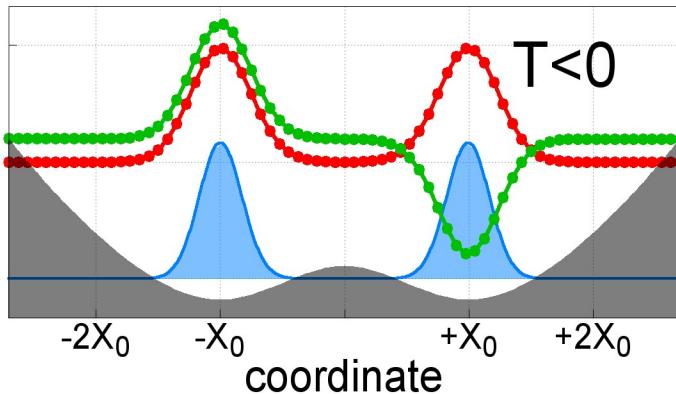


**IV-step:** Measure populations of the sub-clouds propagating with different momentum in  $(+2k, 0k, -2k)$ -channels

$$n_2 = 1-3N^{0k}/2$$



**III-step:** Apply a recombining laser-pulse of a proper phase and momentum  $\mathbf{k}$  at the re-collision



**II-step:** Deflect split parts

**I-step:** Split BEC ... It can be

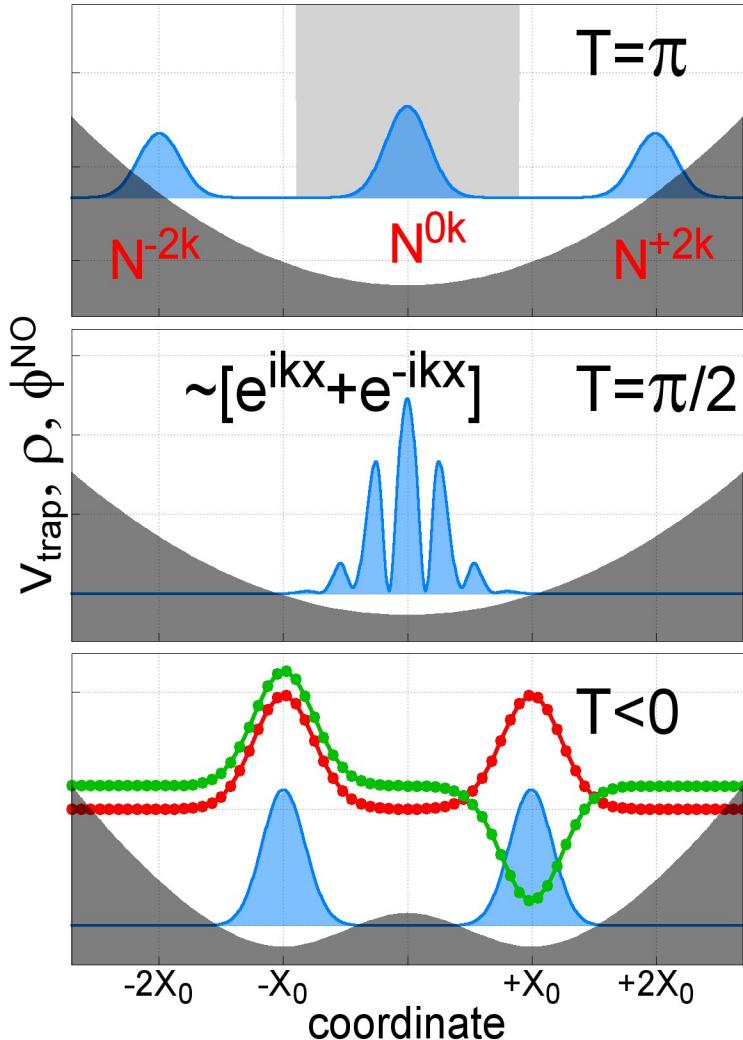
- i) condensed  $n_2 < 5\%$
- ii) depleted  $n_2 < 10\%$
- iii) two-fold fragmented  $n_2 \approx 50\%$

# Fragmentation phenomenon in BECs

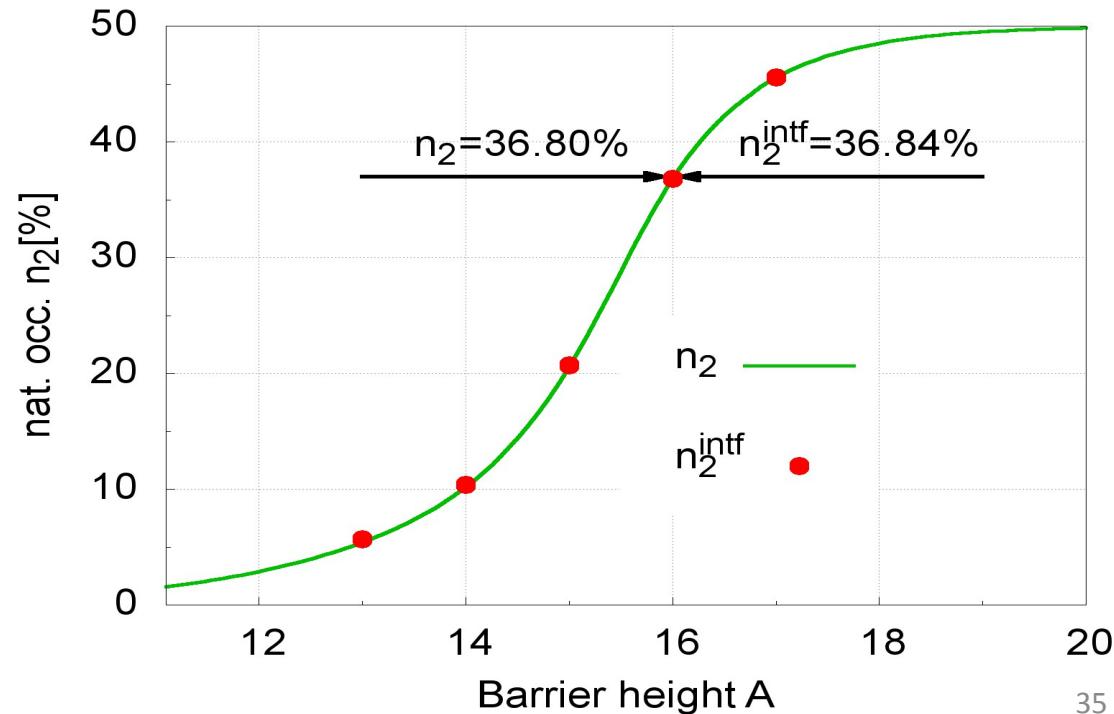
Repulsive, attractive, short-, finite- and long-range interactions

