MCTDHB lab

The laboratory to study quantum many-body dynamics

Center for Quantum Dynamics

http://QD-lab.org

http://mctdhb.org

Many-body theory of bosons group Heidelberg, Germany

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Talk: MCTDHB theory: predictions and applications

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

MCTDHB lab

The laboratory to study quantum many-body dynamics

http://qdlab.org

Talk: MCTDHB theory: predictions and applications

Outline:

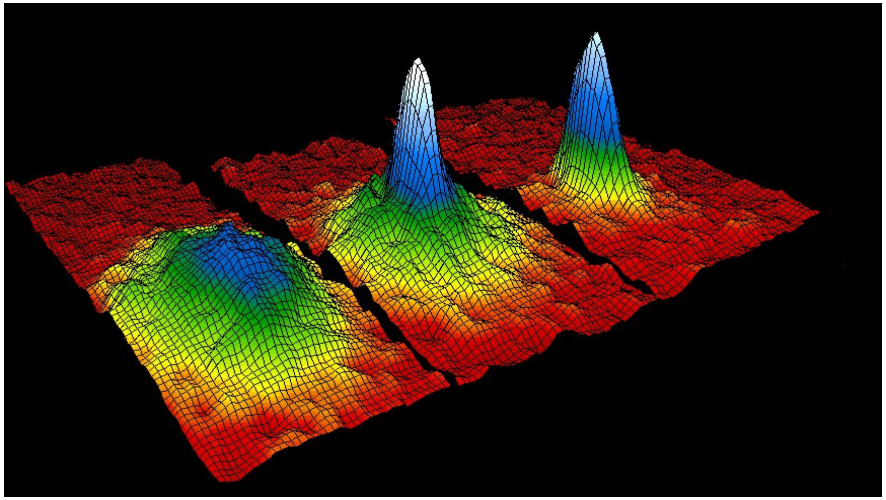
- **Introduction to the field of ultracold atoms and molecules**
- **Idea behind the MCTDHB method and benchmarks**
- **Applications to BECs with Repulsive, Attractive, Short- and Long-range inter-boson interactions in 1-D-, 2-D- ,3-D…**
- **Condensation and Fragmentation: How to measure?**
- **MCTDHB-Laboratory 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)

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

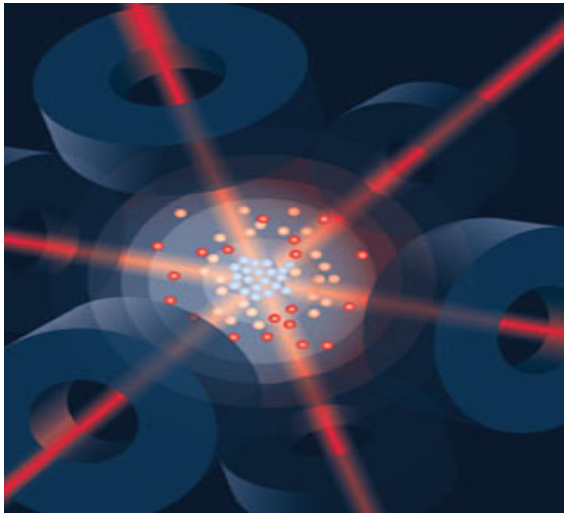
$$\rho(r,r';t) = \int \Psi^*(r,r_2,r_3,\ldots,r_N;t)\Psi(r',r_2,r_3,\ldots,r_N;t)dr_2\ldots dr_N = \sum_{k,q}\rho_{kq}(t)\phi_k^*(r,t)\phi_q(r',t)$$

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

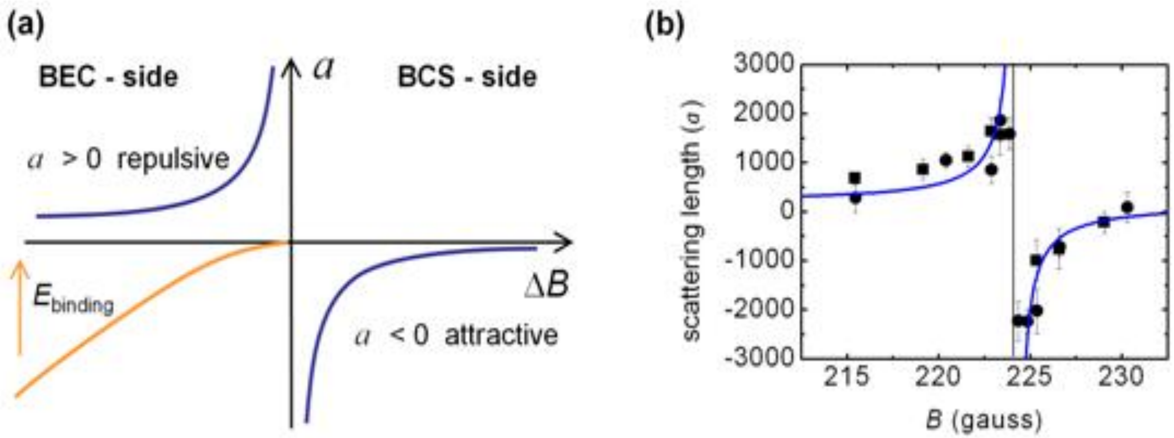
All the terms of the Hamiltonian are under experimental control and can be manipulated

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

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



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



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

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

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

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

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

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

One has to specify initial condition

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

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

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)

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

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

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

Natural analysis (eigenvalues and eigenvectors of the RDM):

n_i – natural occupation numbers ϕ_i^{NO} – natural orbitals

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

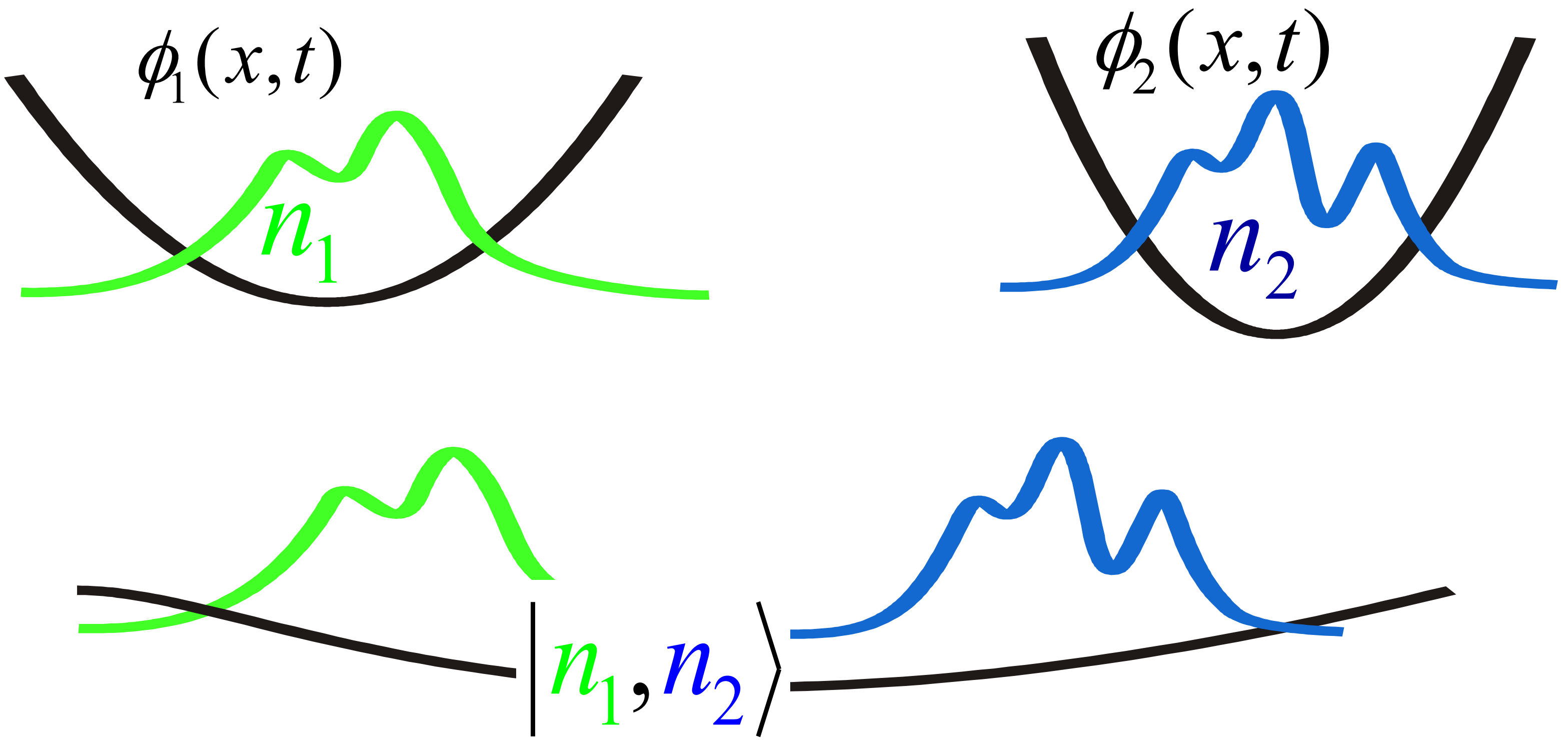
Fragmentation: several NO **macroscopically occupied** J. Phys. France 43, 1133 (1982)

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

Multi-Configurational 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

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

Every permanent $|i_1\, i_2\, i_3\, i_4 \cdots i_M;t\rangle$
is a symmetryzed time-dependent Hartree product

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

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

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

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

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

Gross-Pitaevskii mean-field theory
Aka NLSE

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

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

$$\left\langle\Psi\right| b_k^\dagger b_k^\dagger b_k b_k \left|\Psi\right\rangle = \sum_{i_1,\ldots,i_M} C^*_{i_1,\ldots,i_M} C_{i_1,\ldots,i_M} n_k (n_k - 1)$$

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

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

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

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

e.g. Bosons:

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

- ✓ ***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)
MCTDHF: 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)
O.E. Alon, A.I. Streltsov, and L.S. Cederbaum, J. Chem. Phys. **127**, 154103 (2007)
MCTDH-XY: O.E. Alon, A.I. Streltsov, and L.S. Cederbaum, Phys. Rev. A **76**, 062501 (2007)
MCTDH-*conversion*: O.E. Alon, A.I. Streltsov, and L.S. Cederbaum, Phys. Rev. A **79**, 022503 (2008)
Recursive formulation: O.E. Alon, A.I. Streltsov, L.S. Cederbaum, K. Sakmann, A.U.J. Lode, J. Grond, Chem. Phys. **401**, 2 (2012)
Linear Response: 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)

Benchmarks: PRA **86**, 063606 (2012)

MCTDHB vs. Exact Results

Harmonic Interaction Model (HIM)

HIM is exactly solvable in ***any*** **D** dimensions

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

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

$$\vec{q}_i = \frac{1}{\sqrt{j(j+1)}}\sum_{i=1}^{j}(\vec{r}_{j+1} - \vec{r}_i),\ j = 1,\ldots,N-1;\ \vec{q}_N = \frac{1}{\sqrt{N}}\sum_{i=1}^{N}\vec{r}_i$$

$$\delta_N = \sqrt{\varpi^2 + 2NK_0}$$

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

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

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

MCTDHB vs. Exact Results. Exact HIM Results

HIM Ground State – enormous relevance of the self-consistency

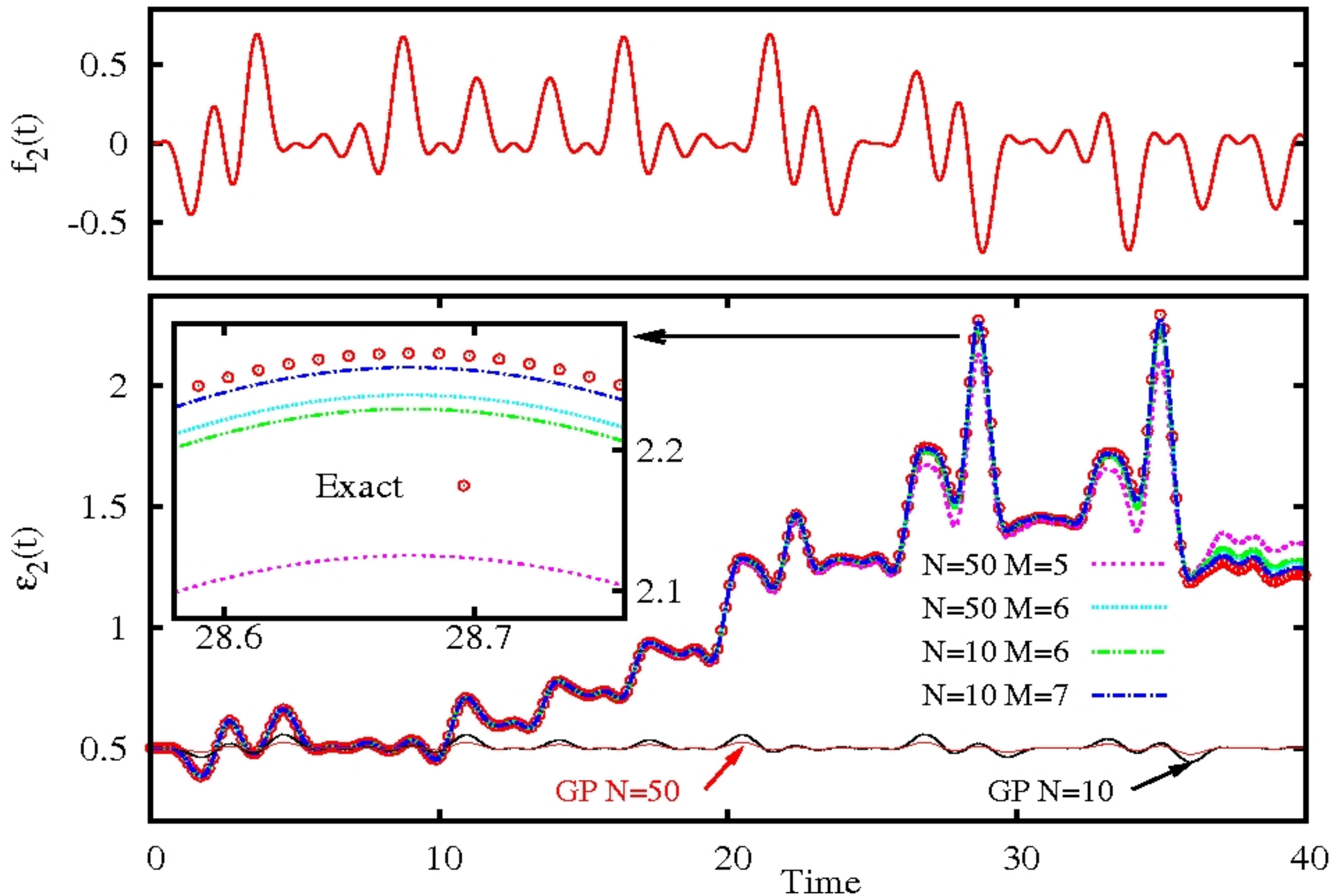
M	N=10	N=100	N=1000
1	7.07106781186548	70.7106781186548	707.106781186548
2	7.03876902630316	70.6801695174716	707.076433425731
3	7.03835065240638	70.6801254121867	707.076428987186
4	7.03834842490991	70.6801253917454	
5	7.03834841534905	70.6801253917376	
6	7.03834841531149		
7	7.03834841531101		
E_{exact}	7.03834841531101	70.6801253917375	707.076428986985

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:

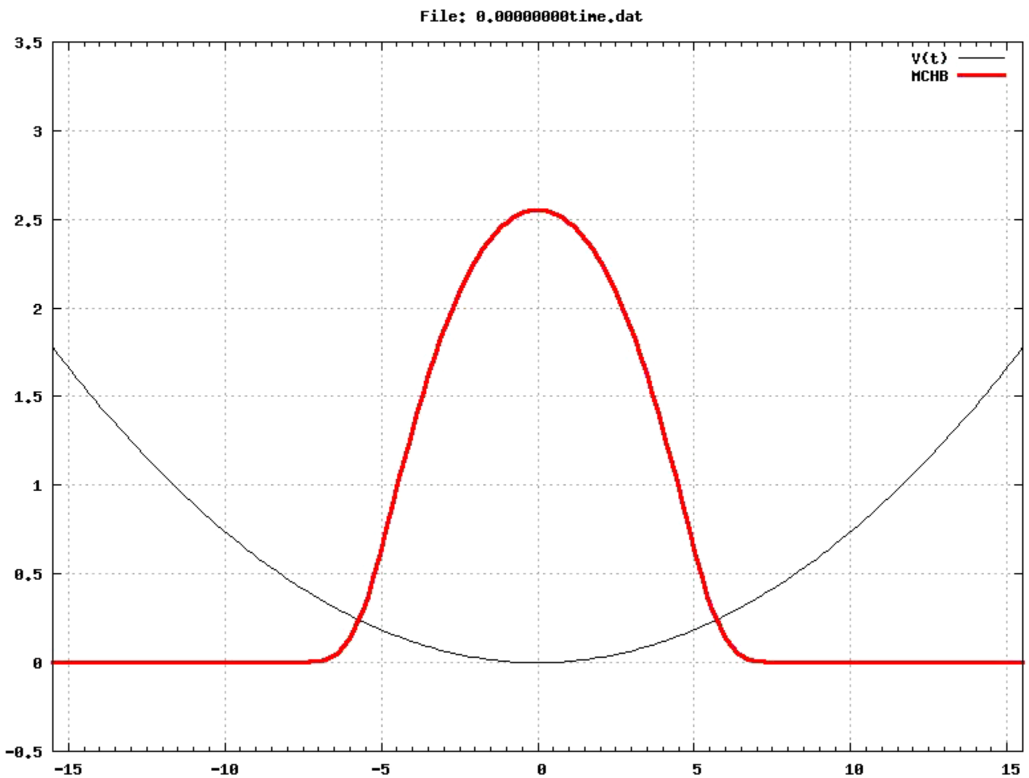
Wave Chaos and depletion: PRA 86, 013630 (2012), J. Phys.: *Conf. Ser.* 488 012032 (2014)

