Universitat Politècnica de Catalunya, Barcelona, Spain

Diffusion Monte Carlo simulation of quantum gases and solids

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GROUP MEMBERS

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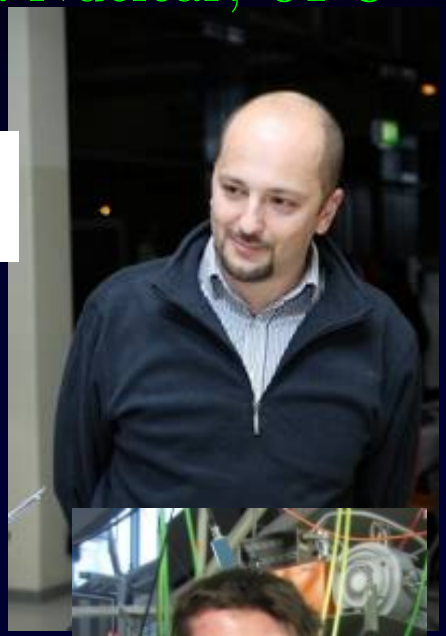

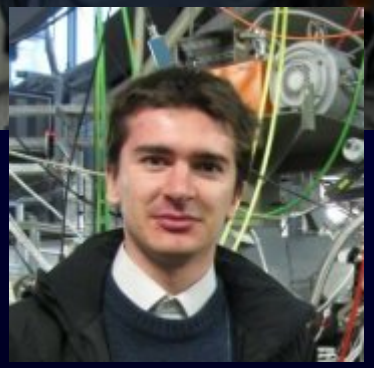

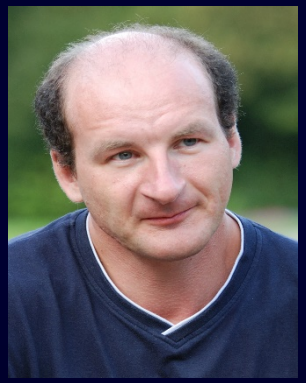

RESULTS OBTAINED USING BSC CLUSTERS

- Y. Lutsyshyn, "*Fast quantum Monte Carlo on a GPU*", Computer Physics Communications 187, 162 (2015)
- Y. Lutsyshyn, *"A coordinated wavefunction for the ground state of liquid helium-4"* arXiv:1506.03752
- A. Iu. Gudyma, G. E. Astrakharchik, Mikhail B. Zvonarev, *"Reentrant behavior of the breathing-mode-oscillation frequency in a one-dimensional Bose gas"*, Phys. Rev. A 92, 021601(R) (2015)
- G. E. Astrakharchik and B. A. Malomed, *"Quantum versus mean-field collapse in a many-body system"*, arXiv:1508.05449 (2015)
- G. Ferre, G. E. Astrakharchik, J. Boronat, *"Phase diagram of a quantum Coulomb wire"*, arXiv:1507.05496 (2015)
- Grigory E. Astrakharchik, Konstantin V. Krutitsky, Maciej Lewenstein, Ferran Mazzanti, *"One-dimensional Bose gas in optical lattices of arbitrary strength"*, arXiv:1509.01424 (2015)
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- G. E. Astrakharchik and J. Boronat, *"Luttinger liquid behavior of one-dimensional 3He"*, Phys. Rev. B 90, 235439 (2014)
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- M. A. Garcia-March, B. Julia-Diaz, G. E. Astrakharchik, Th. Busch, J. Boronat, A. Polls, *"Quantum correlations and spatial localization in one-dimensional ultracold bosonic mixtures"*, New J. Phys. 16, 103004 (2014)
- Y. Lutsyshyn, G. E. Astrakharchik, C. Cazorla, J. Boronat, *"Quantum phase transition with a simple variational ansatz"*, Phys. Rev. B 90, 214512 (2014)
- Z. D. Zhang, G. E. Astrakharchik, D. C. Aveline, S. Choi, H. Perrin, T. H. Bergeman, M. Olshanii, *"Breakdown of the scale invariance in a near-Tonks-Girardeau gas: some exact results and beyond"*, Phys. Rev. A 89, 063616 (2014)
- G. E. Astrakharchik and I. Brouzos, *"Trapped one-dimensional ideal Fermi gas with a single impurity"*, Phys. Rev. A 88, 021602(R) (2013)

STRUCTURE OF THE TALK

INTRODUCTION:

- ULTRACOLD GASES AND SOLIDS
- QUANTUM MONTE CARLO METHODS
- COMPLEXITY OF THE CALCULATION
- ADVANTAGES OF PARALLELIZATION

STUDIED SYSTEMS:

- LIQUID HELIUM
- COULOMB WIRE
- 1D BOSE GAS IN OPTICAL LATTICE
- BILAYER OF DIPOLES
- OSCILLATIONS IN A TRAPPED 1D BOSE GAS
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ULTRACOLD GASES AND SOLIDS

- The main goal is the study of the properties of quantum systems at ultralow temperatures (absolute zero)

- Microscopic ab initio simulation is performed starting directly from the many-body Hamiltonian

$$\hat{H} = \sum_{i=1}^{N} \left[-\frac{\hbar^2}{2m} \Delta_i + V_{ext}(\mathbf{r}_i) \right] + \sum_{i<j} V_{int}(|\mathbf{r}_i - \mathbf{r}_j|)$$

- Describes a system of N particle in an external field with a given interaction potential between the particles.

- Interaction potential can be of a realistic or model type:

  - Helium interacton potential [Aziz II], Hydrogen, Coulomb, Yukawa, dipoles, Rydberg, Van der Waals, etc.
  - model potentials: hard sphere, soft sphere, square well, delta-pseudopotentials, etc.