Static and highly-non-equilibrium dynamics, 2- 3- 4- fold fragmentation

How to measure natural occupations? With Interferometric Protocol!



**I-step: Split repulsive BEC  
by Gaussian barrier A**  
It can be condensed  $n_2 < 5\%$ , depleted  $n_2 < 10\%$  or  
two-fold fragmented  $n_2 \approx 50\%$

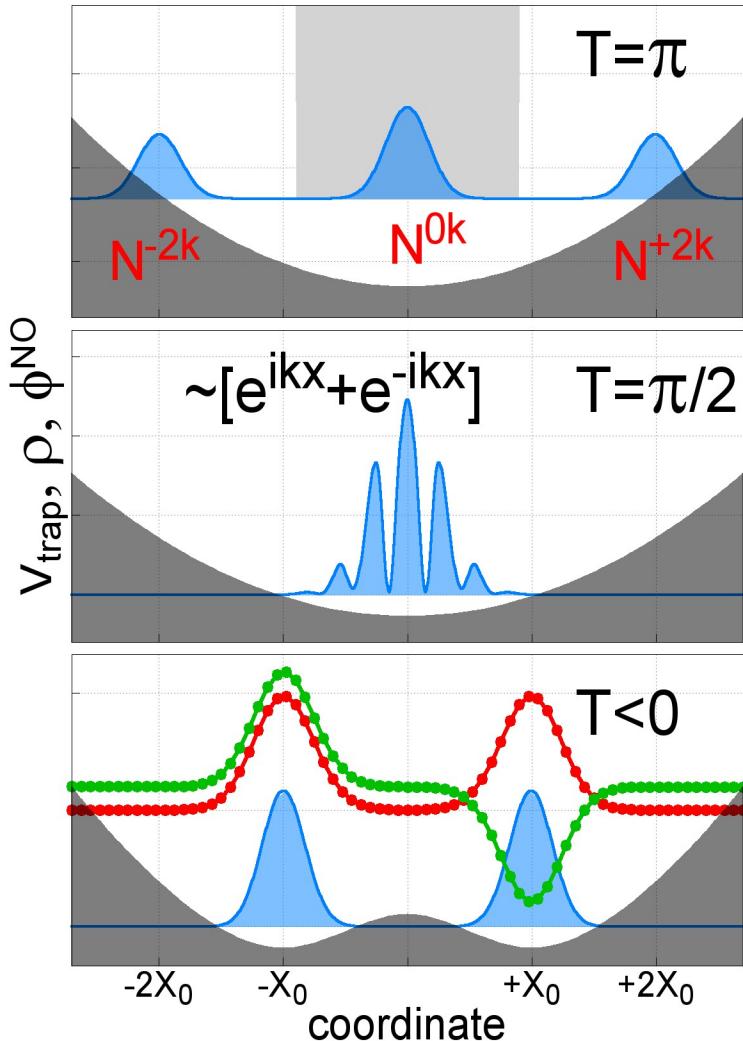


# Fragmentation phenomenon in BECs

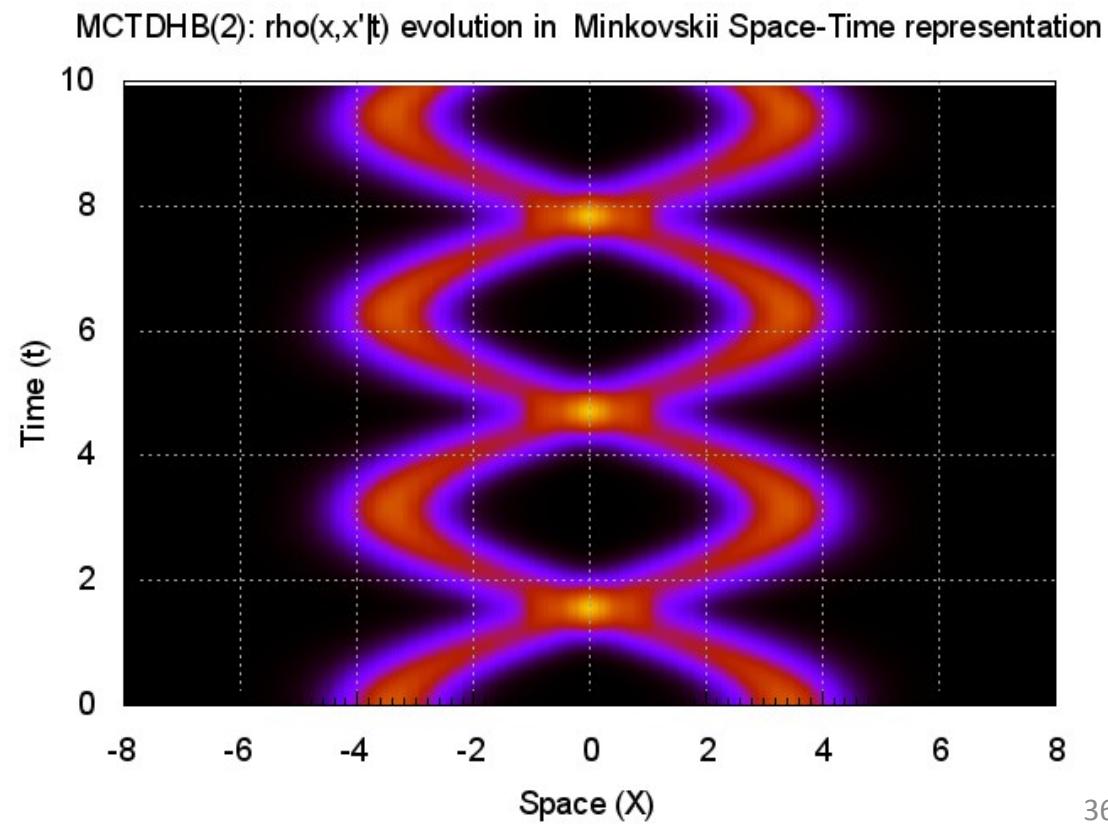
Repulsive, attractive, short-, finite- and long-range interactions