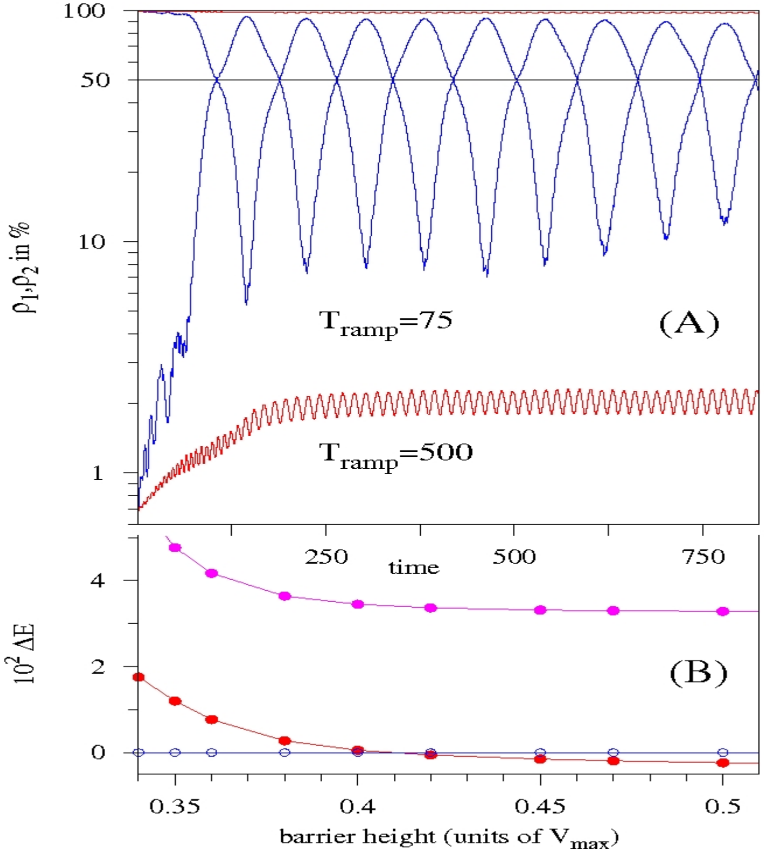
Just/recently started: Aarhus, Berkeley, Barcelona, Basel, Cambridge, Dubna, Haifa, Hamburg, Hannover, Kaiserslautern, São Paulo, Stanford, Ulm, …

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*

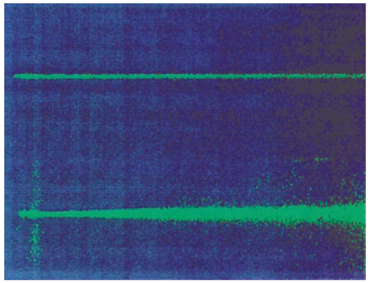
(ii)Inverse regime *time-dependent state stays condensed during all the evolution and thereby evolves to a non-ground many-body eigenstate*

http://QDlab.org

REVIEW

Optical Spatial Solitons and Their Interactions: Universality and Diversity

George I. Stegeman[1] and Mordechai Segev[2,3]



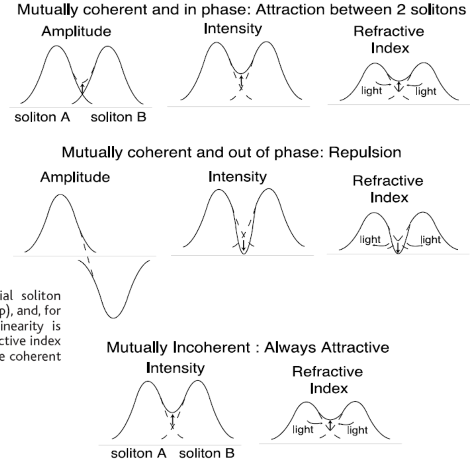


Fig. 2 (above). A top view photograph of a 10-μm-wide spatial soliton propagating in a strontium barium niobate photorefractive crystal (top), and, for comparison, the same beam diffracting naturally when the nonlinearity is "turned off" (bottom). (*23*). **Fig. 3 (right).** Schematic of the refractive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

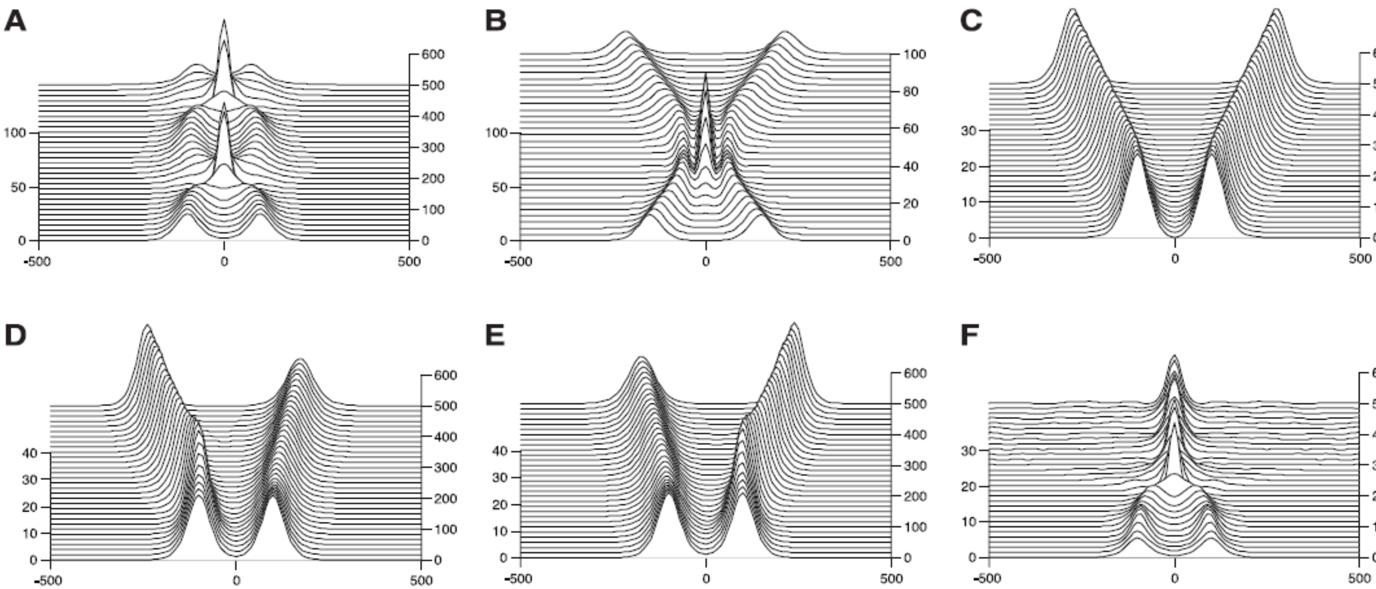


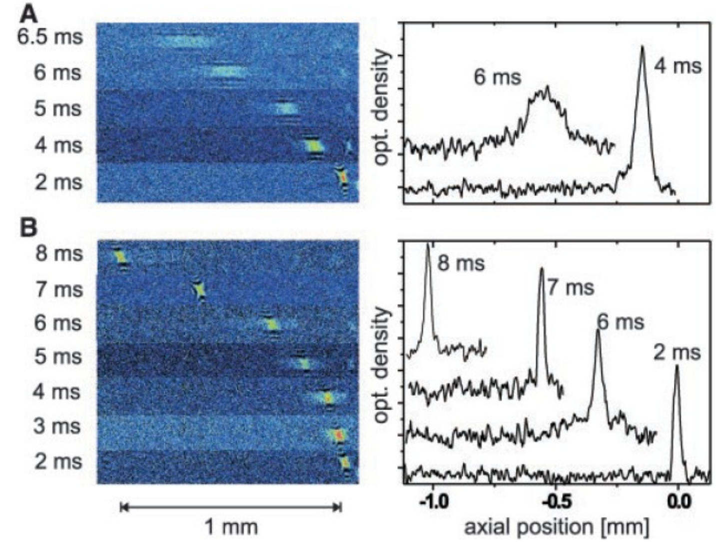
Fig. 4. Beam evolution calculations of the interactions between two solitons for the following cases: (**A**) Parallel input trajectories, in-phase Kerr solitons; (**B**) converging input trajectories, in-phase Kerr solitons; (**C**) parallel input trajectories, out-of-phase Kerr solitons; (**D**) parallel 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.

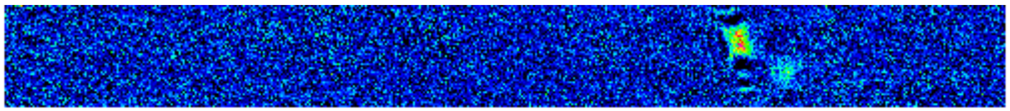
Formation of a Matter-Wave Bright Soliton

L. Khaykovich,[1] F. Schreck,[1] G. Ferrari,[1,2] T. Bourdel,[1] J. Cubizolles,[1] L. D. Carr,[1] Y. Castin,[1] C. Salomon[1]*

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.

Fig. 3. Absorption images at variable delays after switching off the vertical trapping beam. Propagation of an ideal BEC gas (**A**) and of a soliton (**B**) in the horizontal 1D waveguide in the presence of an expulsive potential. Propagation without dispersion over 1.1 mm is a clear signature of a soliton. Corresponding axial profiles are integrated over the vertical direction.





Absorption images at variable delays (2–8ms) 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*

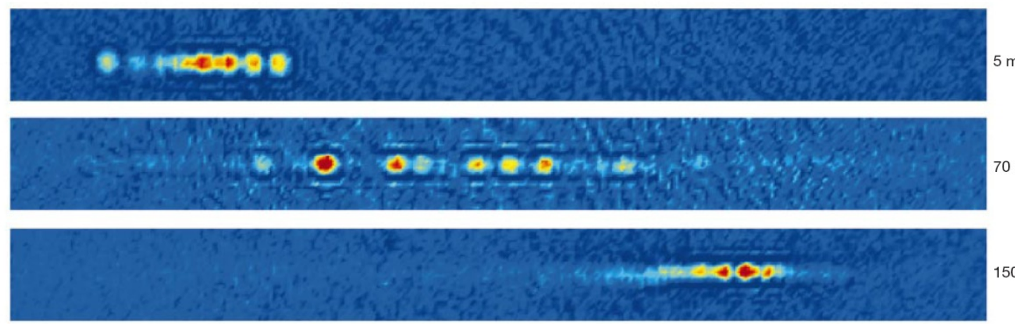


Figure 4 Repulsive interactions between solitons. The three images show a soliton train near the two turning points and near the centre of oscillation. The spacing between solitons is compressed at the turning points, and spread out at the centre of the oscillation. A simple model based on strong, short-range, 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.

NATURE | VOL 417 | 9 MAY 2002 | www.nature.com

PRL **96,** 170401 (2006) PHYSICAL REVIEW LETTERS

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

Simon L. Cornish,[1,*] Sarah T. Thompson,[2] and Carl E. Wieman[2]

PRL **112,** 060401 (2014) PHYSICAL REVIEW LETTERS week ending 14 FEBRUARY 2014

Evaporative Production of Bright Atomic Solitons

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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}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

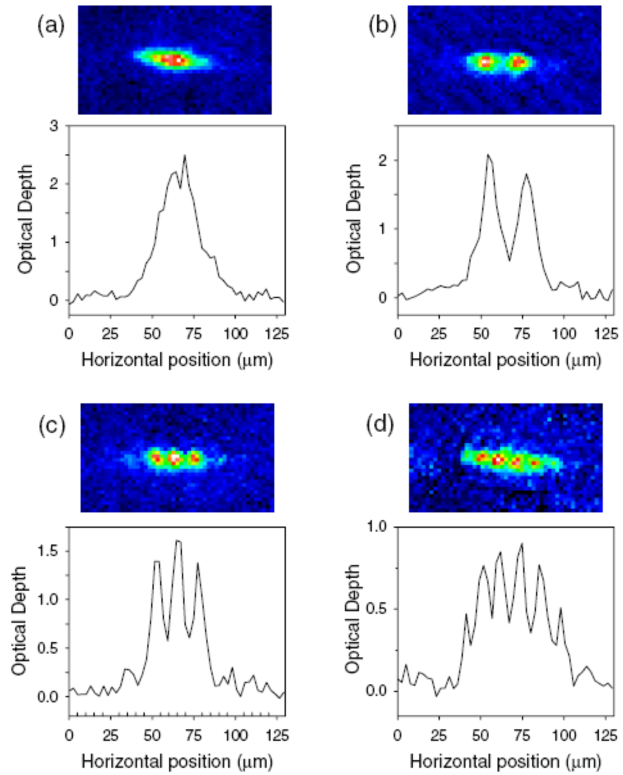


FIG. 3 (color online). Images and cross sections of remnant condensates. (a) When the magnitude of a_{collapse} is sufficiently small a single remnant condensate containing less than the critical number is observed to survive the collapse. When the magnitude of a_{collapse} is larger and/or larger initial 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 × 129 μm.

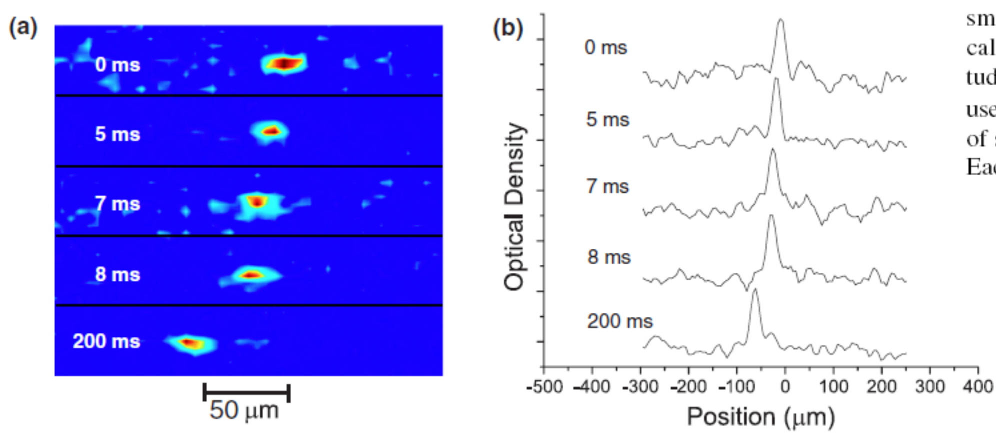
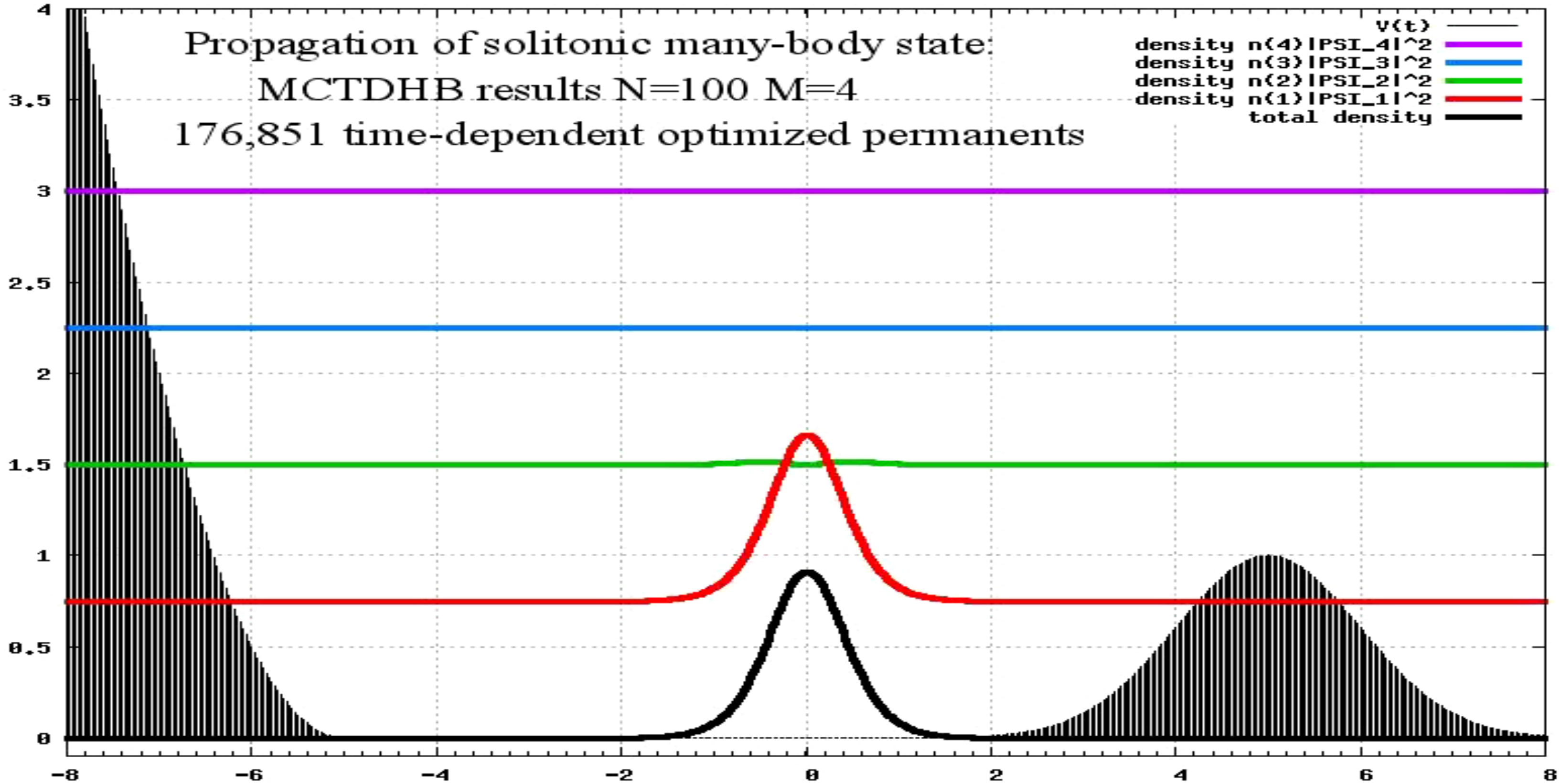