QUANTUM MONTE CARLO METHODS

- Ground-state properties are found using quantum Monte Carlo methods

- Is an efficient way of evaluating $3N$ – dimensional integrals

  - Variational Monte Carlo (VMC) method:
    - the many-body wave function $\psi_T(\mathbf{r}_1, ..., \mathbf{r}_N; \alpha, \beta, ...)$is proposed
    - variational principle applies (minimal energy when is ψ_T exact)
    - variational parameters $\alpha, \beta, ...$ are optimized

  - Diffusion Monte Carlo (DMC) method
    - solves the Schrödinger equation in imaginary time
    - provides the ground-state energy exactly

- Energetic and structural properties are studied
  - energy, equation of state, excitation spectrum, gap, etc.
  - pair correlation function, density profile, static structure factor, one-body density matrix, etc.

COMPLEXITY OF THE CALCULATION

- A typical choice of the trial wave function contains a pair-product of two body terms (Bijl-Jastrow wave function)

$$\psi_T(\mathbf{r}_1, ..., \mathbf{r}_N) = \prod_{i=1}^{N} f_1(\mathbf{r}_i) \prod_{j<k}^{N} f_2(|\mathbf{r}_j - \mathbf{r}_k|)$$

- Even for a short-range interaction potential the complexity scales as N^2 with the number of particles for bosons

- N^3 complexity for fermions (Slater determinants, etc)

- Homogeneous system simulated in a box with periodic boundary conditions (PBC) : typical convergence $1/N$

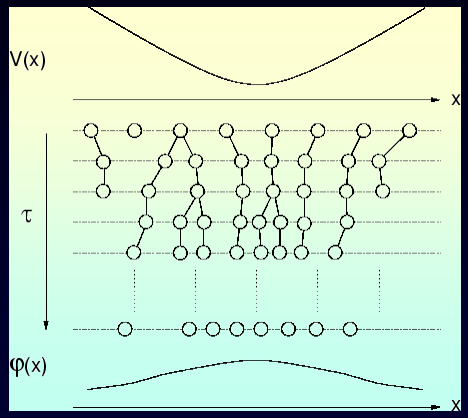
- Typical number of particles in a simulation $N \sim$ 100 - 1000

ADVANTAGES OF PARALLELIZATION

- Generally QMC can parallelized efficiently

  - on the level of single-particle updates (VMC)

  - on the level of *walkers*
  (quantum system is replicated many times)



- Speed-up factors of 40 - 140 can be achieved
  (compared to an optimized code on a single CPU)