Static and highly-non-equilibrium dynamics, 2- 3- 4- fold fragmentation

**How to measure natural occupations?** With Interferometric Protocol!



**II-step:** To deflect the split parts we switch off  
the Gaussian barrier  $A=0$

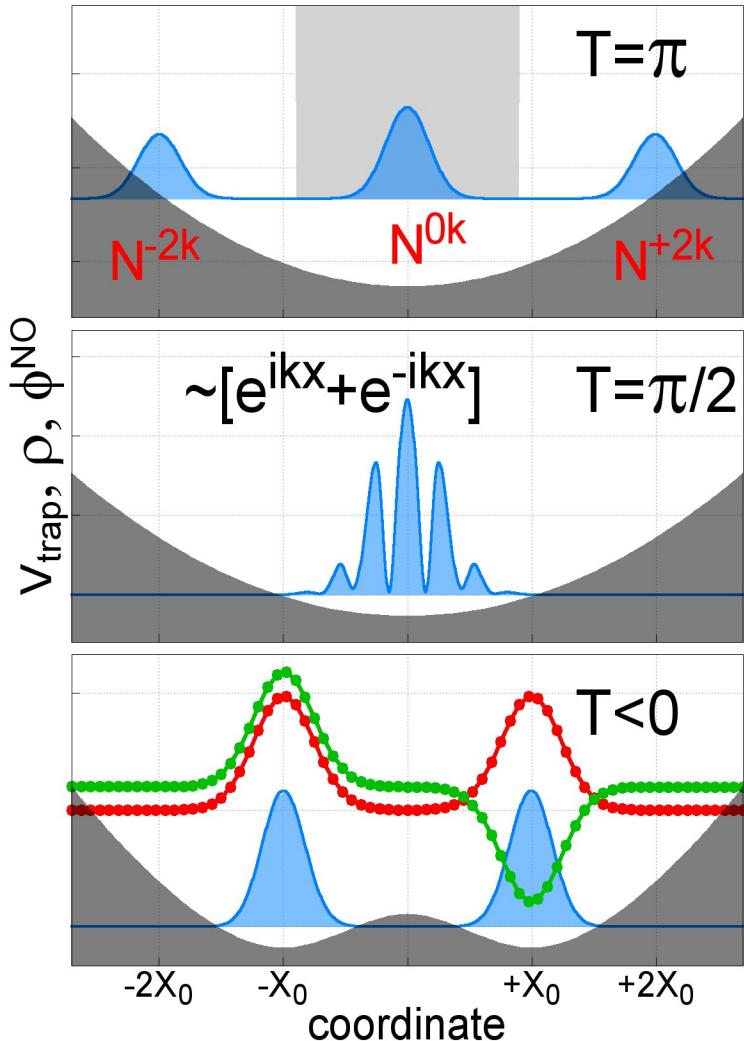


# Fragmentation phenomenon in BECs

Repulsive, attractive, short-, finite- and long-range interactions

Static and highly-non-equilibrium dynamics, 2- 3- 4- fold fragmentation

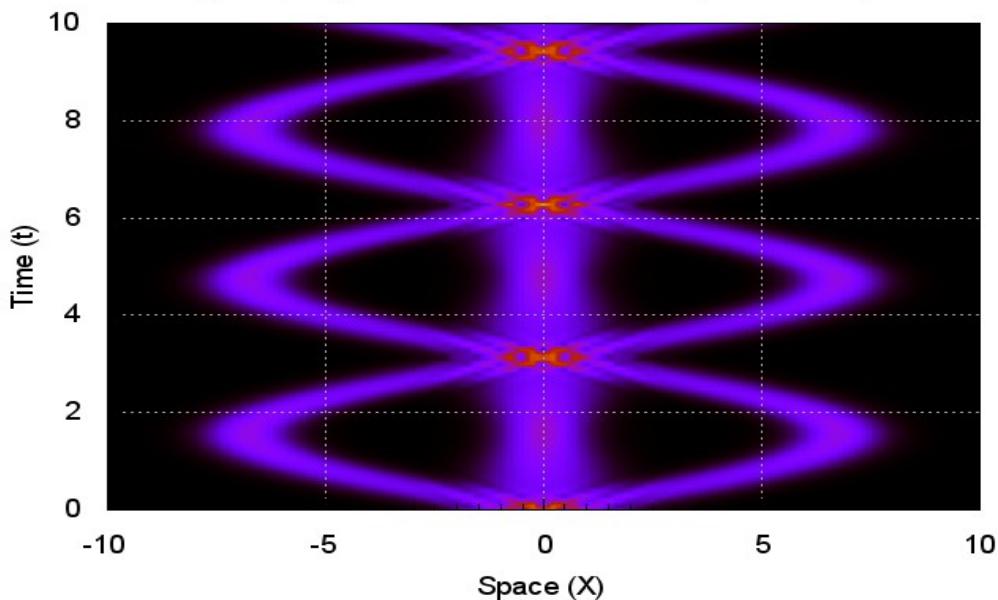
**How to measure natural occupations?** With Interferometric Protocol!