FIG. 2 (color online). (a) Absorption images and (b) axial profiles of solitons after various 1D times of flight in an expulsive waveguide, with curvature at the center of $|\omega| = 2\pi \times 20$ Hz for all but the 200 ms time of flight experiment, which had $|\omega| = 2\pi \times 5$ Hz. Each picture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

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

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



Initial wave-packet: location at x=0, velocity $\vec{v} = -1.0$

Left: wall $(x+5)^2/2$ Right: barrier $Exp(-(x-5)^2/2)$

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)

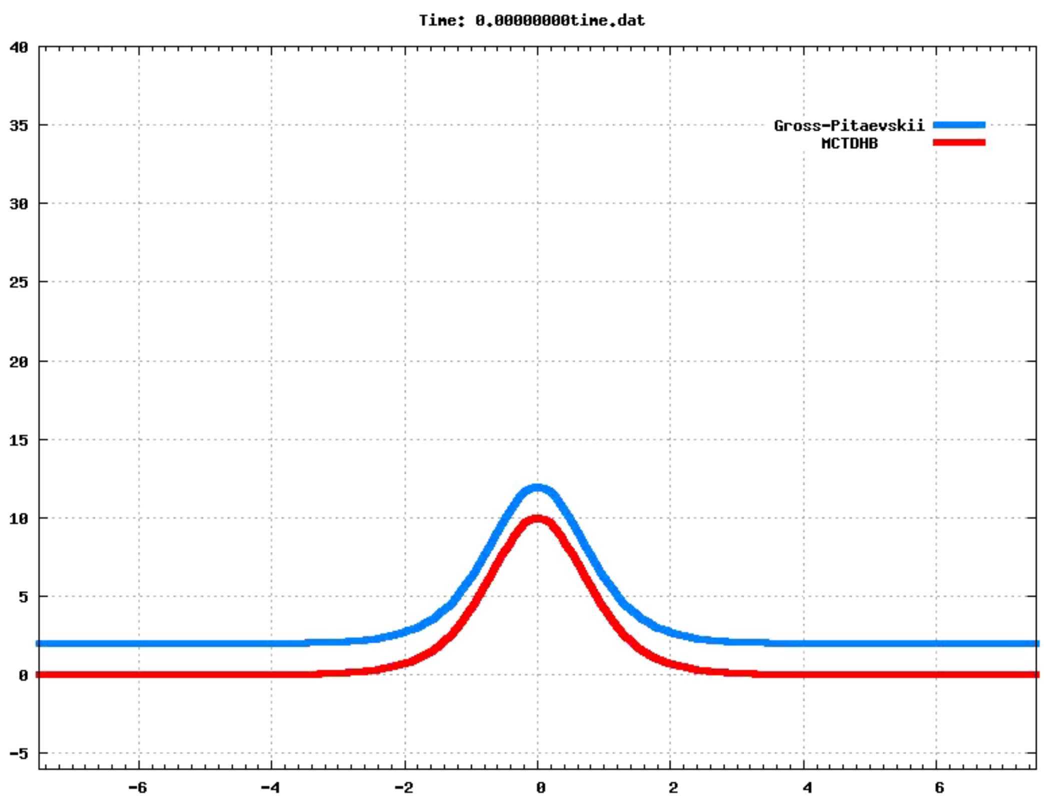
Catons: Formation PRA 80, 043616 (2009)

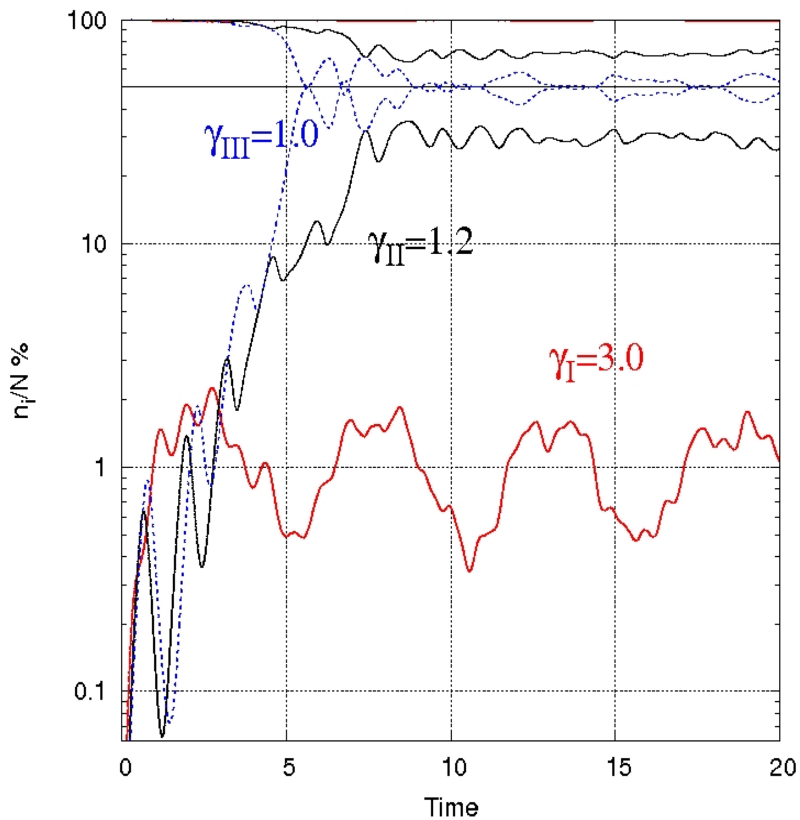
Efficient generation JPB 42, 091004 (2009)

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:*

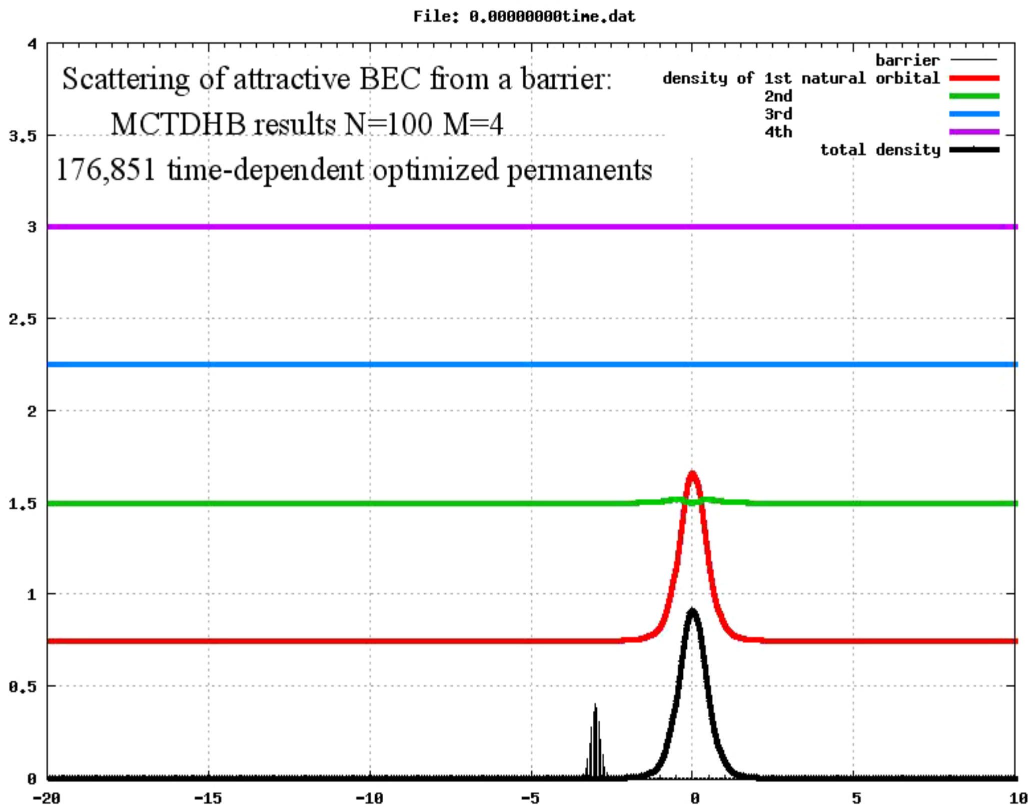
(1)two-fold fragmented, (2) propagates almost without dispersion (3) delocalized NO

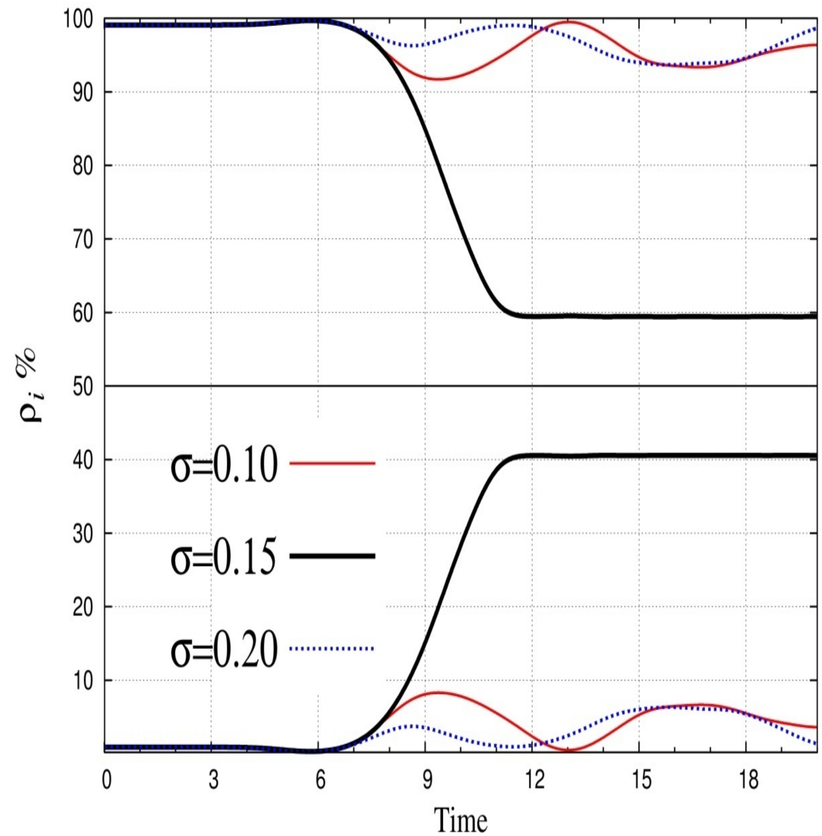
http://QDlab.org

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**)





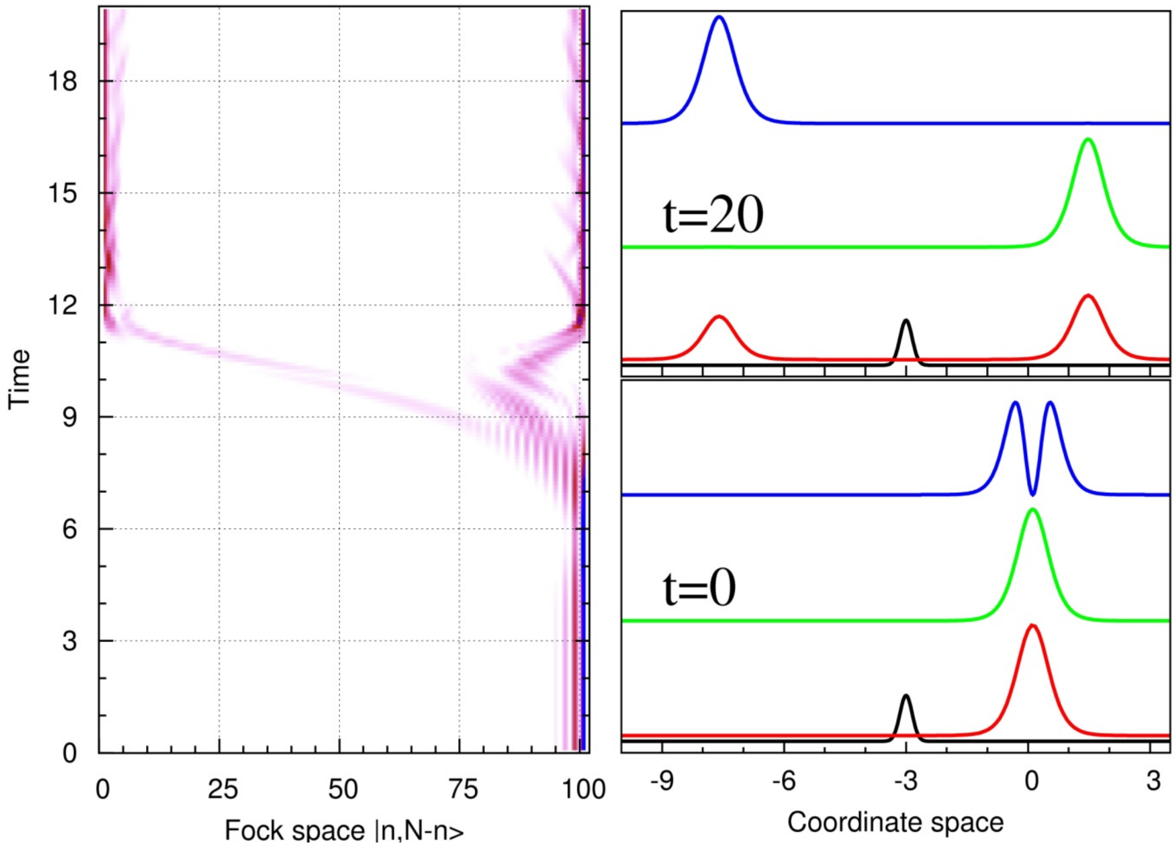
Efficient generation of Schrödinger cats JPB 42, 091004 (2009)

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⟩,|N-1,1⟩,...,|1,N-1⟩,|0,N⟩ configurations



t=20:

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

t=0:

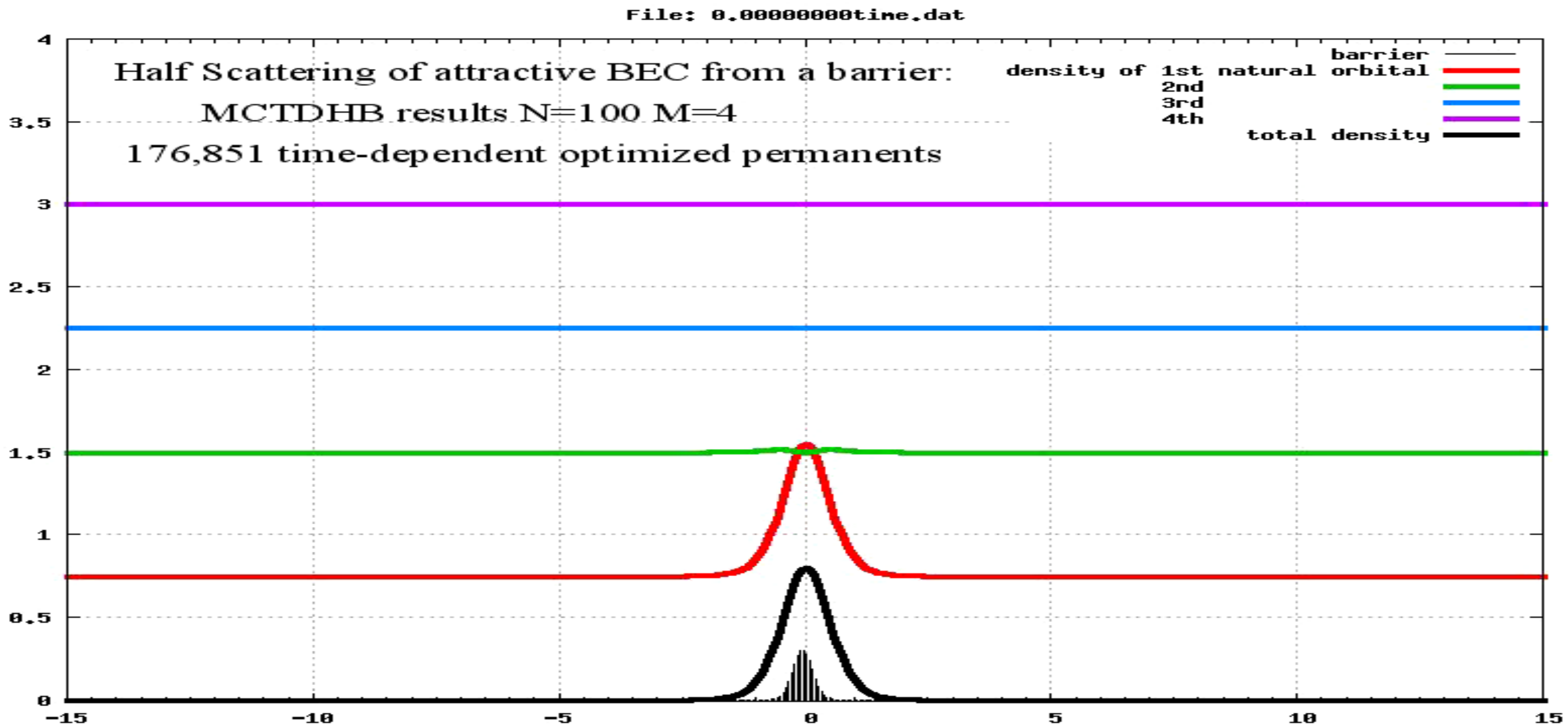
mainly |0,N⟩ contribute

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

MCTDHB: Efficient generation of Schrödinger cats :

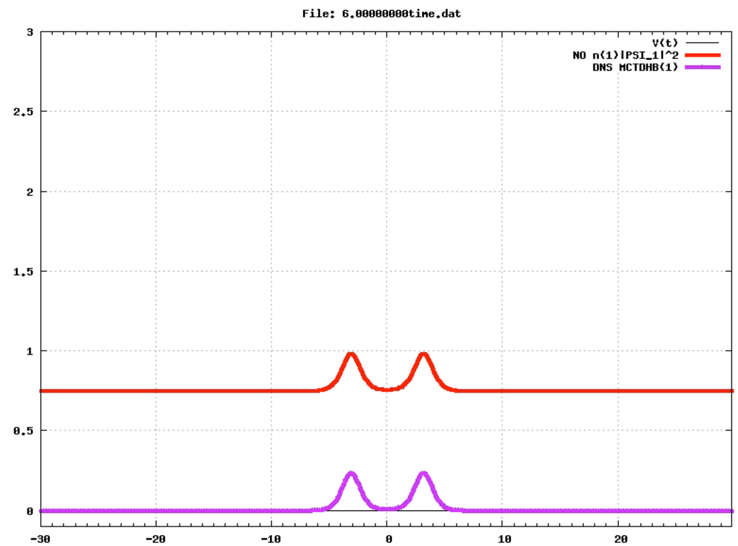
Attractive BEC is threaded by a potential barrier JPB, 42 091004 (2009)

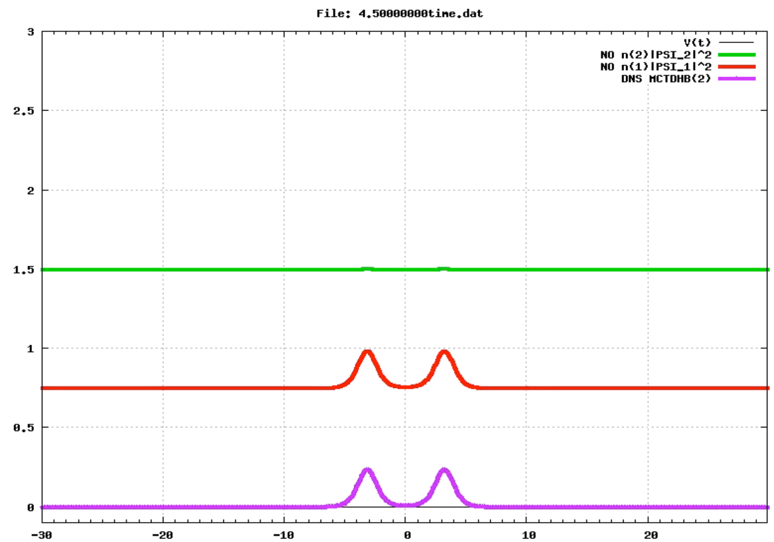
$$\rho(r,r';t)=\int \Psi^*(r,r_2,\ldots,r_N;t)\Psi(r',r_2,\ldots,r_N;t)dr_2\ldots dr_N=\sum_{k,q}\rho_{kq}(t)\phi_k^*(r,t)\phi_q(r',t)=\sum_i n_i\left|\phi_i^{NO}(r=r',t)\right|^2$$

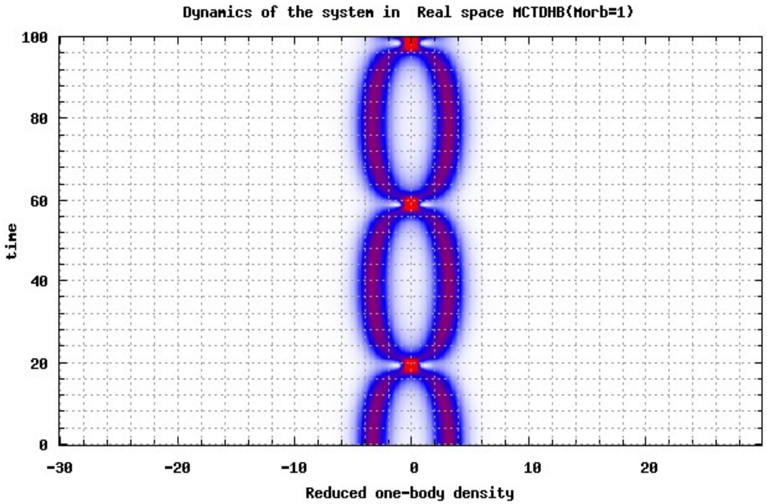


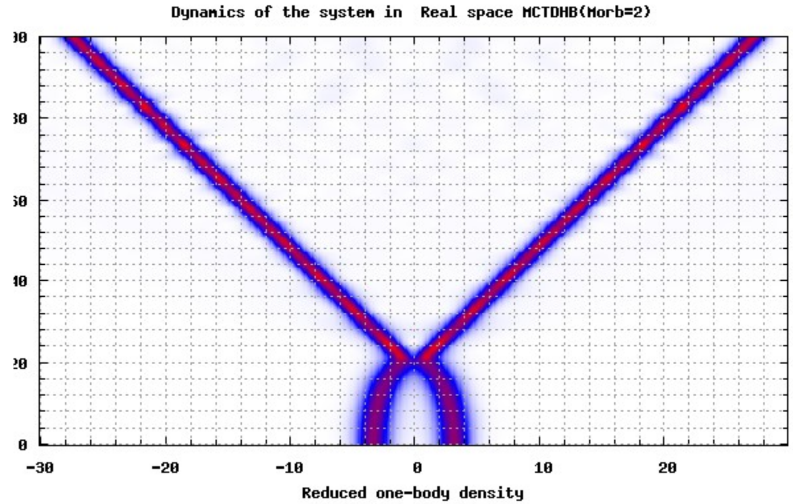
The time-dependent **Schrödinger cat** state – **CATon** is formed

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





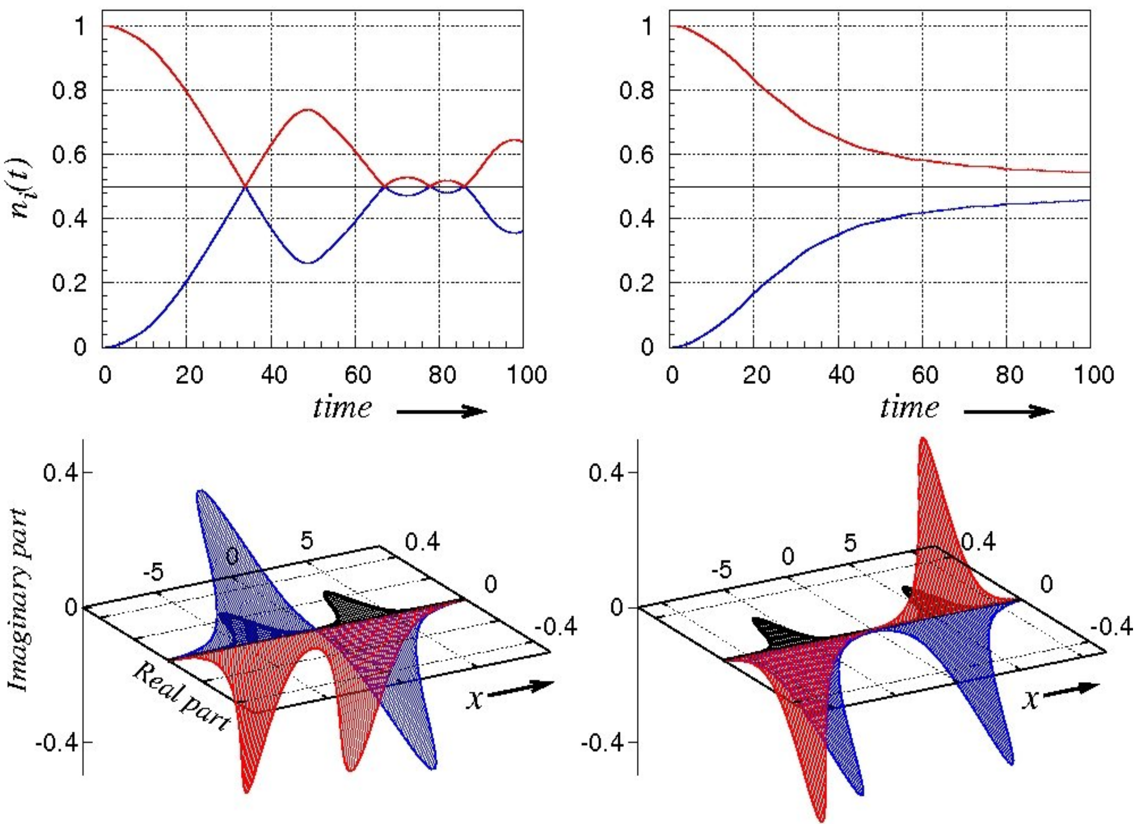


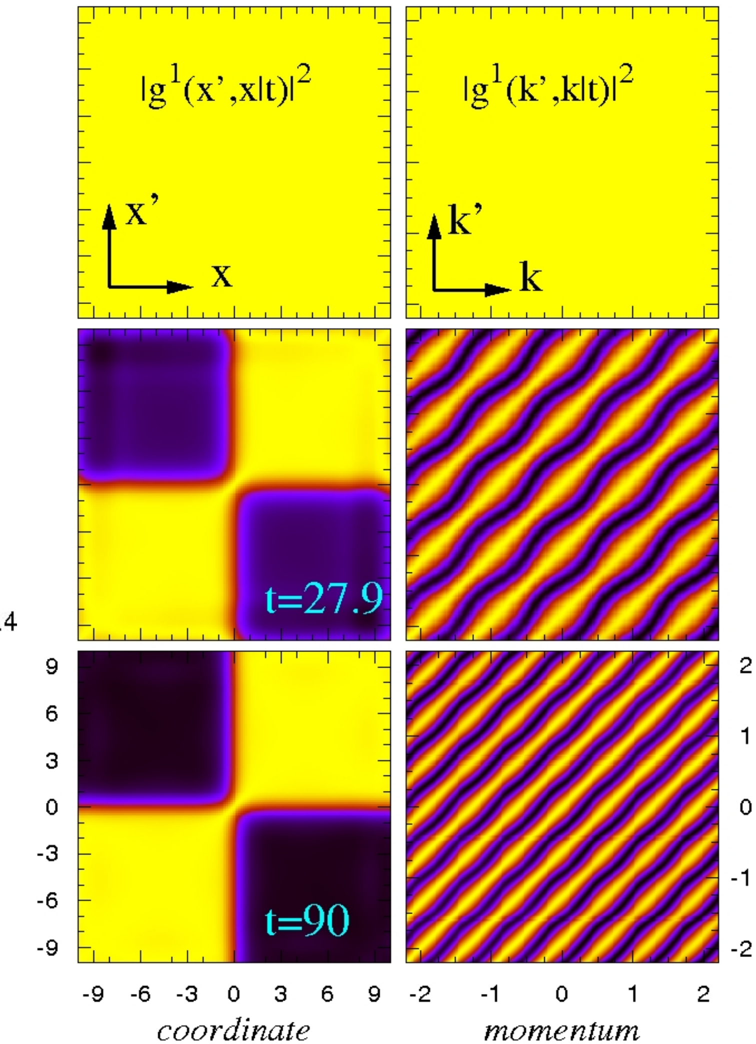


Fragmentation phenomena with *the* MCTDHB

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)

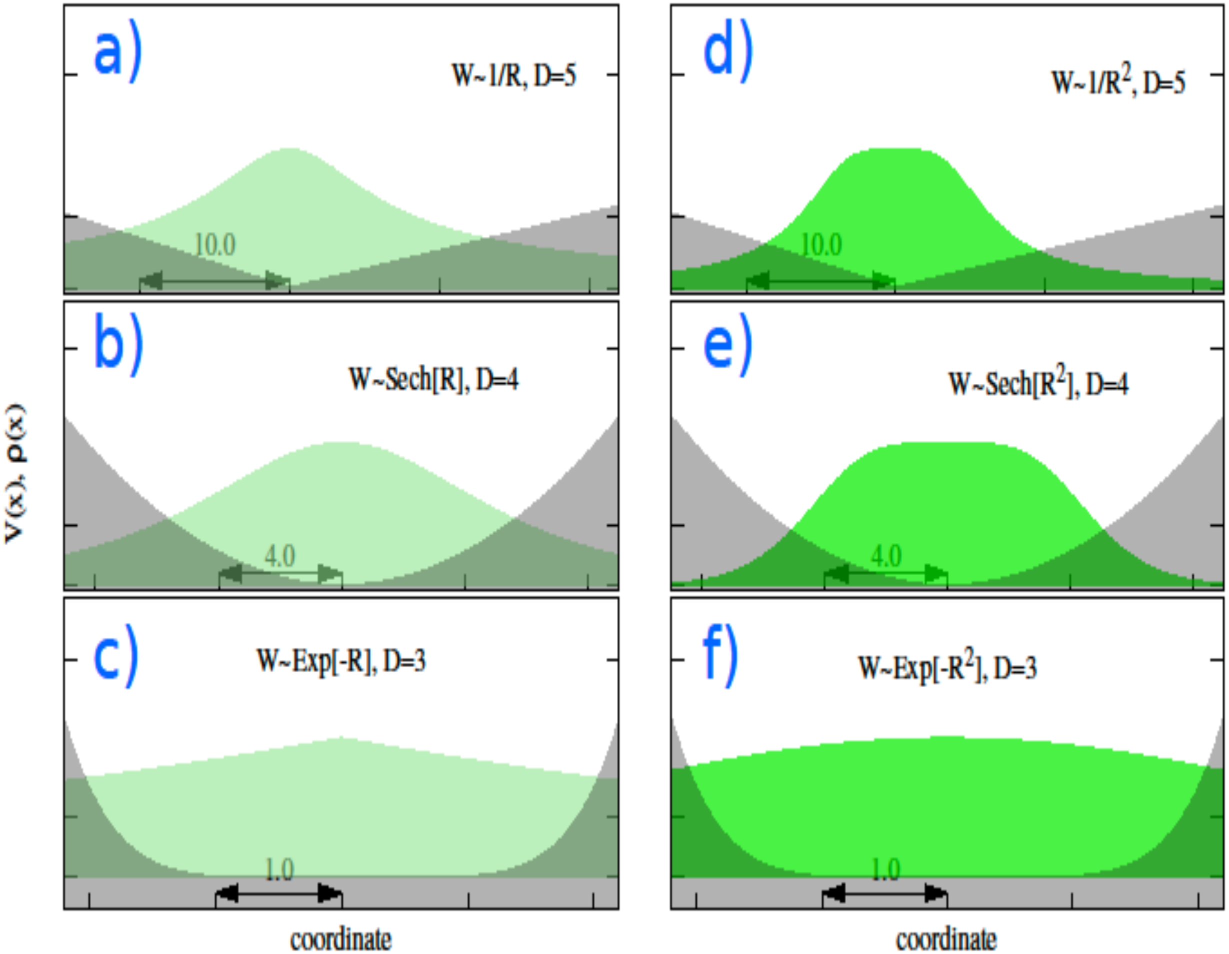
- ✓ ***The initially coherent wave-packet threaded by (scattered from) a barrier (can) dynamically dissociate into two parts***
- ✓ ***The time-dependent GP theory applied to similar initial state does not show up the splitting***
- ✓ ***The split object CATon possesses remarkable properties:***