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QUANTUM LIQUID HELIUM

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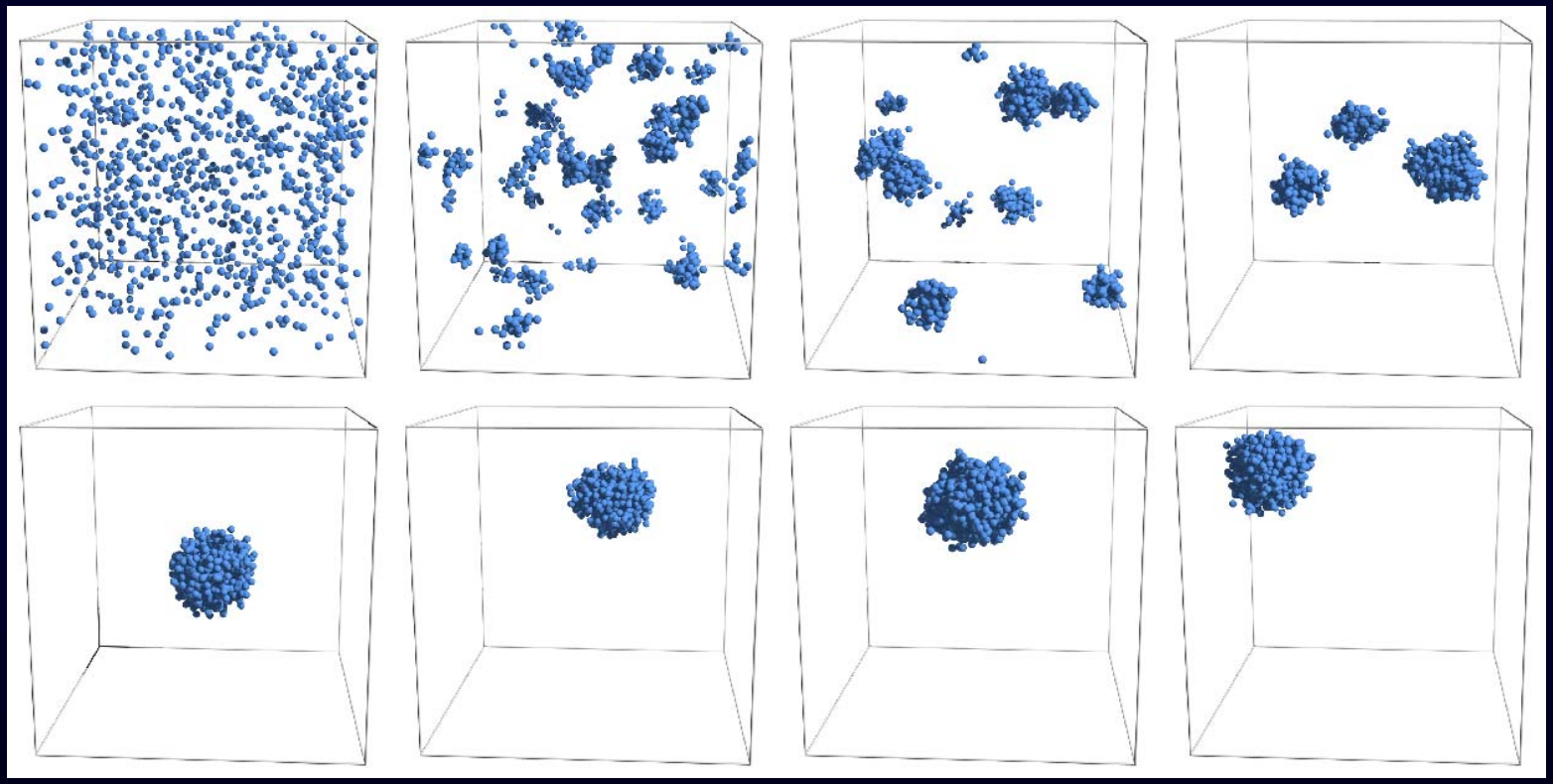
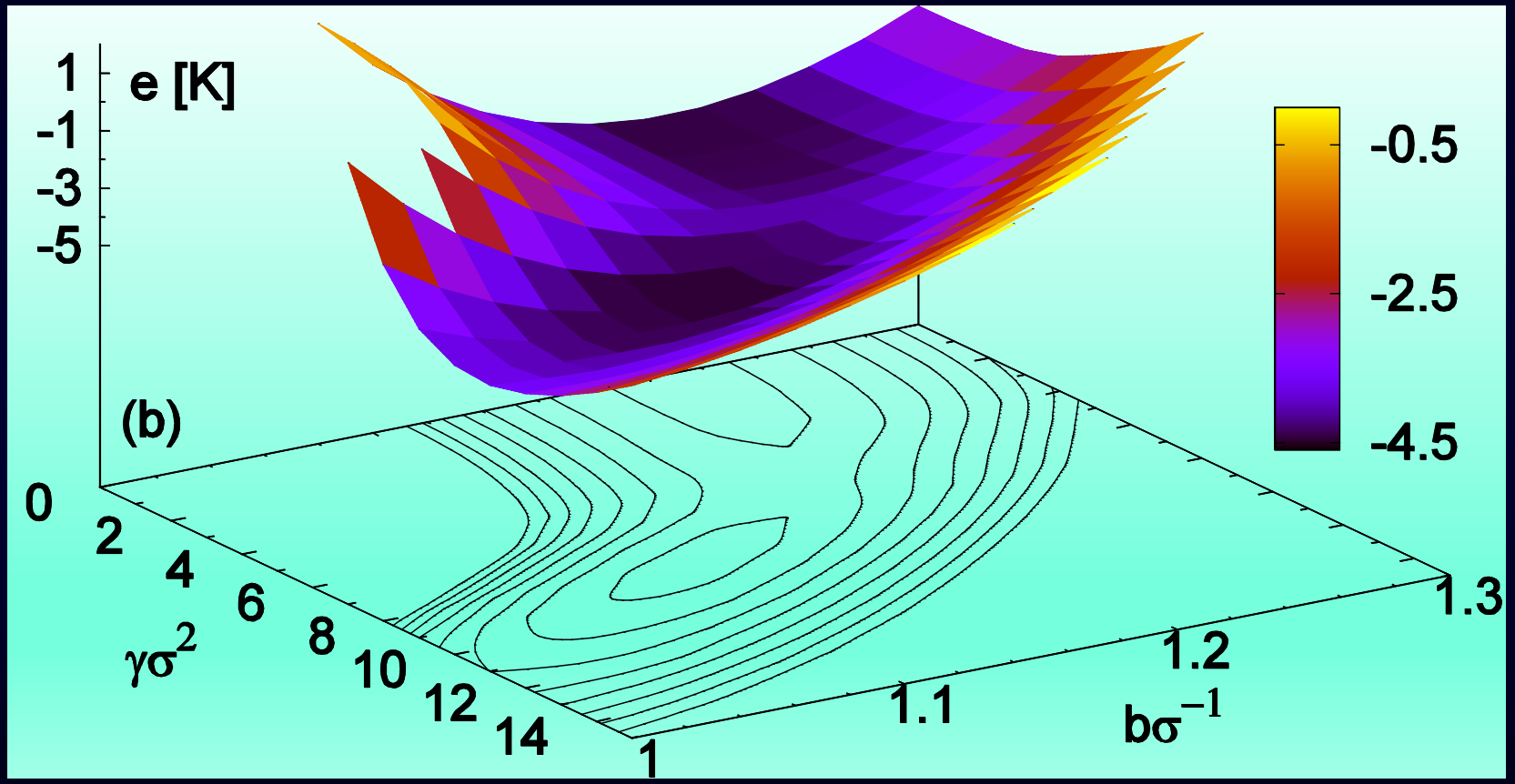


- Progression of Markov chain during Metropolis sampling of a system with $N = 1000$ atoms. A droplet gets formed.