**III-step:** Apply a recombining Kapitza-Dirac  
laser-pulse of a proper phase and momentum  
 $k = X_0$  ( $k^2/2m = X_0^2/2$ )  
at the re-collision time  $T_{rc}$

$$\Psi_{MB}(x_1, x_2, \dots, x_N, t = T_{rc}) \prod_{j=1}^N \left[ e^{+ikx_j} + e^{-ikx_j - i\chi} \right]$$

MCTDHB(2):  $\rho(x, x' | t)$  evolution in Minkovskii Space-Time representation

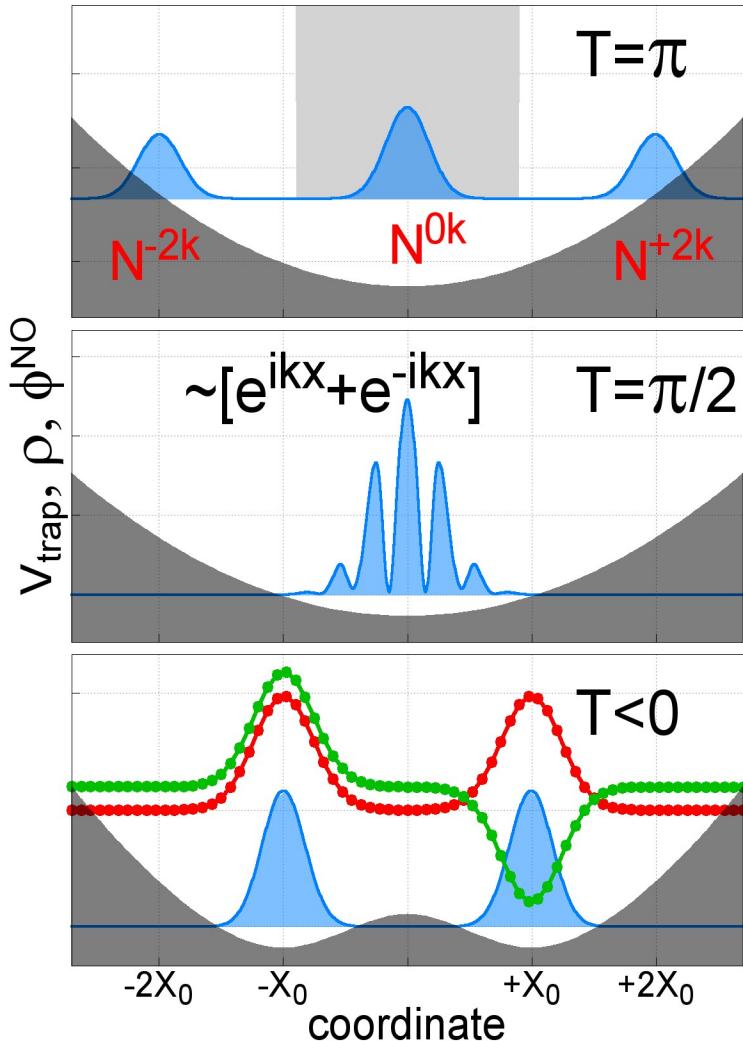


# Fragmentation phenomenon in BECs

Repulsive, attractive, short-, finite- and long-range interactions

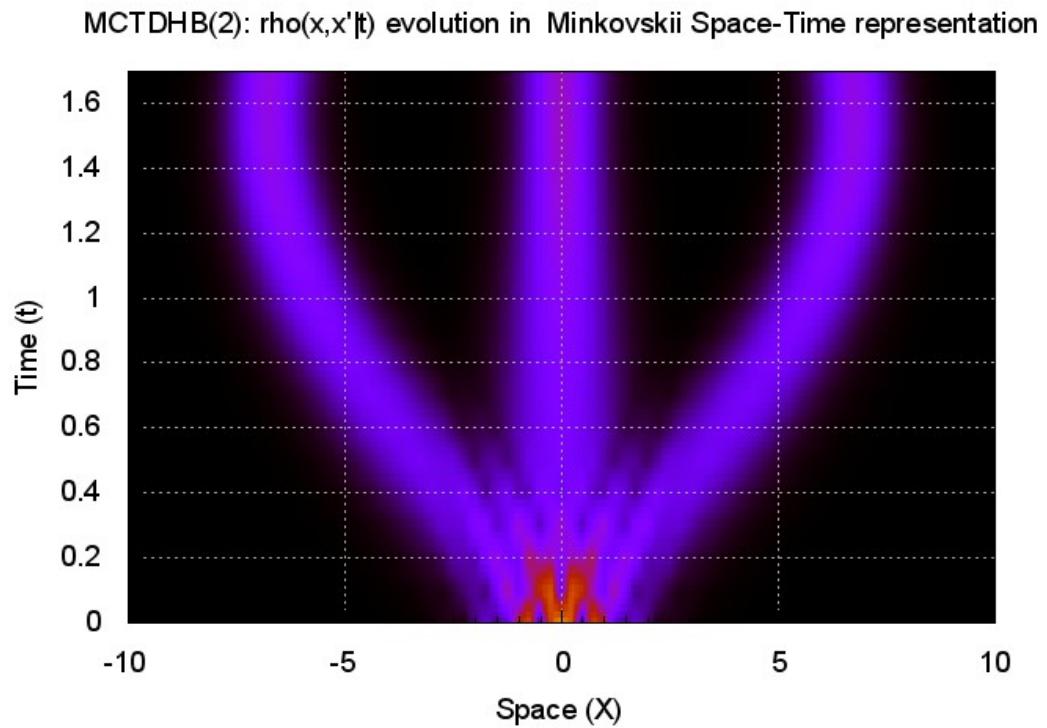
Static and highly-non-equilibrium dynamics, 2- 3- 4- fold fragmentation