(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)



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

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

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

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

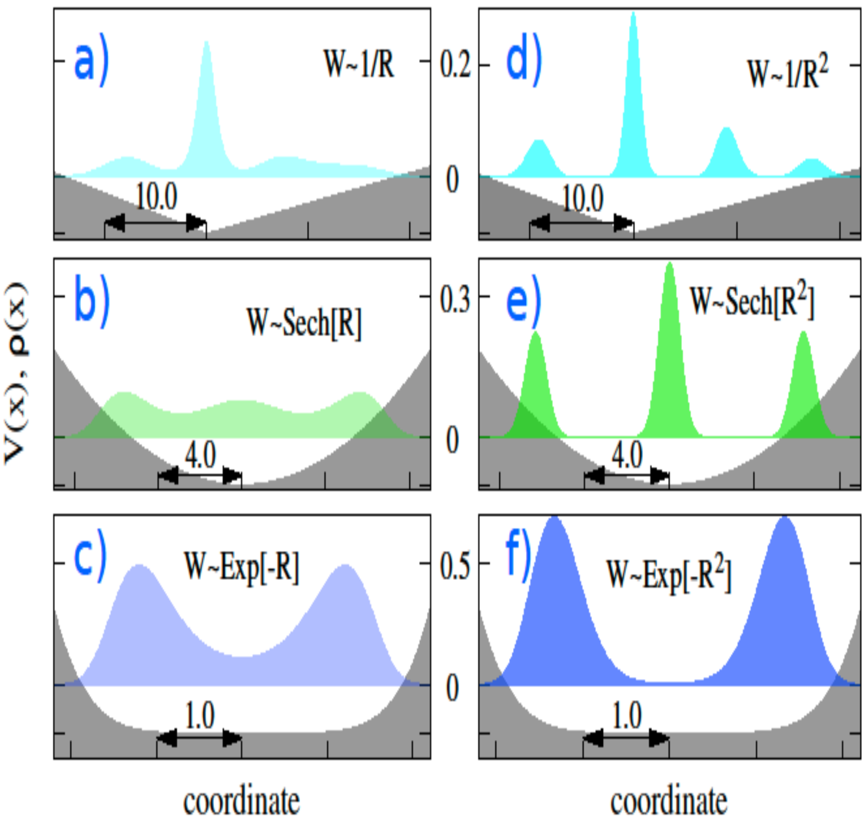
$$\mathbf{W(R)} = \mathbf{Exp}\left[-\tfrac{1}{2}\left(\frac{|x-x'|}{D}\right)^{n}\right]$$

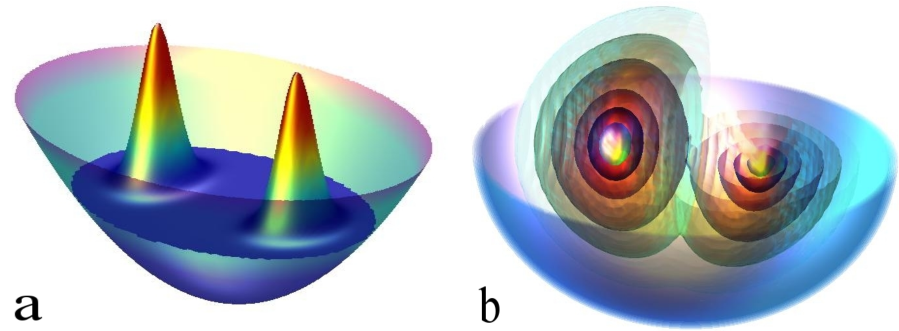
$$\mathbf{V}(x) = \tfrac{1}{2}x^6$$

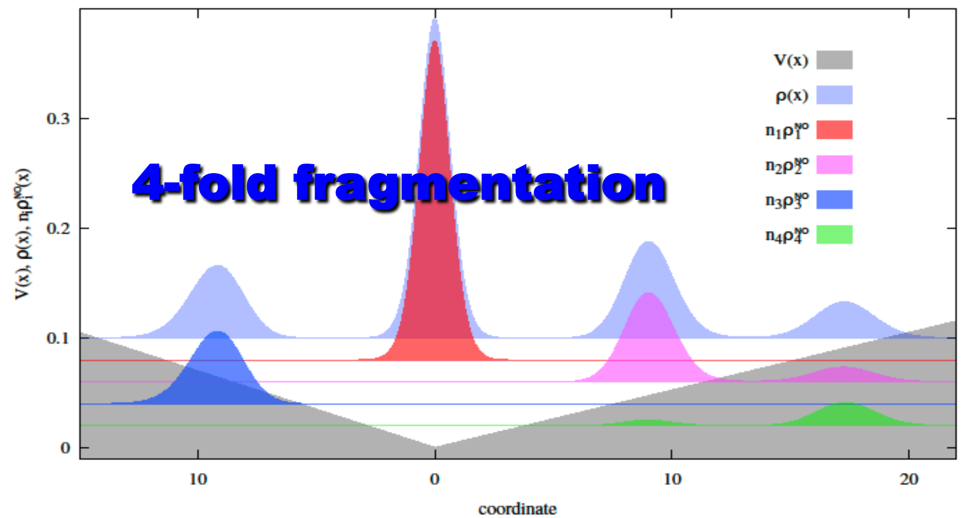
W(R) depicted on the left and right panels have the same range (width) D, but tails of the right ones are "shorter"

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)







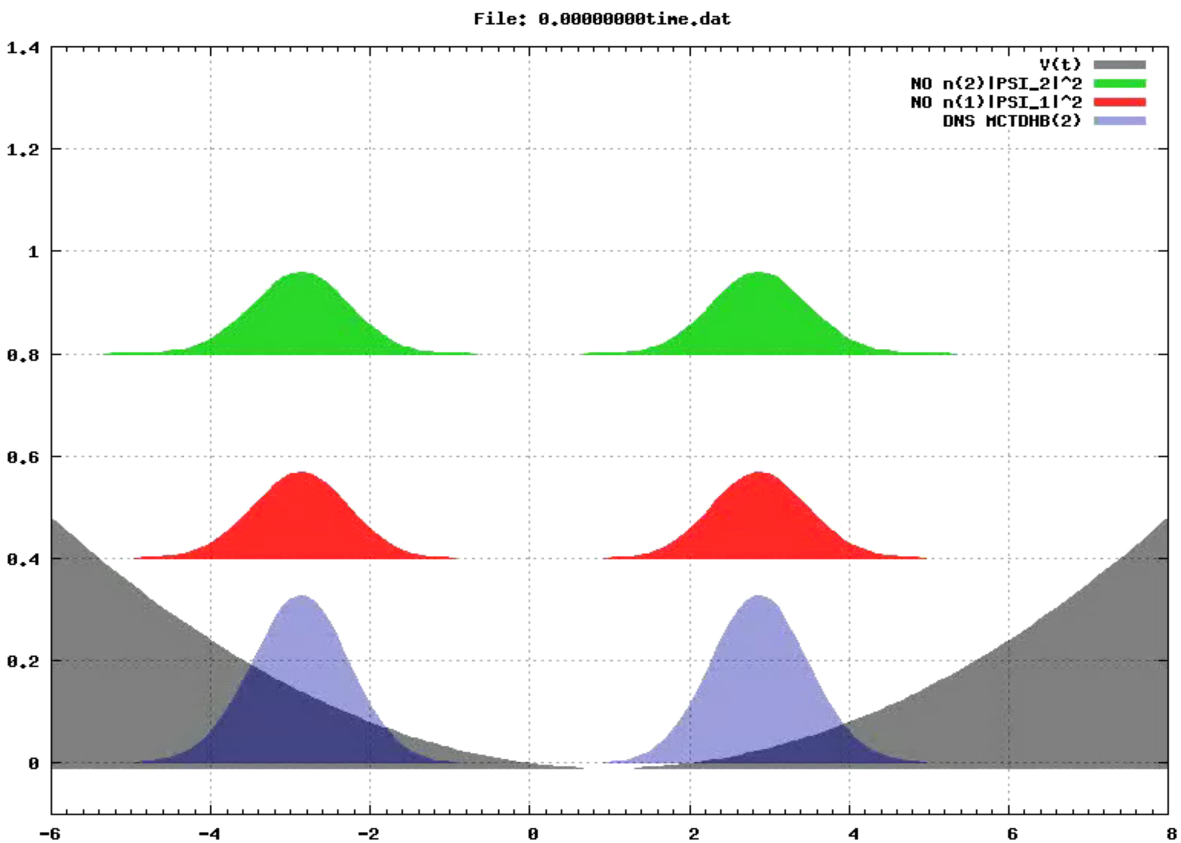
Irrespective to the shapes of inter-particle W(R) and trapping V (r) strong inter-particle repulsion leads to formation of multi-hump localized fragmented structures …

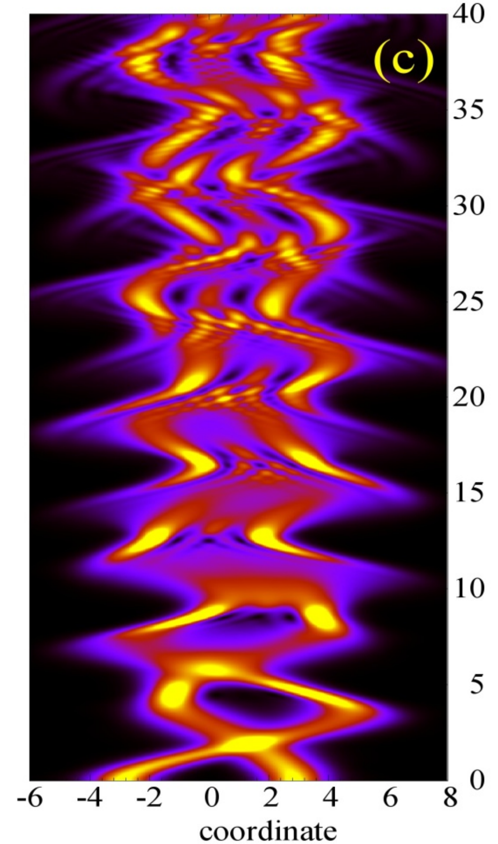
Non-violent regime ↔ under-a-barrier AND Violent, explosive regime ↔ over-a-barrier dynamics (when the induced barriers are not high enough to keep the sub-clouds apart from each other)

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

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

$$V(x)=\tfrac{1}{2}x^2 \rightarrow V(x-1) \qquad \lambda_0 = 0.5 \rightarrow 0.1$$

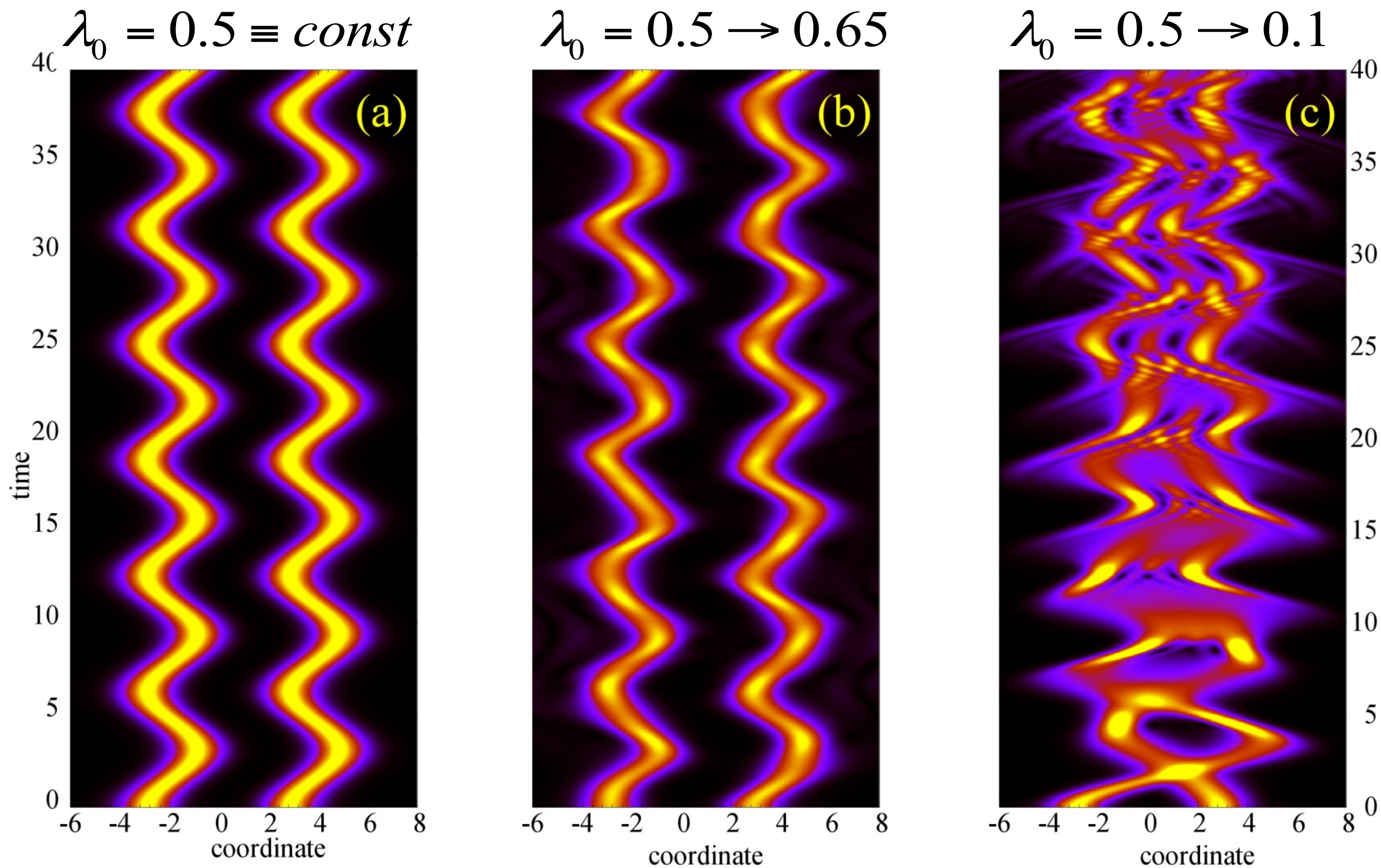




To visualize wave-packet dynamics we utilize Minkovskii-like space-time representation as a 2D plot

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

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



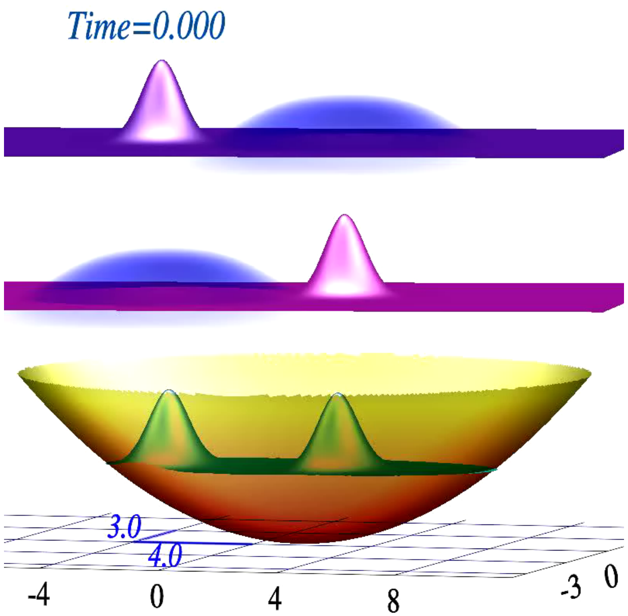
Message: Two generic regimes: (i) non-violent (under-a-barrier) and (ii) Explosive (over-a-barrier)

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

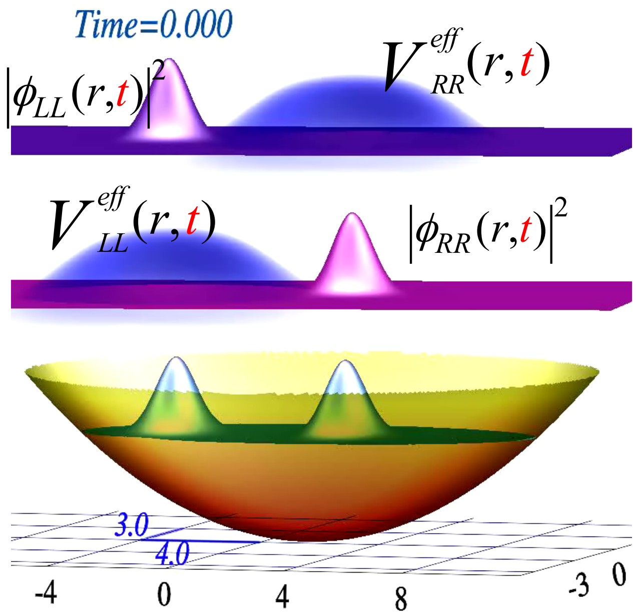
$$\mathbf{V}(x,y)=\tfrac{1}{2}x^2+\tfrac{3}{2}y^2 \rightarrow \mathbf{V}(x-1.5,y-0.5)$$