LIQUID HELIUM

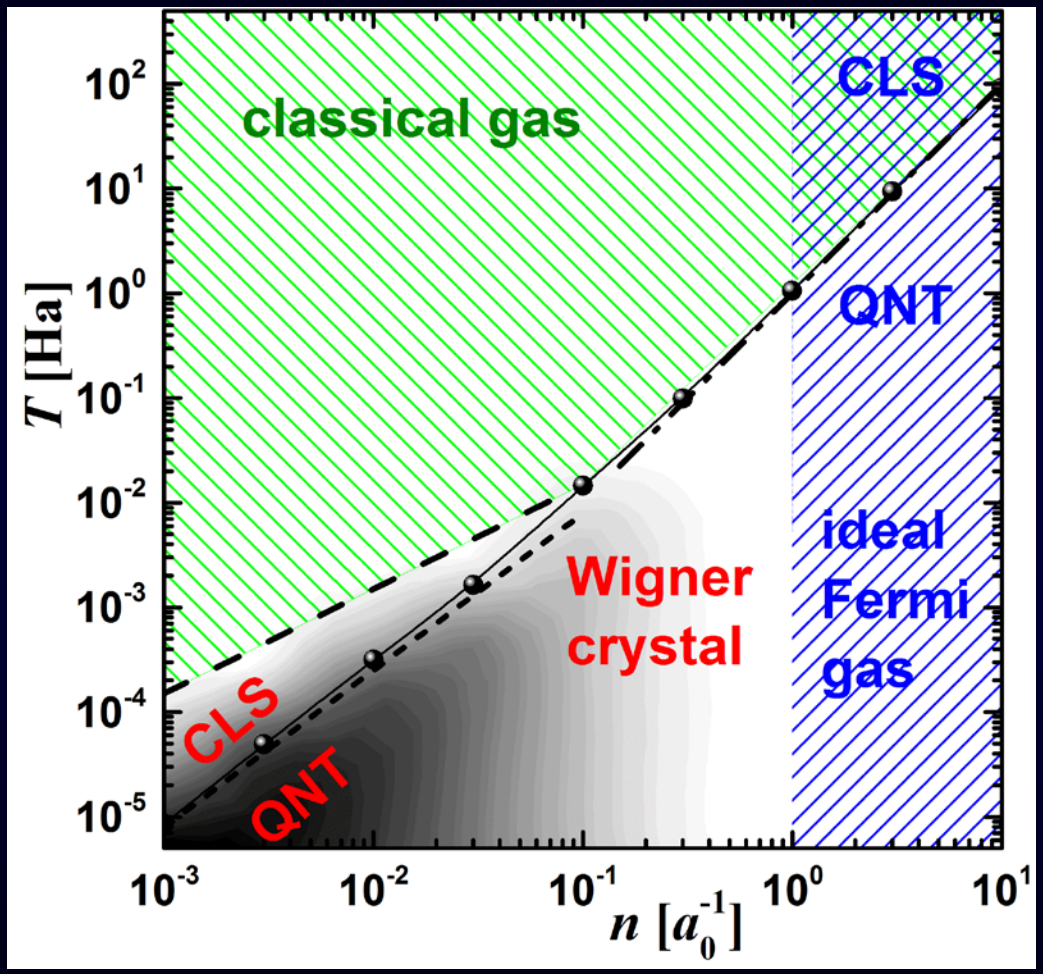
- Y. Lutsyshyn, G. E. Astrakharchik, C. Cazorla, J. Boronat, "Quantum phase transition with a simple variational ansatz", Phys. Rev. B 90, 214512 (2014)



- Energy per particle in liquid-solid coexistence region,
- two separate local minima exist (liquid phase, solid phase)

COULOMB WIRE

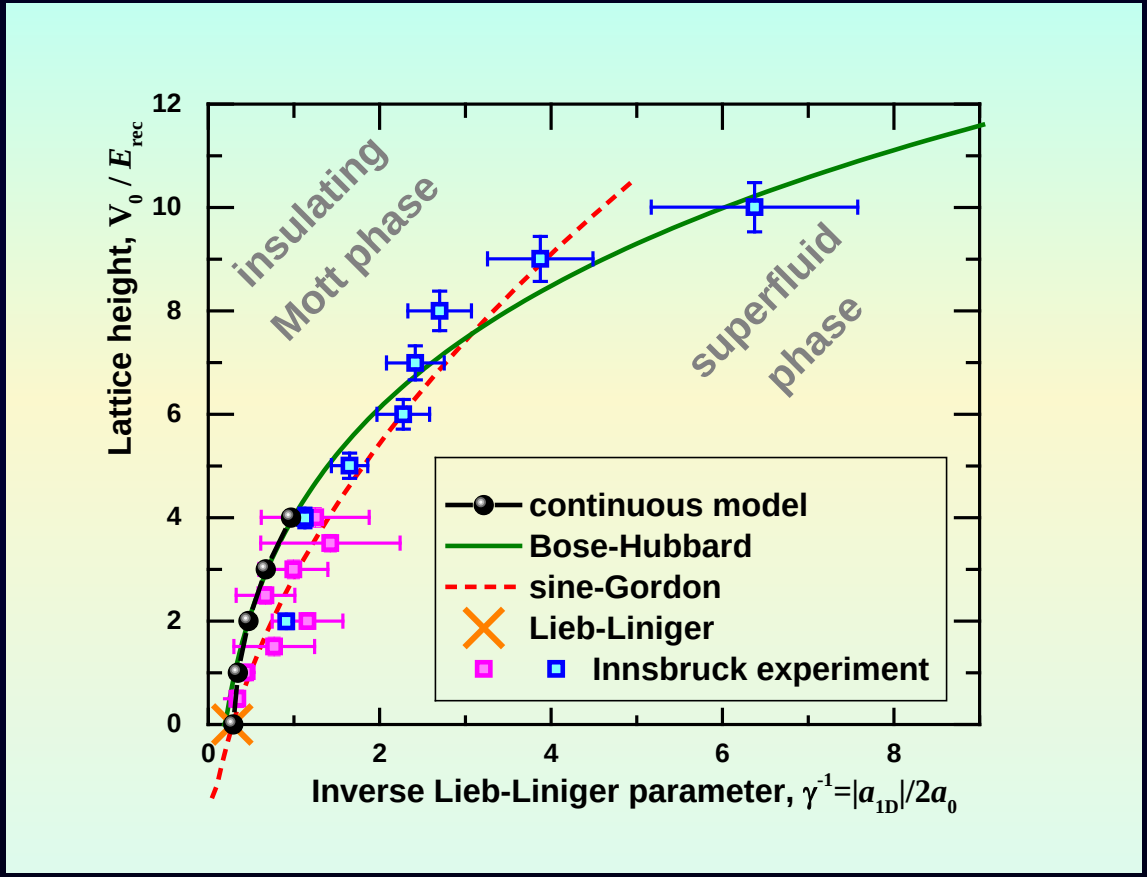
- G. Ferre, G. E. Astrakharchik, J. Boronat, "Phase diagram of a quantum Coulomb wire", arXiv:1507.05496 (2015)



- Temperature - density phase diagram.