**How to measure natural occupations?** With Interferometric Protocol!



**IV-step:** Measure the populations of the sub-clouds at  $T=\pi$  propagating with different momentum ( $k$ -channels)

$$n_2 = 1-3N^{0k}/2$$

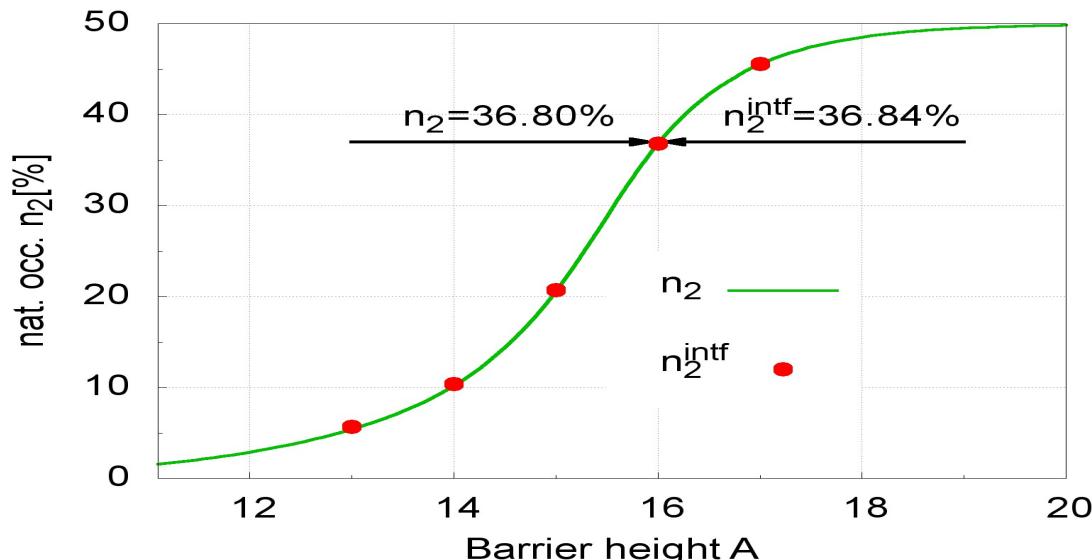
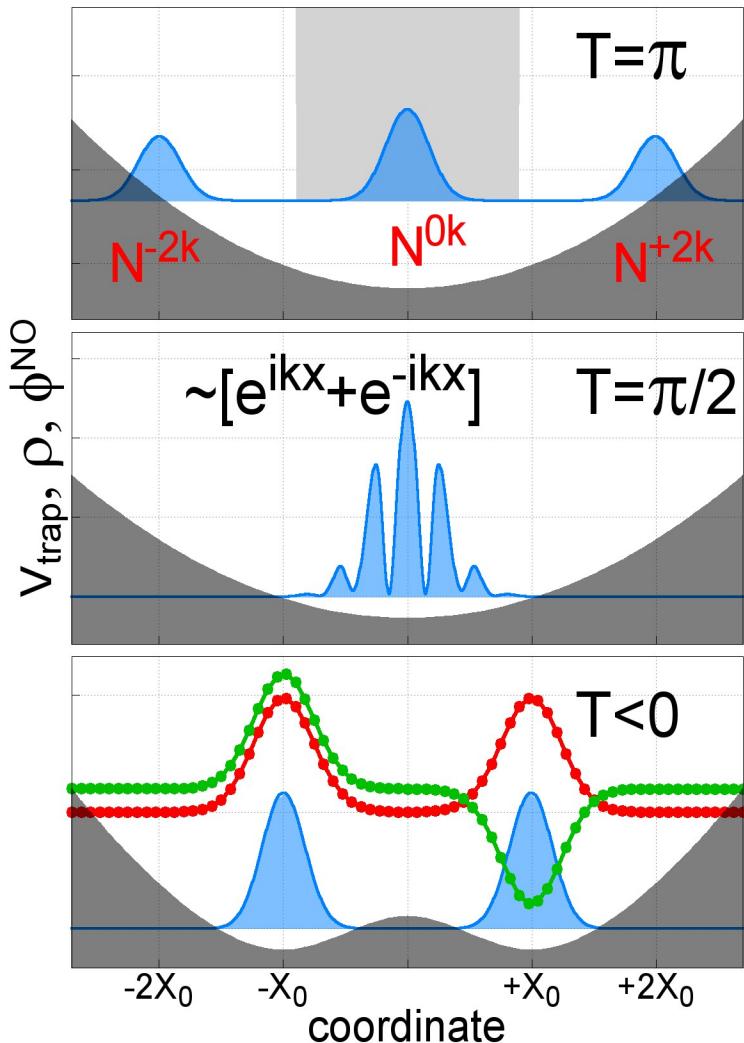


# Fragmentation phenomenon in BECs

Repulsive, attractive, short-, finite- and long-range interactions

Static and highly-non-equilibrium dynamics, 2- 3- 4- fold fragmentation

Interferometric Protocol to measure natural occupations works!