$\lambda_0 = 0.5 \rightarrow 0.1$

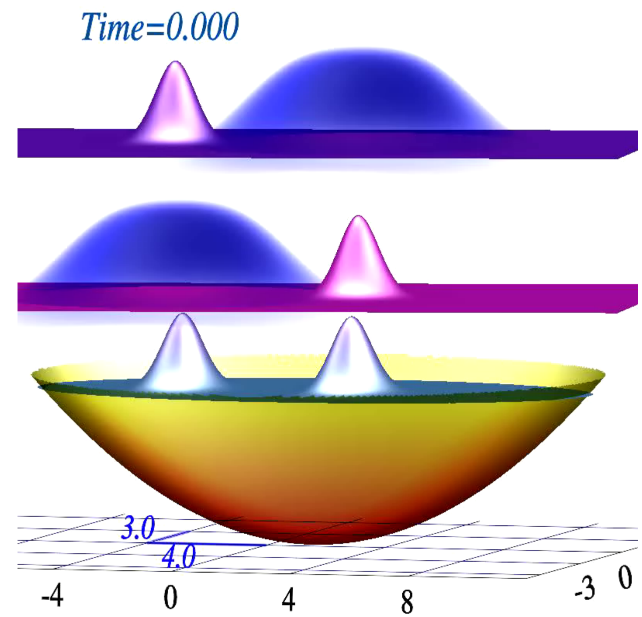


$V_{ii}^{eff}(r,t)\times 40$

$\lambda_0 = 0.5 \rightarrow 0.7$



$\lambda_0 = 0.5 \rightarrow 0.8$



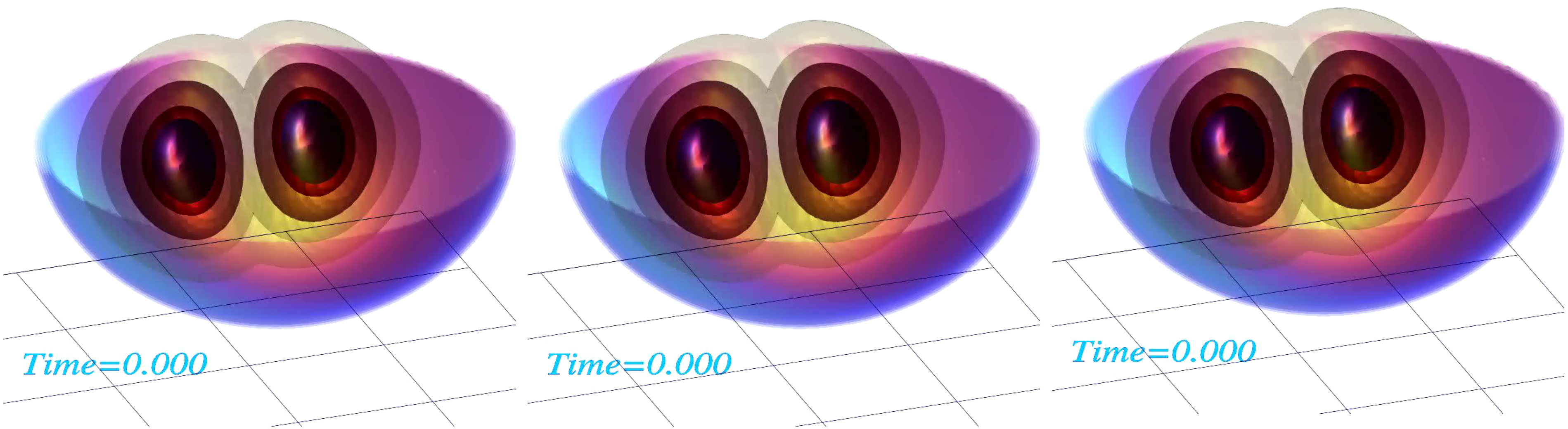
Two generic regimes: (i) non-violent (under-a-barrier) and (ii) Explosive (over-a-barrier)

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

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

$\lambda_0 = 0.5 \rightarrow 0.1$ $\lambda_0 = 0.5 \rightarrow 0.7$ $\lambda_0 = 0.5 \rightarrow 0.8$



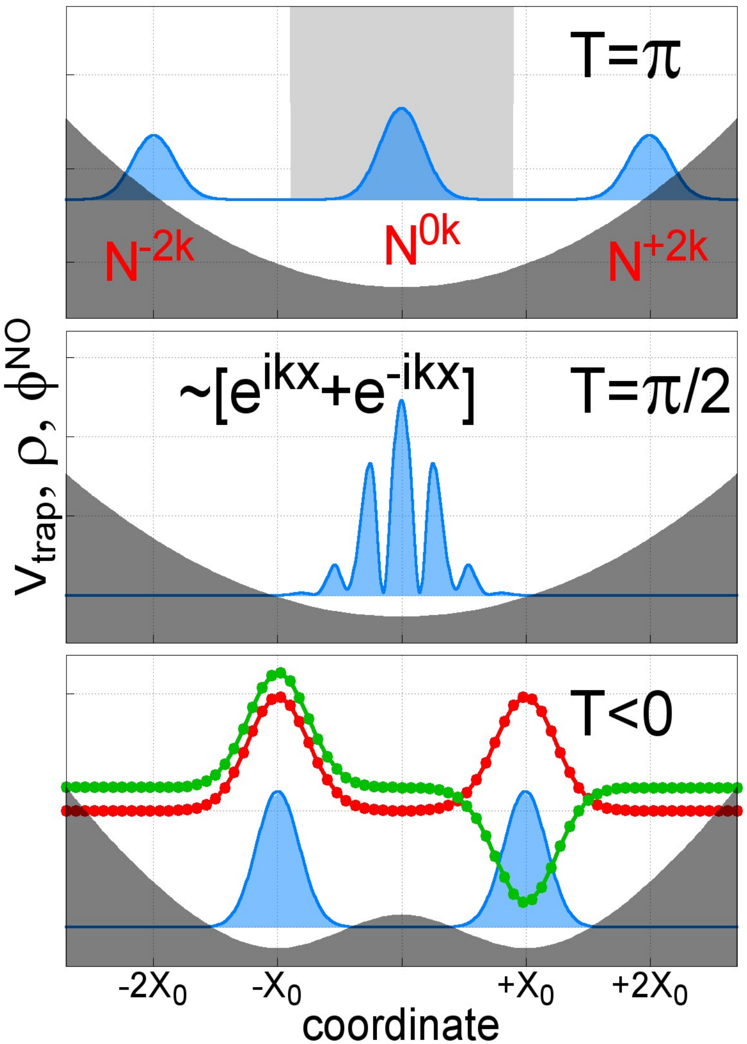
Two generic regimes: (i) non-violent (under-a-barrier) and (ii) Explosive (over-a-barrier)

Fragmentation phenomenon in BECs

Repulsive, attractive, short-, finte- 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 momenum in (+2k,0k,-2k)-channels

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

III-step: Apply a recombining laser-pulse of a proper phase and momentum 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 $n_2\approx50\%$

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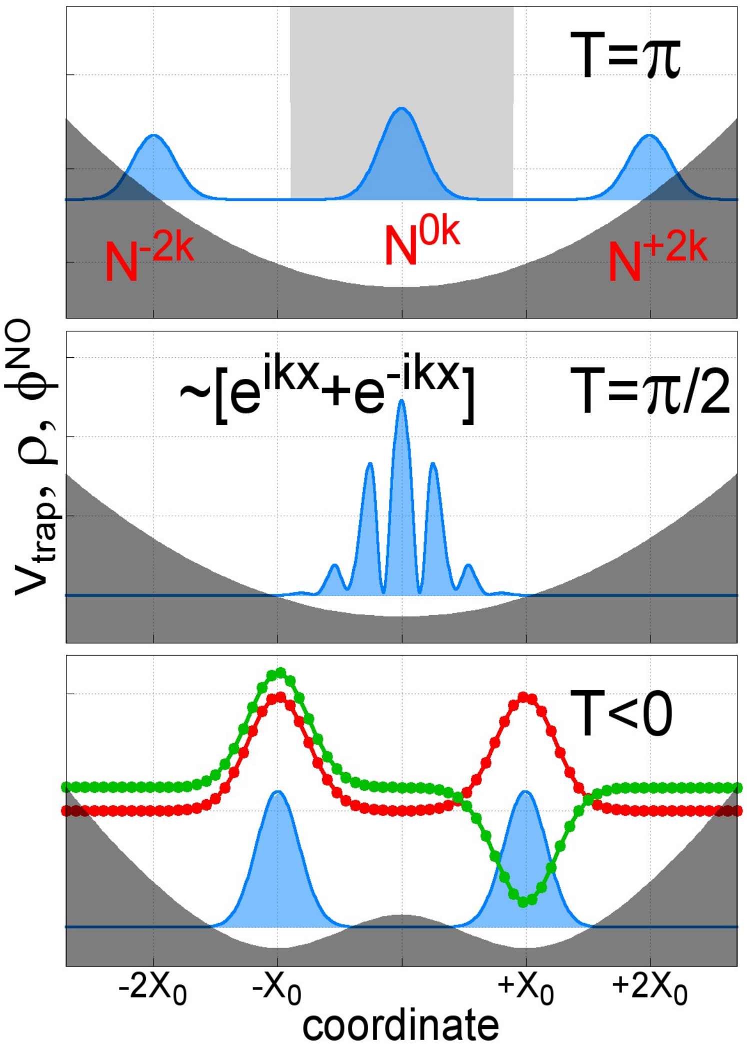
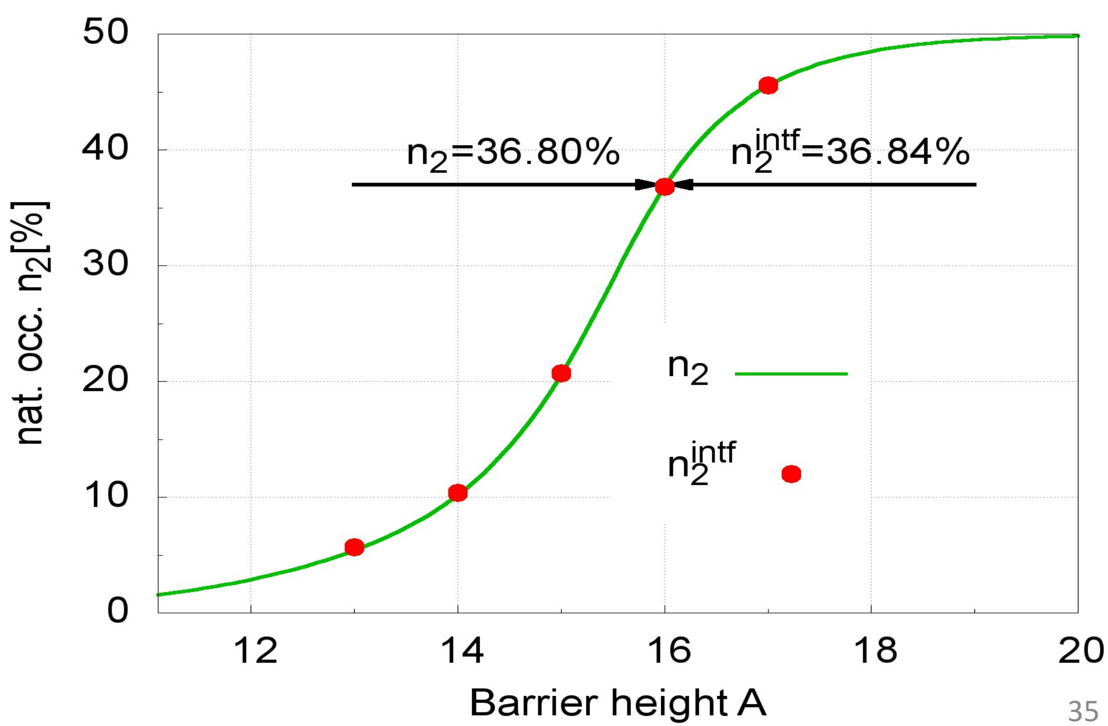


I-step: Split repulsive BEC by Gaussian barrier A

It can be condensed $n_2<5\%$, depleted $n_2<10\%$ or two-fold fragmented $n_2 \approx 50\%$



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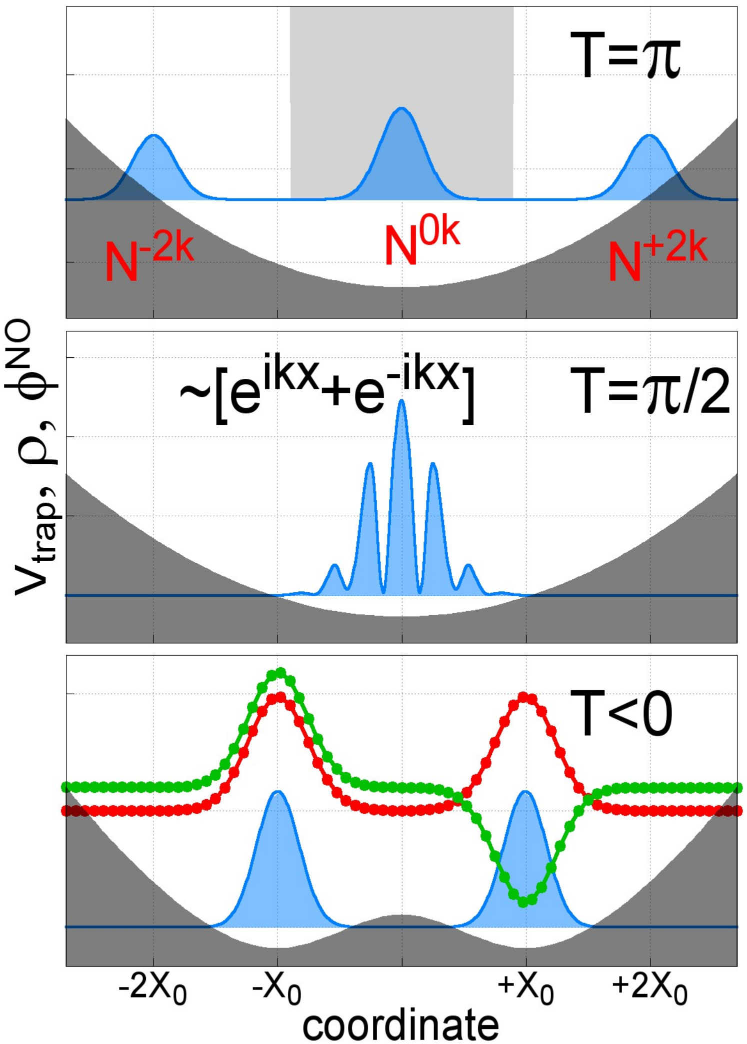
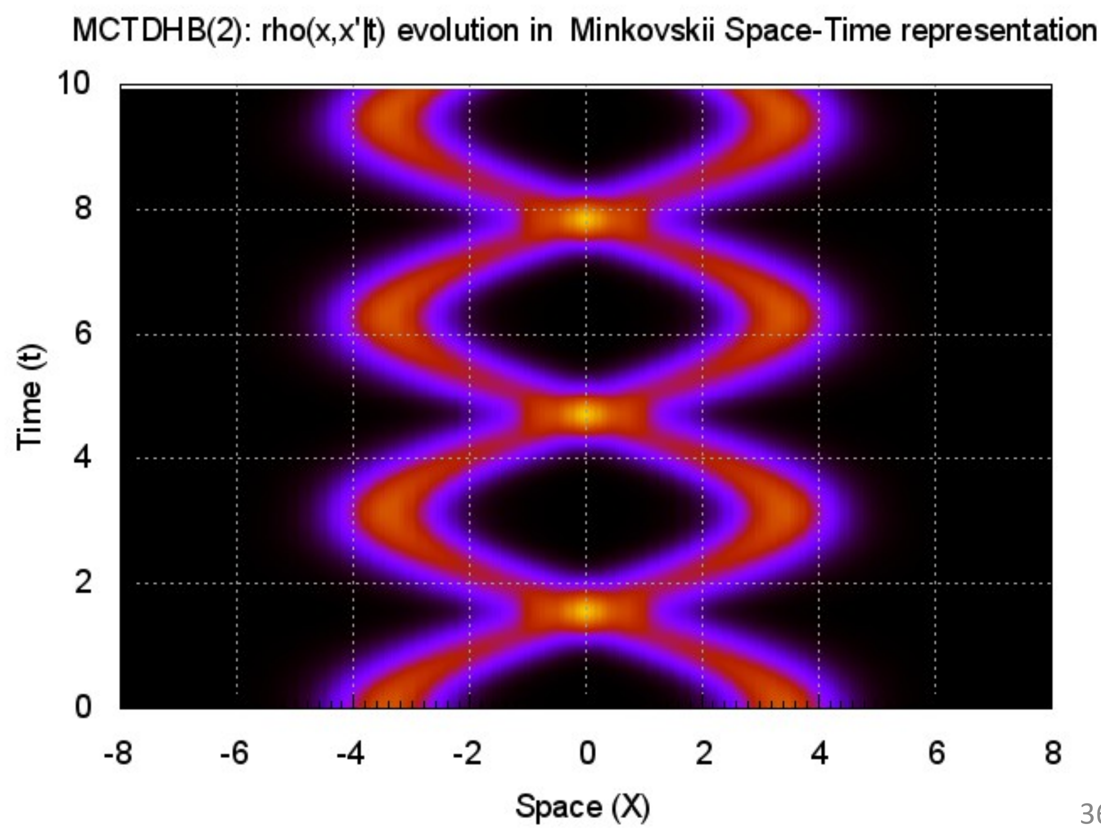