1D BOSE GAS IN OPTICAL LATTICE

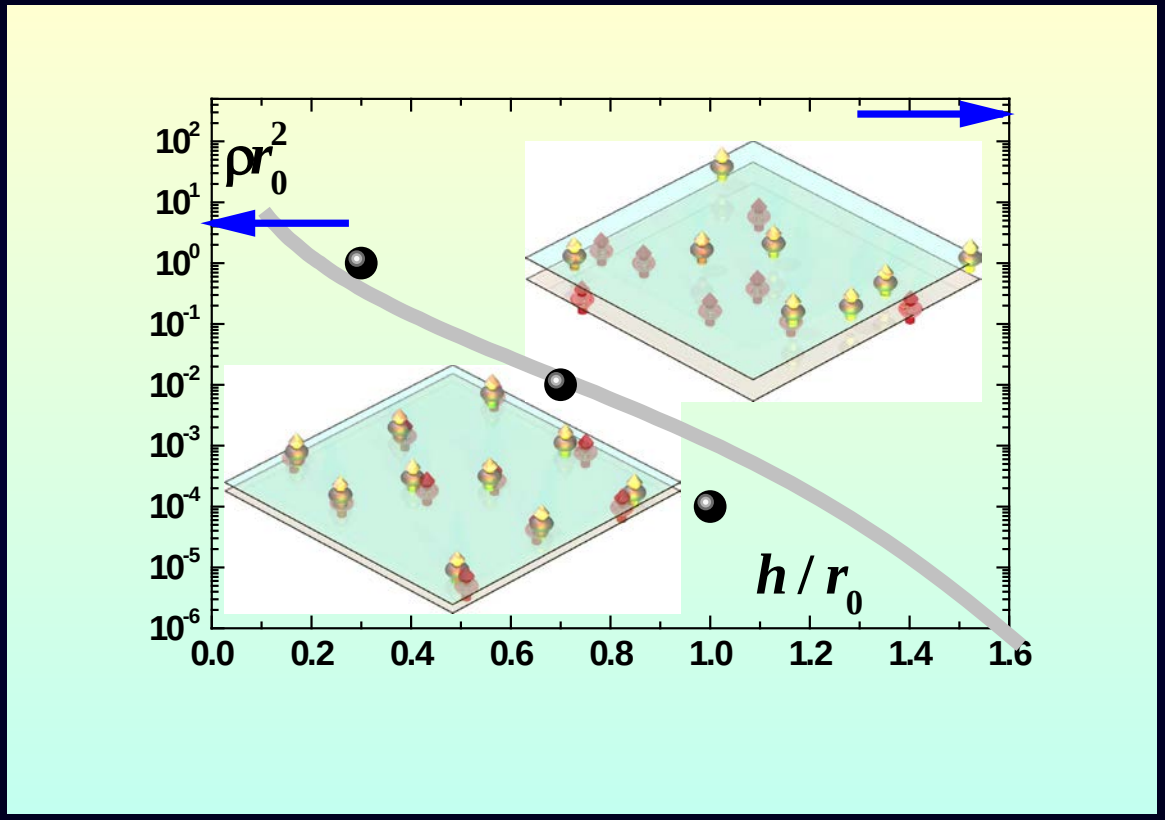
- Grigory E. Astrakharchik, Konstantin V. Krutitsky, Maciej Lewenstein, Ferran Mazzanti, "One-dimensional Bose gas in optical lattices of arbitrary strength", arXiv:1509.01424 (2015)



The $T = 0$ phase diagram of the continuous model as a function of the s-wave scattering length a_{1D}/a_0 and the optical lattice intensity V_0/E_{rec}. Compared to sine-Gordon and Bose-Hubbard model.

BILAYER OF DIPOLES

- A. Macia, G. E. Astrakharchik, F. Mazzanti, S. Giorgini, J. Boronat, "Single-particle versus pair superfluidity in a bilayer system of dipolar bosons", Phys. Rev. A 90, 043623 (2014)



Phase diagram featuring the single-particle (upper region) and the pair superfluid (lower region). The dots correspond to the transition points as obtained from DMC simulations. The two arrows show the freezing density of a single layer of particles (right) and of dimers (left).

OSCILLATIONS IN A TRAPPED 1D BOSE GAS

- A. Iu. Gudyma, G. E. Astrakharchik, Mikhail B. Zvonarev, "*Reentrant behavior of the breathing-mode-oscillation frequency in a one-dimensional Bose gas*", Phys. Rev. A 92, 021601(R) (2015)
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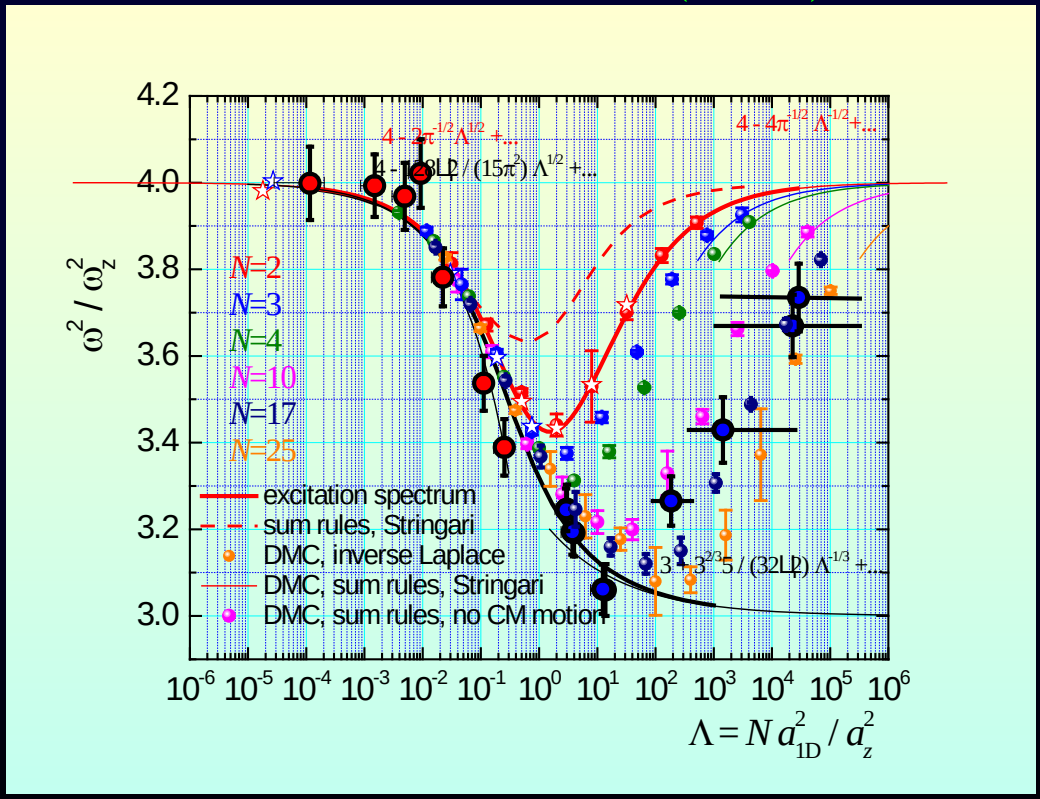