At  $A=13$ : RDM  $n_2=5.43\%$  Interfer.  $n_2\approx 5.67\%$

At  $A=14$ : RDM  $n_2=10.20\%$  Interfer.  $n_2\approx 10.37\%$

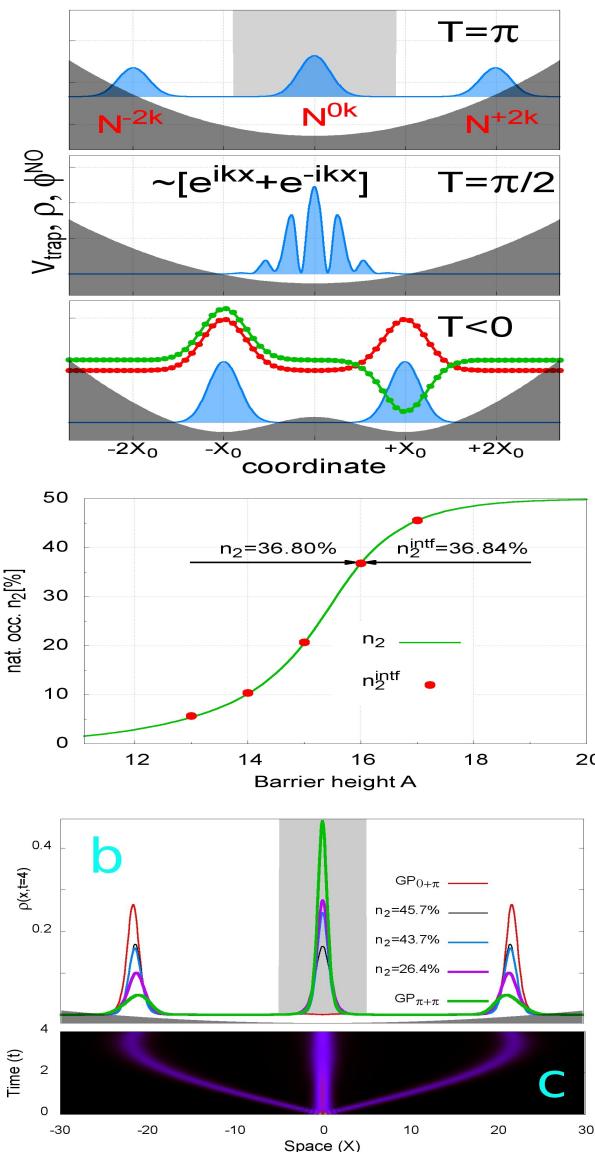
At  $A=17$ : RDM  $n_2=45.53\%$  Interfer.  $n_2\approx 45.59\%$

Small differences due to approximations:

- 1)  $\mathbf{k}=\mathbf{m}\omega\mathbf{X}_0$  (strict only for Gaussian sub-clouds)
- 2) As  $\mathbf{X}_0$  we took minima of the double-well trap

# Conclusions on How to measure fragmentation?

arXiv:1412.4049



## Interferometric Protocol

Universal:

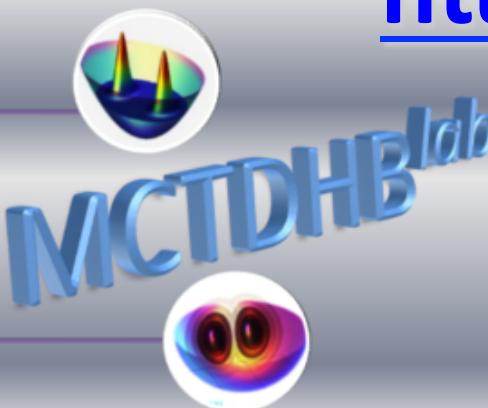
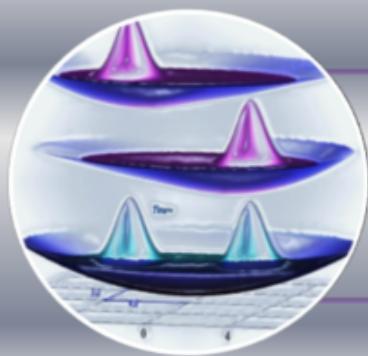
- Repulsive, attractive, short-, finite- and long-range interactions
  - Static states and highly-non-equilibrium dynamics
- Simple:
- Accessible from a single-shot measurement - does not require statistical averages

Quantitative:

- “Interferometric” natural occupations  $n_i$  are very close to the exact, theoretical ones obtained by diagonalizing the RDM (for example RDM  $n_2=45.53\%$  Interfer.  $n_2 \approx 45.59\%$ )

Selective:

- Varying the phase  $X$  of the applied laser Dirac-Kapitza pulse:  $e^{[-ikx]} + e^{[+ikx+iX]}$
- one can select which occupation number to measure. In the above double-well example to access  $n_2$  we use  $X=0$ , to access  $n_1$  one should use  $X=\pi$



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dynamics

Linux:

click to launch  
MCTDHB-Lab

MCTDHBLab V1.5

Project

Hamiltonian Computation Analysis Control Package Help About us & MCTDHB

Hamiltonian Computation Analysis: MCTDHB Analysis: LR-MCTDHB

Computer Home mctdhb-Lab

Terminal

```
File Edit View Terminal Help
GOOD file existence
Global variable: projectPathDef
Global variable: defaultPLTPath
Global variable: commonConfigP
Global variable: bosonEXDefault
MKLFFT
Global variable: propertiesEXE
ifort_MKLFFT
Global variable: envNAMEDefault
Global variable: envVALUEDef
WARNING: com.sun.javafx.css.parser.CssParser parse.css Error parsing jar!/resource/home/alexej/MCTDHB-Lab/MCTDHBLabV1_5.jar!/mctdhblabv1/mctdhblab.css: Expected RBR ACE at [21,1]
INFO: com.sun.javafx.css.StyleManager loadStylesheetUnPrivileged Could not find stylesheet: jarfile: /home/alexej/MCTDHB-Lab/MCTDHBLabV1_5.jar!/AlertDialog_css/
AlertDialog.css
INFO: com.sun.javafx.css.StyleManager loadStylesheetUnPrivileged Could not find stylesheet: jarfile: /home/alexej/MCTDHB-Lab/MCTDHBLabV1_5.jar!/GUI/new/src/mctdhblabv1/mctdhblab.css
INFO: com.sun.javafx.css.StyleManager loadStylesheetUnPrivileged Could not find stylesheet: jarfile: /home/alexej/MCTDHB-Lab/MCTDHBLabV1_5.jar!/mctdhblabv1/analysis/mctdhblab.css
set up!
```