II-step: To deflect the split parts we switch off the Gaussian barrier A=0



Fragmentation phenomenon in BECs

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

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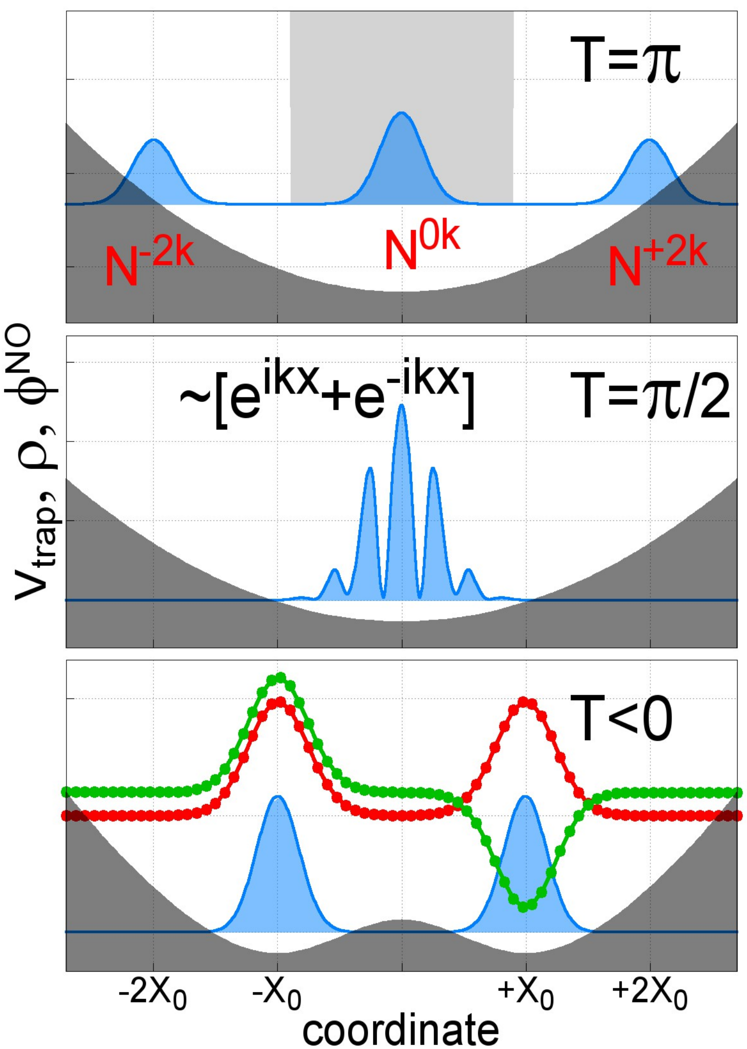
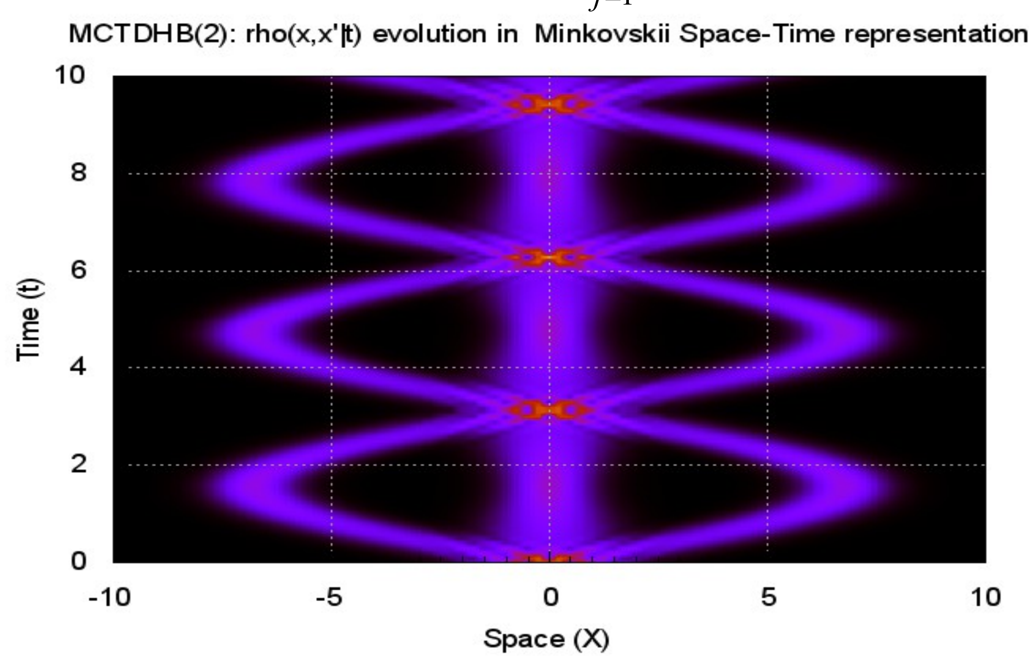


III-step: Apply a recombining Kapitza-Dirac laser-pulse of a proper phase and momentum $k=X_0$ ($k^2/2m=X_0^2/2$) at the re-collision time T_{rc}

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

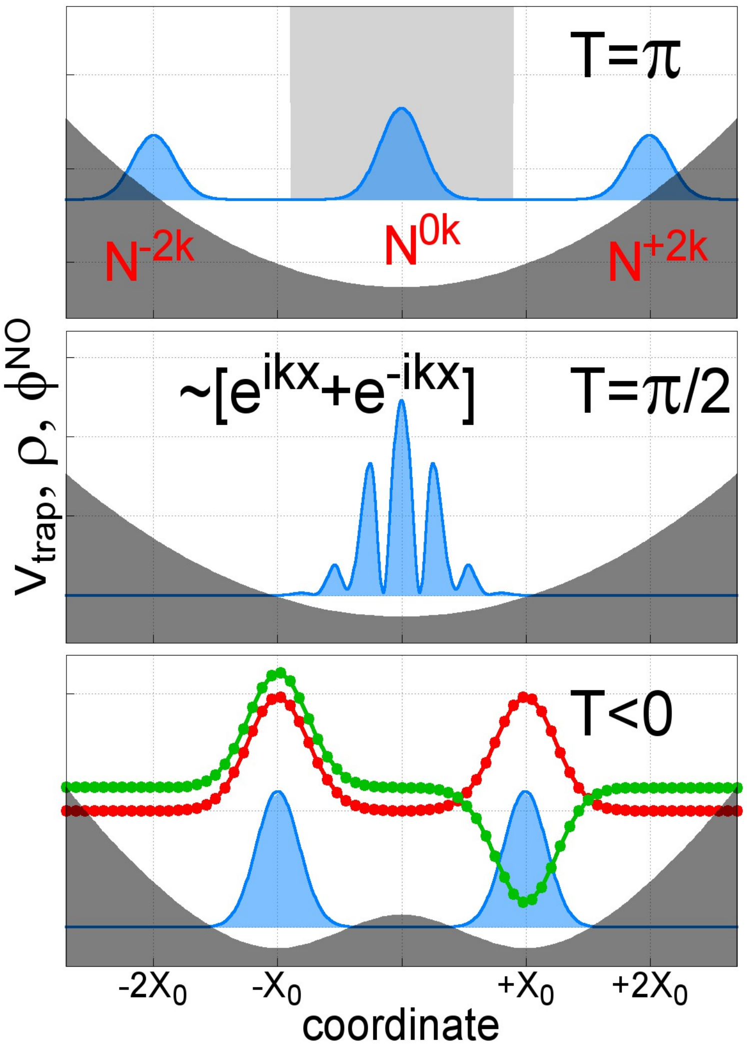


Fragmentation phenomenon in BECs

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

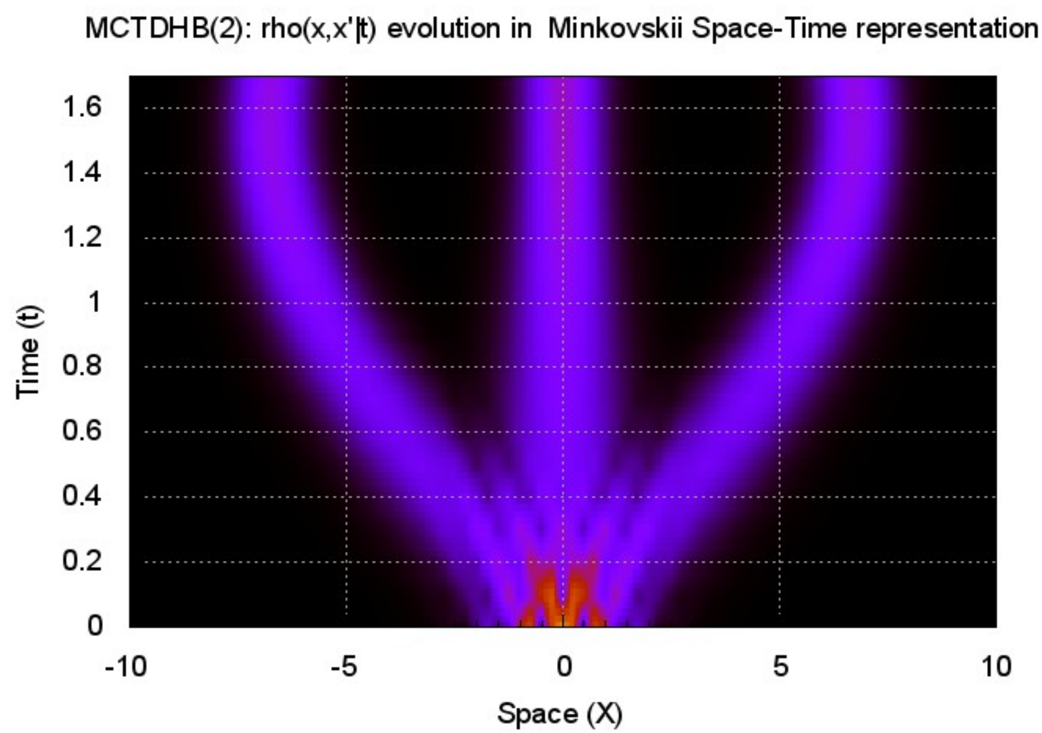
Static and highly-non-equilibrium dynamics, 2- 3- 4- fold fragmentation

How to measure natural occupations? With Interferometric Protocol!



IV-step: Measure the populations of the sub-clouds at T=π propagating with different momenum (k-channels)

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

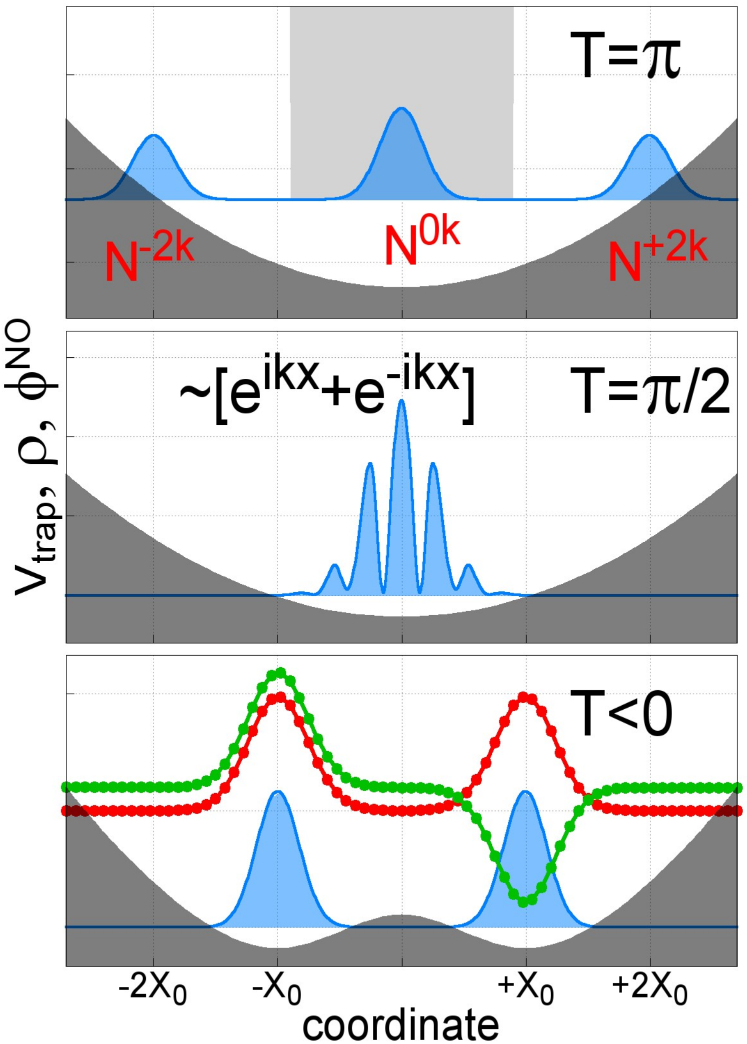


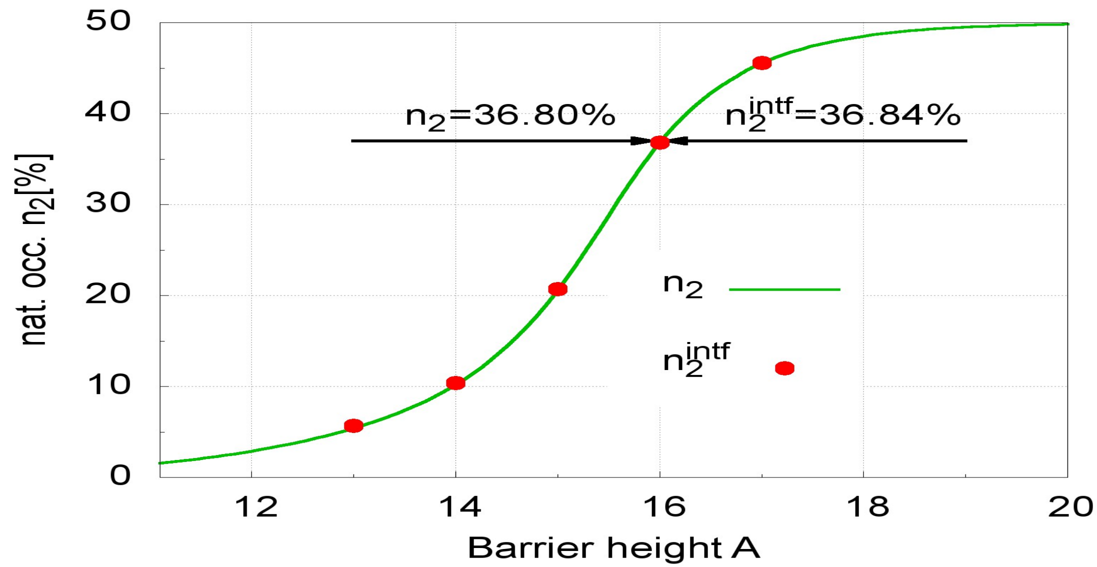
Fragmentation phenomenon in BECs

Repulsive, attractive, short-, finte- 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≈ 5.67%

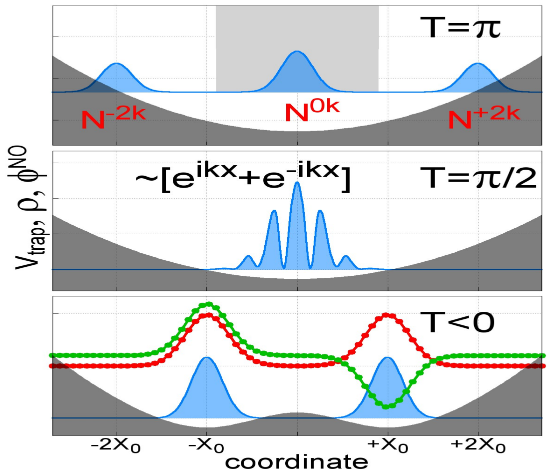
At A=14: RDM n_2=10.20% Interfer. n_2≈10.37%

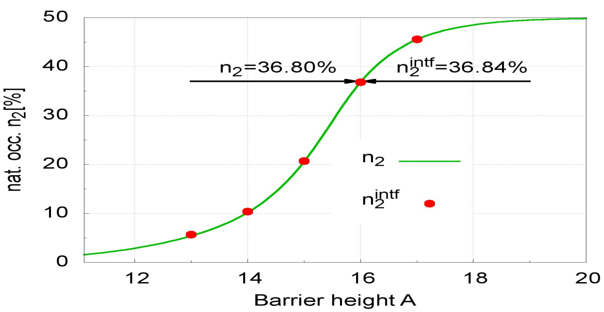
At A=17: RDM n_2=45.53% Interfer. n_2≈45.59%