BOSE GASES

- Solitons: G. E. Astrakharchik and B. A. Malomed, "*Quantum versus mean-field collapse in a many-body system*", arXiv:1508.05449 (2015)

- 1D trapped Bose gases:
- M. A. García-March, B. Juliá-Díaz, G. E. Astrakharchik, J. Boronat, A. Polls, "Distinguishability, degeneracy, and correlations in three harmonically trapped bosons in one dimension", Phys. Rev. A 90, 063605 (2014)

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AMDAHL´S LAW (CPUs ONLY)

Y. Lutsyshyn, "*Fast quantum Monte Carlo on a GPU*", Computer Physics Communications 187, 162 (2015)

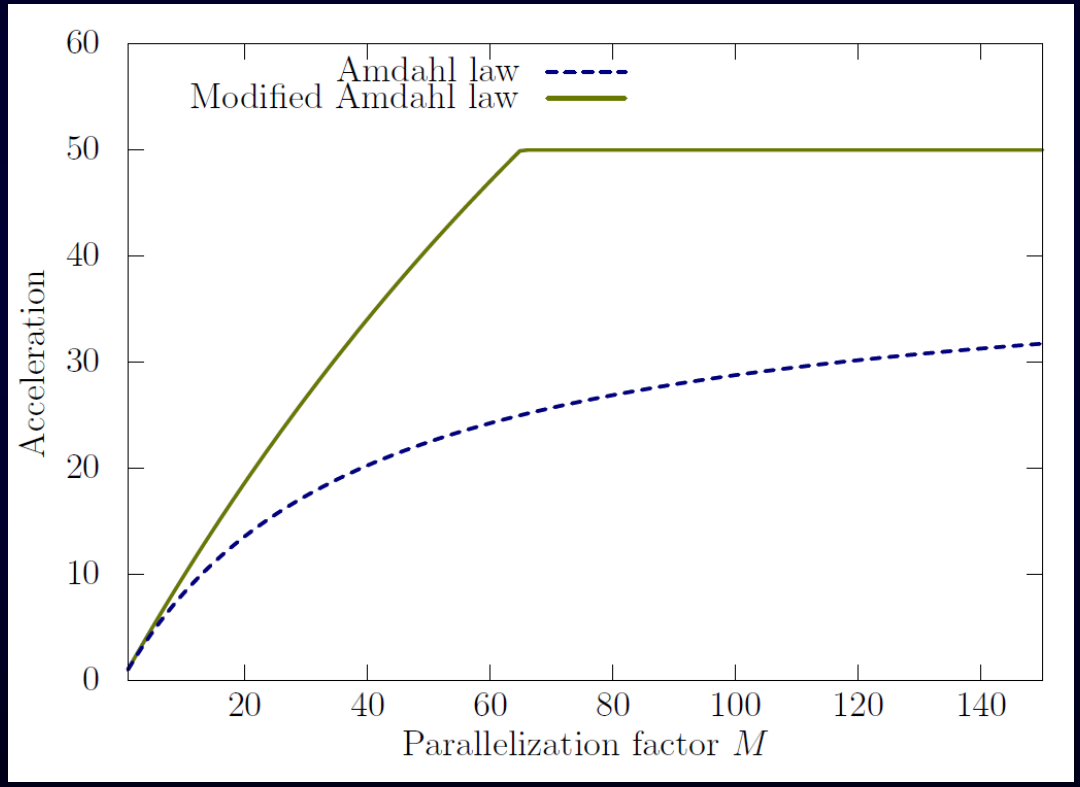
Amdahl's law: maximum speedup using multiple processors.

With increased parallelization, even a small serial fraction inevitably becomes a bottleneck. Given that S is the serial and P the parallel fractions of the program ($S + P = 1$), and M is the number of parallel threads or processes, the achievable acceleration A is given by

$$A = \frac{S+P}{S+P/M} = \frac{1}{S+(1-S)/M} < \frac{1}{S}.$$

MODIFIED AMDAHL´S LAW (CPU+GPU)