About us & MCTDHB

MCTDHB members

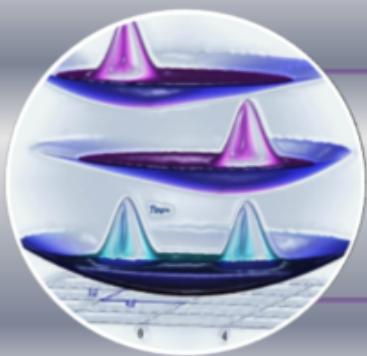
MCTDHB Team

MCTDHB will be done in sec. 0% LR-MCTDHB not done yet 0% processing... DATA 0%

Java-Interface

Lab-console

Fri Mar 13, 15:25



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Mac OS:

The screenshot shows a Mac OS desktop environment. In the center is the MCTDHBlab V1.5 application window. The window title is "MCTDHBlab". The main interface includes a navigation menu with "Hamiltonian", "Computation", "Analysis", "Control", and "Package". Below the menu is a large 3D visualization of quantum states, similar to the inset in the top left. A red circle highlights the top-left corner of the window, with the text "Click here to Maximise window". At the bottom of the window, there is a Java console window titled "Java-Console" with the following text:  

```
MAX_HEAP_SIZE      1024M
open files          (-n) 2560
pipe size          (512 bytes, -p) 1
stack size         (kbytes, -s) 8192
cpu time          (Seconds, -t) user:unlimited
max user processes (-u) 999
virtual memory     (kbytes, -v) unlimited
bosonexe-/Applications/MCTDH-Lab.app/Contents/Resources/bin/
boson_MCTDH_gnu_FFTW
properties=/Applications/MCTDH-Lab.app/Contents/Resources/bin/
boson_MCTDH_gnu_FFTW
Warning: Applications may hold too many file handles open. Update them by running 'port selfupdate'.
grubdir is set to /opt/local/bin/grubplot
BBB: Be superB with mctdh8
J A V A version:
java version "1.8.0_25"
Java(TM) SE Runtime Environment (build 1.8.0_25-b17)
Java HotSpot(TM) 64-Bit Server VM (build 25.25-b02, mixed mode)
Mon 13, 2015 2:52:39 PM com.sun.javafx.css.StyleManager
loadStylesheetInPrivileged
Tried to find stylesheet: jar:file:/Applications/MCTDH-Lab.
Contents/Resources/MCTDHBlabV1.5.jar!/AlertDialog.css
GOOD file exitence!
Global variable: connectWithDefault -> Applications/MCTDH-Lab.app/
```

Below the Java console, there is a message: "Drag files on window to process them". At the bottom right of the window, there is a button labeled "Cancel". To the right of the window, a context menu is open, with a red circle highlighting the "Open in Finder" option. The desktop background features a blue and green abstract pattern. The Dock at the bottom contains various icons, including a magnifying glass, a rocket, a compass, a browser, a terminal, a word processor, a presentation slide, a file folder, a coffee cup, and a trash can. The Dock also has a red circle highlighting the MCTDHBlab icon.

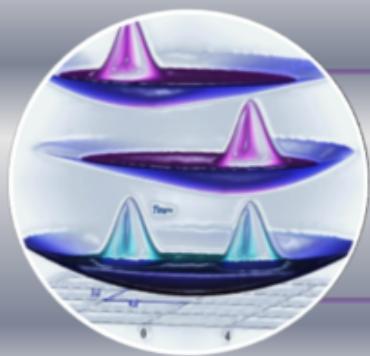
Java-Interface

Click here to Maximise window

MCTDHBlab will be done in sec.

Cancel

Open in Finder



MCTDHB<sup>lab</sup>



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## Windows:

Papierkorb

mctdhb-Lab

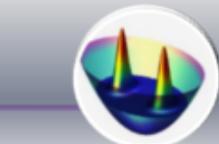
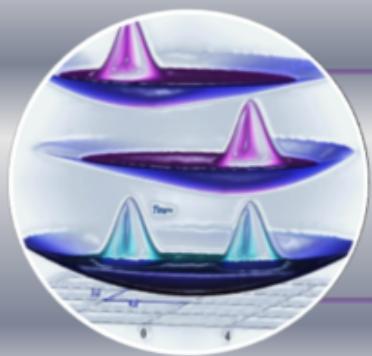
mctdhb-Lab

```
WARNING: bad driver version detected, device disabled. Please update to at least version 8.15.10.2302
Mar 14, 2015 8:31:15 PM com.sun.javafx.css.StyleManager loadStyle
ed
INFO: Could not find stylesheet: jar:file:/C:/MCTDHB-Lab/MCTDHBla
b/Lab/mctdhblab1/stylesheet.css
GOOD file extension
Global variable: projectPathDefault = C:/MCTDHB-Lab/
Global variable: defaultPLTPath = C:/PROGRAM/2/gnuplot4.6.6/bin/gnup
Global variable: commonConfigPath = C:/MCTDHB-Lab/...
Global variable: mctdhbPath = C:/MCTDHB-Lab/...
Global variable: mctdhbExePath = C:/MCTDHB-Lab/...
Global variable: envINOMODE=default=nr_1_ROOT
Global variable: envJVMUIDefault=0
Mar 14, 2015 8:31:30 PM com.sun.javafx.css.StyleManager loadStyle
ed
INFORMATION: Could not find stylesheet: jar:file:/C:/MCTDHB-Lab/M
r!/mctdhblab1/analysislr/mctdhblab.css
Mar 14, 2015 8:31:33 PM com.sun.javafx.css.StyleManager loadStyle
ed
INFORMATION: Could not find stylesheet: jar:file:/C:/MCTDHB-Lab/M
r!/GUI/new/src/mctdhblabv1/mctdhblab.css
set up!
```