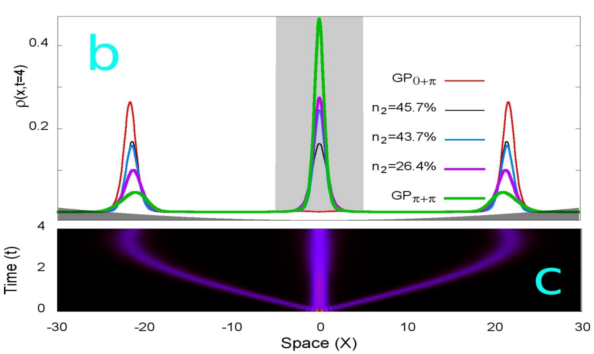
Small differences due to approximations:

1) **$k=m\varpi X_0$** (strict only for Gaussian sub-clouds)
2) **As X_0 we took minima of the dowble-well trap**

Conclusions on How to measure fragmentation?
arXiv:1412.4049







Interferometric Protocol

Universal:

- **Repulsive, attractive, short-, finte- 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≈45.59%)**

Selective:

- **Varying the phase χ of the applied laser Dirac-Kapitza pulse:**

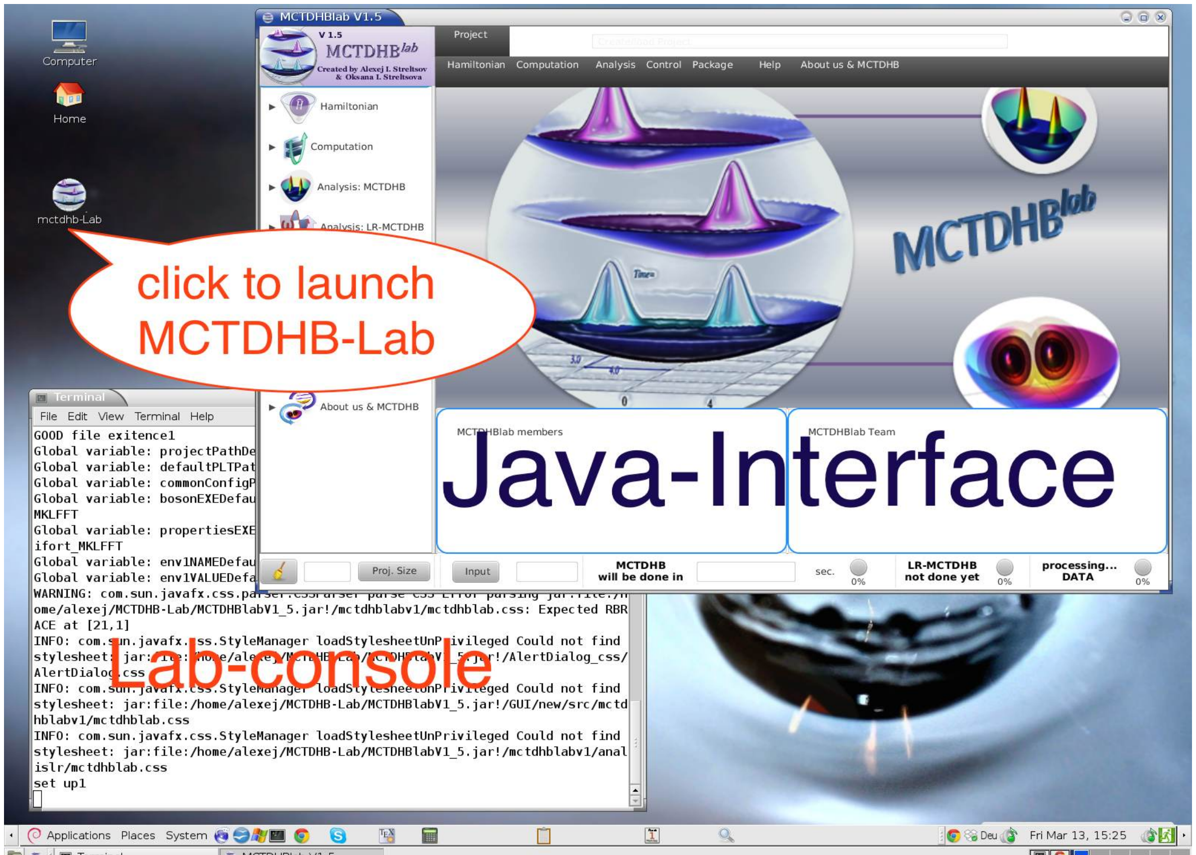
$$e^{[-ikx]}+e^{[+ikx+i\chi]}$$

one can select which occupation number to measure. In the above double-well example to access n_2 we use $\chi=0$, to access n_1 one should use $\chi=\pi$

http://www.QD-lab.org

The laboratory to study quantum many-body dynamics

Linux:



http://www.QD-lab.org

MCTDHB^lab

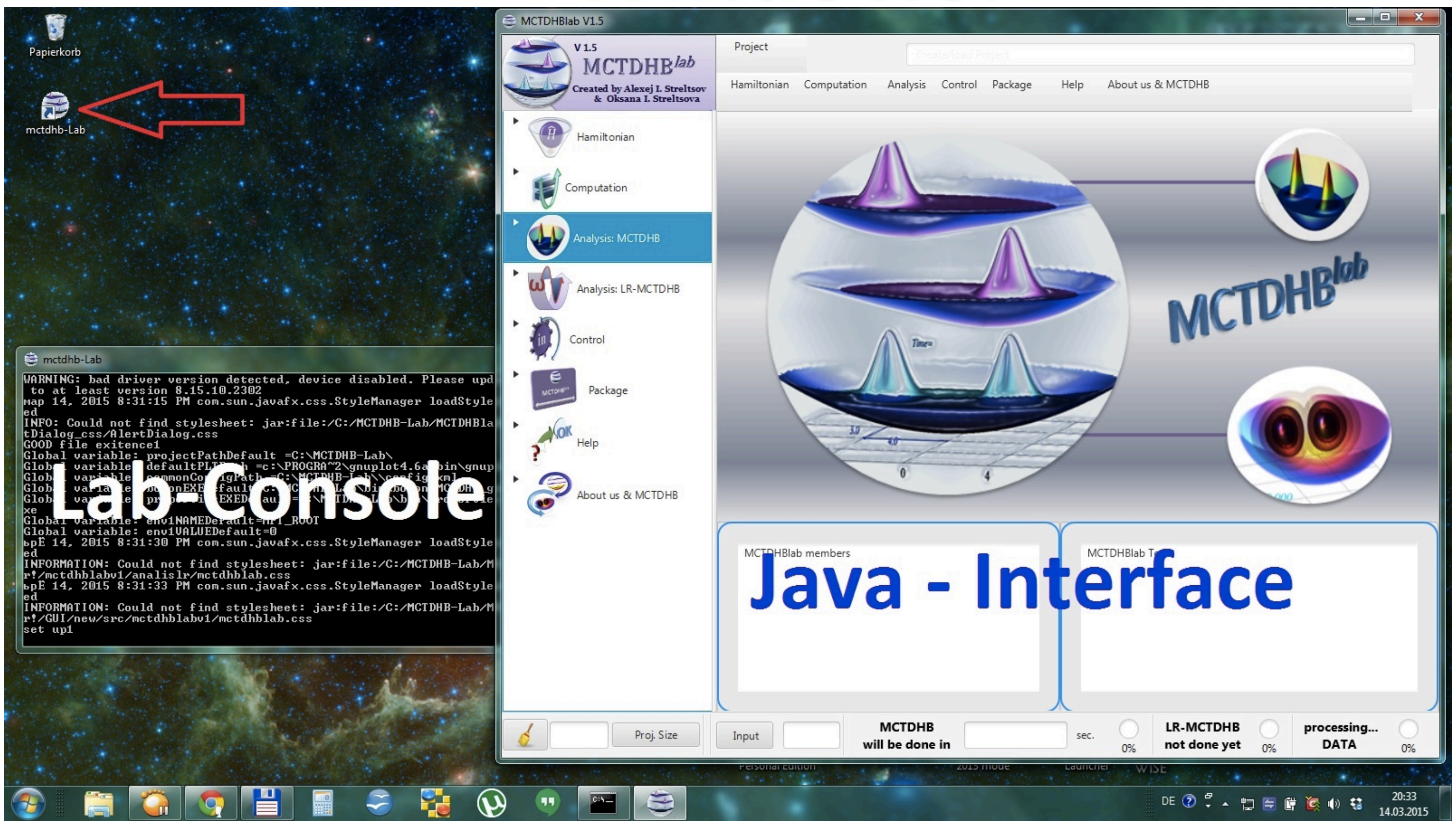
The laboratory to study quantum many-body dynamics

Mac OS:

http://www.QD-lab.org

The laboratory to study quantum many-body dynamics

Windows:



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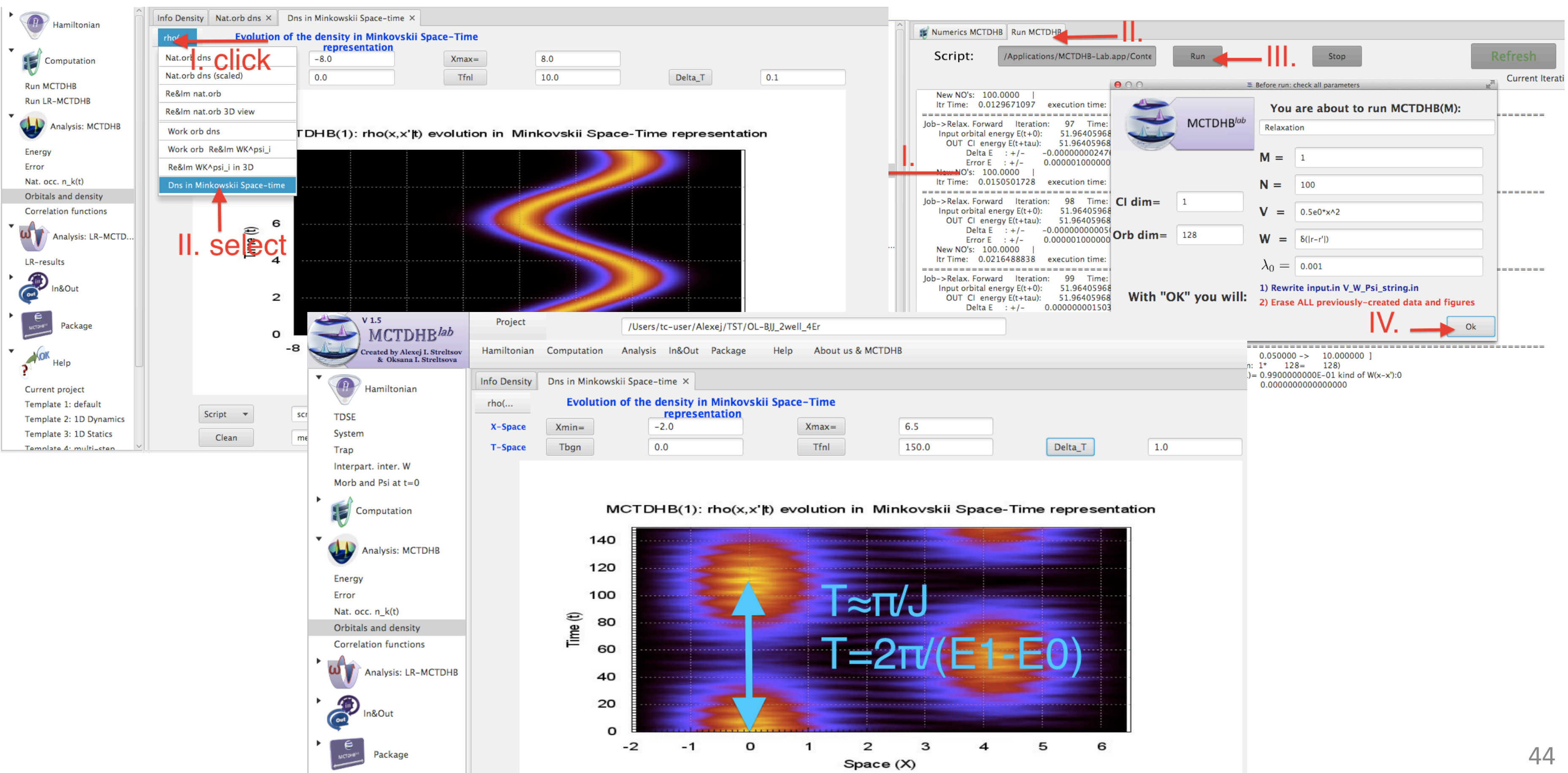
The laboratory to study quantum many-body dynamics

Win&Mac&Linux:



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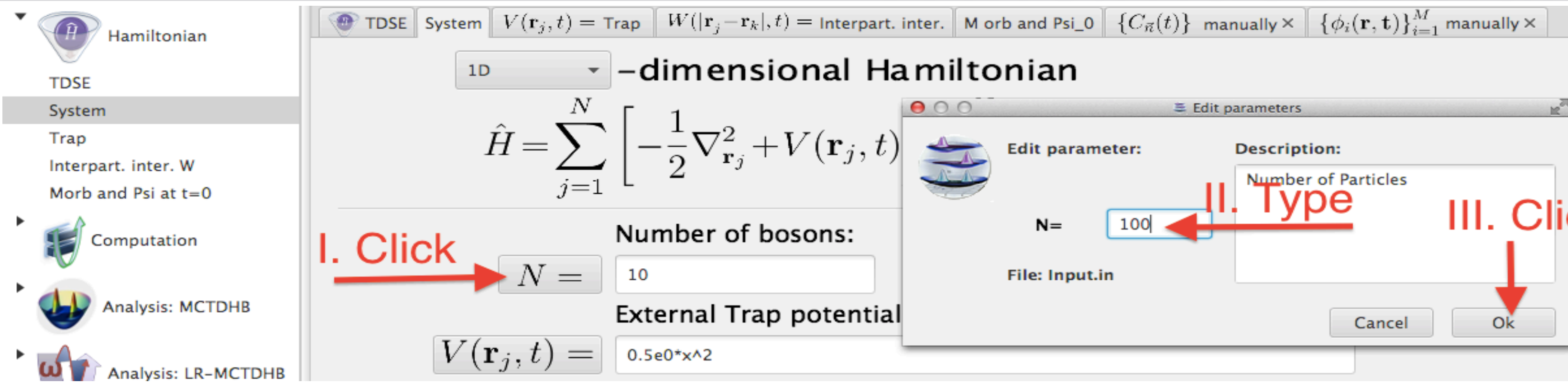

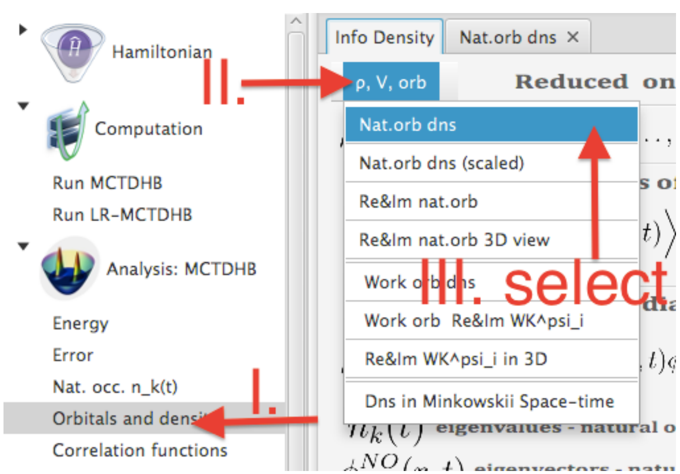

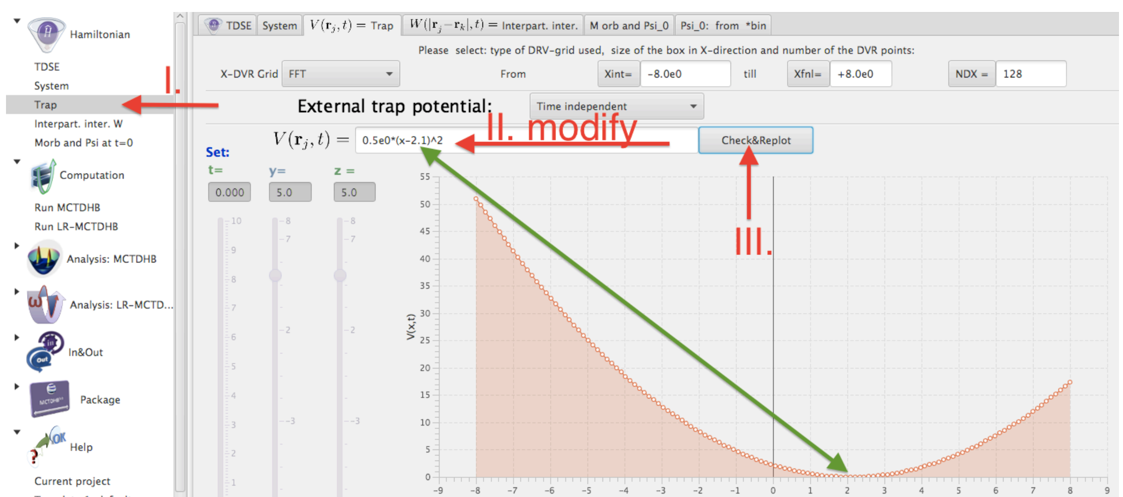

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Julian Grond (Graz, Austria)

Axel Lode (HD, Basel)

Raphael Beinke (HD)

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

The laboratory to study quantum many-body dynamics