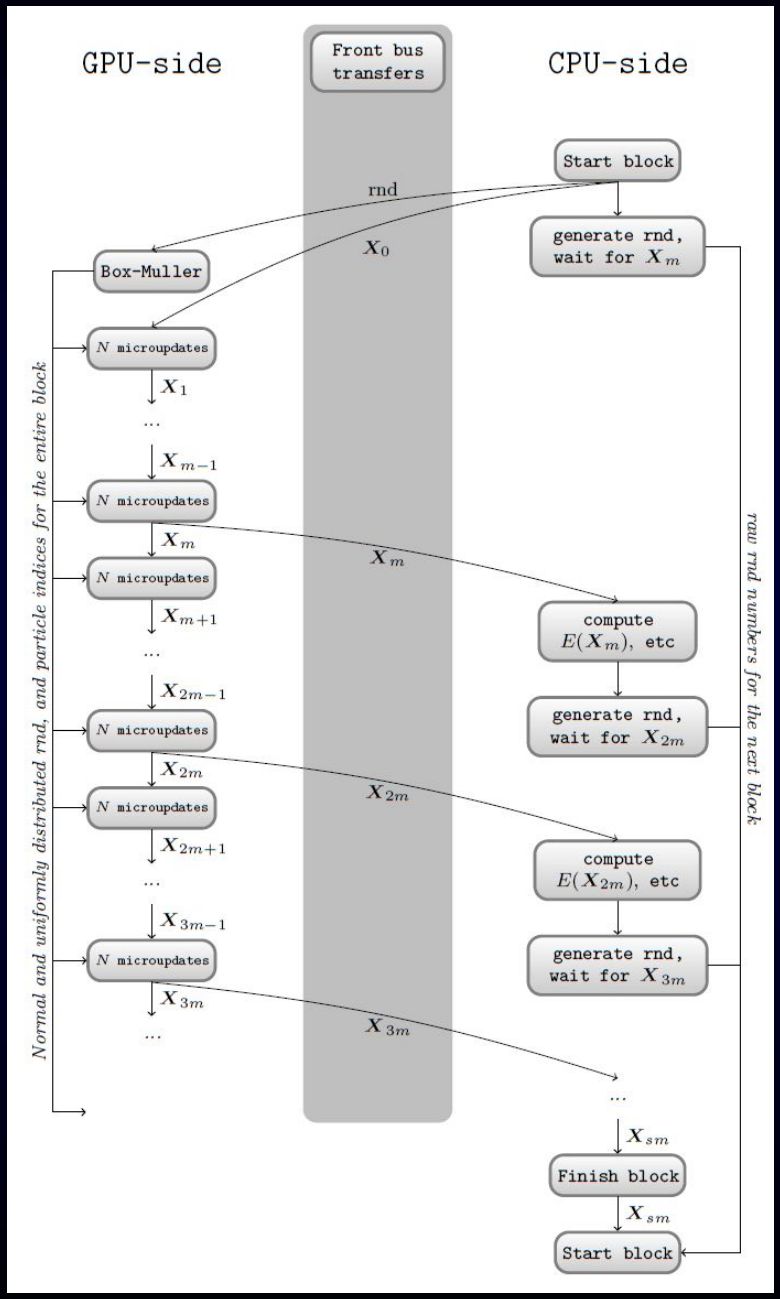
The load masking leads to a modified form of the Amdahl law. Suppose that R_{CPU} is the code fraction that remains on the CPU, and the serial and parallelizable parts that are moved to the GPU are S_{GPU} and P_{GPU}. Thus $R_{\mathrm{CPU}} + S_{\mathrm{GPU}} + P_{\mathrm{GPU}} = 1$.



If the parallel portion of the GPU code may be accelerated by a factor M, the resulting speed-up is

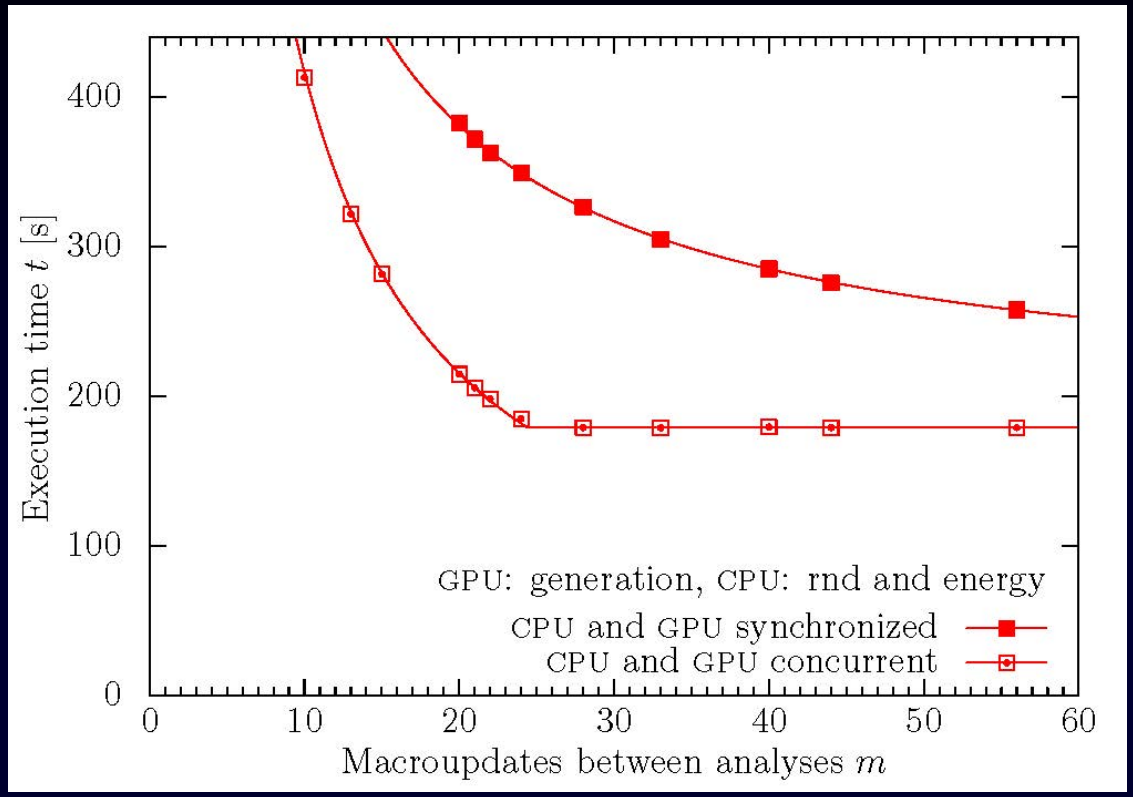
$$A_{\mathrm{mask}}(M) = \frac{1}{\max(R_{\mathrm{CPU}}, S_{\mathrm{GPU}} + M^{-1} P_{\mathrm{GPU}})}$$