MCTDHB members

MCTDHB will be done in sec. 0% LR-MCTDHB not done yet 0% processing... DATA 0%

Personal Edition 2015 mode Launcher WINE DE ? + Task View 20:33 14.03.2015



MCTDH<sup>b</sup>  
lab



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dynamics

Win&Mac&Linux:

**I. click**

**II. select**

**III.**

**IV. Ok**

**Evolution of the density in Minkovskii Space-Time representation**

**TDHB(1): rho(x,x'|t) evolution in Minkovskii Space-Time representation**

**MCTDHb lab v 1.5**

**Project**: /Users/tc-user/Alexej/TST/OL-BJj\_2well\_4Er

**Hamiltonian**   **Computation**   **Analysis: MCTDH**   **In&Out**   **Package**

**Info Density**   **Dns in Minkovskii Space-time**

**rho(...)**

**X-Space**: Xmin= -2.0   Xmax= 6.5   Tfnl= 150.0   Delta\_T= 1.0

**T-Space**: Tbg= 0.0

**Evolution of the density in Minkovskii Space-Time representation**

**MCTDHb(1): rho(x,x'|t) evolution in Minkovskii Space-Time representation**

**Time (t)**: 0 to 140

**Space (X)**: -2 to 6

$\Delta t \approx \pi/J$   
 $\Delta t = 2\pi/(E_1 - E_0)$

**Numerics MCTDHb**   **Run MCTDHb**

**Script:** /Applications/MCTDH-Lab.app/Conte

**Run**   **Stop**

**Before run: check all parameters**

**You are about to run MCTDH(M):**

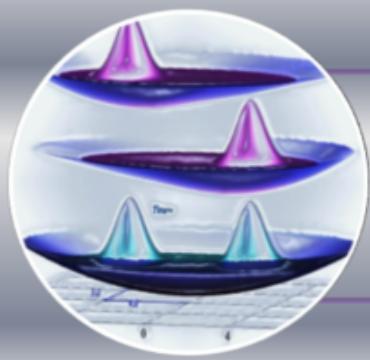
**M** = 1   **N** = 100   **V** = 0.5e0\*x^2   **W** = 8(|r-r'|)   **Orb dim** = 128   **Cl dim** = 1

**Relaxation**

**With "OK" you will:**

- 1) Rewrite input.in V\_W\_Psi\_string.in
- 2) Erase ALL previously-created data and figures

0.050000 -> 10.000000 ]  
1= 128   2= 28  
0= 0.9000000000e-01 kind of W(x-x'): 0.00000000000000



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Win&Mac&Linux:

TDSE System  $V(\mathbf{r}_j, t) = \text{Trap}$   $W(|\mathbf{r}_j - \mathbf{r}_k|, t) = \text{Interpart. inter.}$  M orb and Psi\_0  $\{C_{\vec{n}}(t)\}$  manually  $\{\phi_i(\mathbf{r}, t)\}_{i=1}^M$  manually

1D -dimensional Hamiltonian

$$\hat{H} = \sum_{j=1}^N \left[ -\frac{1}{2} \nabla_{\mathbf{r}_j}^2 + V(\mathbf{r}_j, t) \right]$$

I. Click  $N =$  10

Number of bosons: 10

External Trap potential  $V(\mathbf{r}_j, t) = 0.5e^*x^2$

II. Type N= 100

III. Click OK

Edit parameter: Description: Number of Particles  
File: Input.in

Hamiltonian TDSE System Trap Interpart. inter. W Morb and Psi at t=0

Computation Run MCTDHB Run LR-MCTDHB

Analysis: MCTDHB Energy Error Nat. occ. n\_k(t)

Orbitals and density Correlation functions

Info Density Nat.orb dns X

p, V, orb Reduced on Nat.orb dns

II. select III. select

II. I. II. III.

External trap potential: Set: t= 0.000 y= 5.0 z= 5.0

External trap potential:  $V(x, t) = 0.5e^*(x-2.1)^2$

Check&Replot

Time independent

X-DVR Grid FFT From Xint= -8.0e0 till Xfnl= +8.0e0 NDX = 128

Graph showing the potential  $V(x, t)$  versus position  $x$ . The potential is a parabolic well centered at  $x = 2.1$  with depth  $0.5e^*$ .

# Acknowledgments

**Ofir E. Alon (Haifa, Israel)**

**Lorenz S. Cederbaum (HD)**

**Oksana I. Streltsova (Dubna, Russia)**

**Luis Santos (Hannover), Michael Fleischhauer  
(Kaiserslautern)**

Shachar Klaiman (HD)

Kaspar Sakmann (Stanford, Vienna)

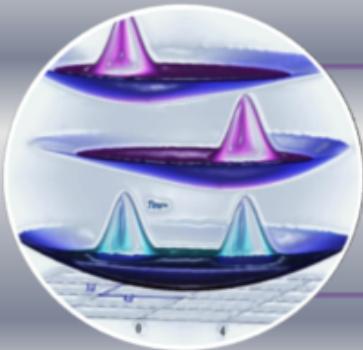
Hans-Dieter Meyer (HD),

Julian Grond (Graz, Austria)

Axel Lode (HD, Basel)

Raphael Beinke (HD)

BwGRiD & Cray XE6 clusters “Hermit” and “Hornet”  
& K100 & HybriLIT <http://www.QDLab.org>



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