BLOCK DIAGRAM



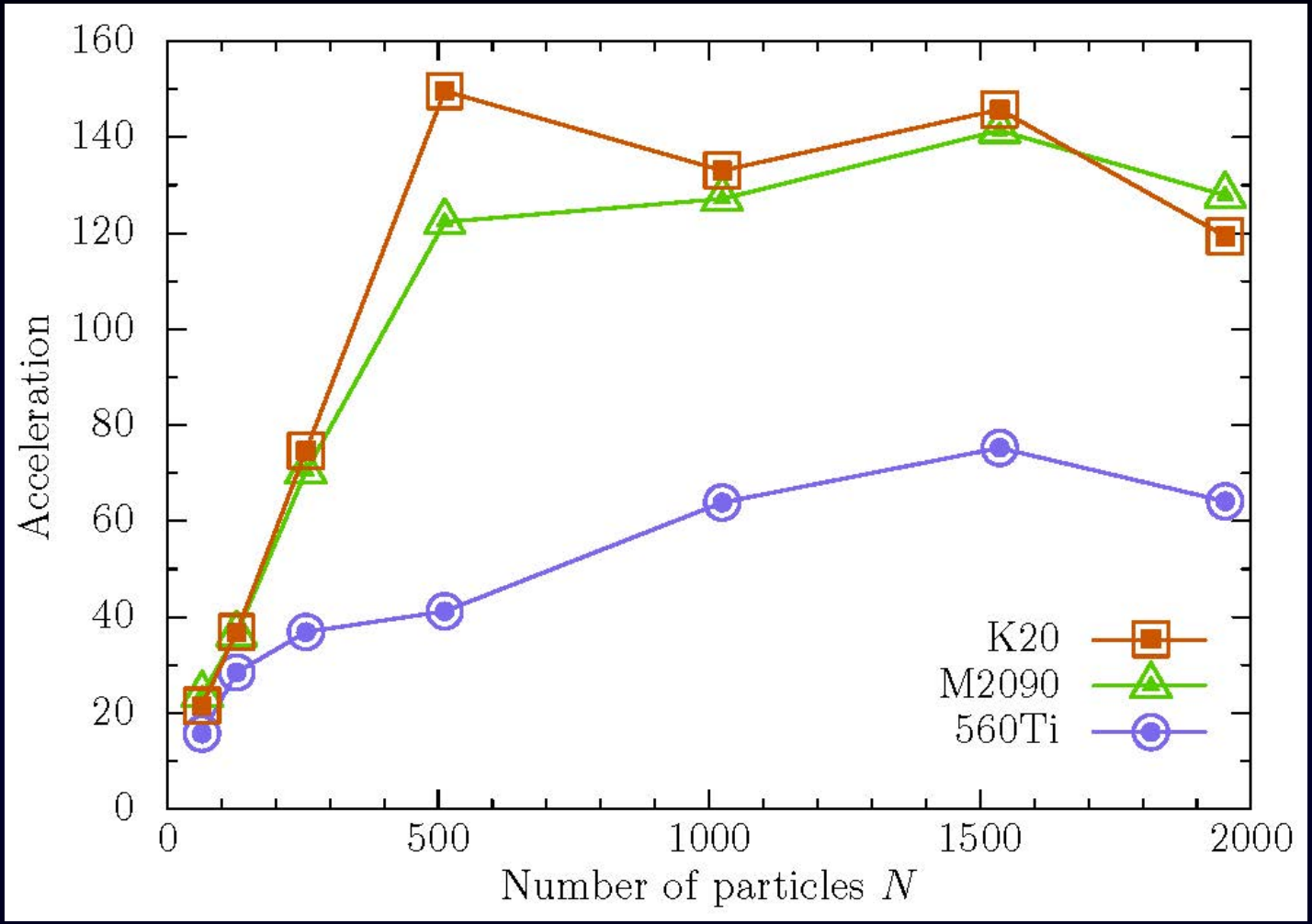
- CPU-side generates raw random numbers and sends them to the GPU-side.
- Once the GPU obtains the starting configurations, it starts the Markov chain.
- Every m macroupdates N^2(threadblocks), the GPU sends the configurations back to the CPU for processing.
- Meanwhile, the GPU continues the generation.
- When the CPU-side is not occupied, it generates new raw random numbers to be used in the next block.
- The size of a block is limited by the GPU global memory, typically at 2^{28}=$268 \cdot 10^6$ microupdates.

FAST QUANTUM MONTE CARLO ON GPU



Load masking in a calculation with $N = 512$ particles and eight independent Markov chains on a GTX560Ti. The plots show the total execution time in seconds vs the number of macroupdates between analyses. The vertical axis shows the total execution time in seconds. All lines are fits to the corresponding regions in the form $a + b/m$.

ACCELERATION



Acceleration: ratio of execution times measured with or without GPU acceleration.(optimized 1CPU code)

Blue bullets: 560Ti; green triangles: M2090; red squares: K20.

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THANK YOU
FOR YOUR ATTENTION !

Table 1: Configuration of the computers used for benchmarking. The top column shows the labels used to refer to the corresponding machine in the text. M2090s were accessed on a BullX GPU cluster in the Barcelona Supercomputing Center. The 560Ti and K20 were installed on a workstation.

	560Ti	**M2090**	**K20**
Architecture	Workstation	Cluster	Workstation
CPU			
make	Intel	Intel	Intel
type	i5-2500	Xeon E5649	i5-3570
clock frequency	3.3 GHz	2.5 GHz	3.4 GHz
memory	16 GB	24 GB	12 GB
L3 cache	6 MB	12 MB	6 MB
GPU			
series	GeForce	Tesla	Tesla
architecture	Fermi	Fermi	Kepler
chipset	GF114	T20A	GK110
model	GTX 560 Ti	M2090	K20
compute capability	2.1	2.0	3.5
number of cores	384	512	2496
SM(SMX) count	8	16	13
cores per SM	48	32	192
clock frequency	1.8 GHz	1.3 GHz	0.71 GHz
global memory	1.0 Gb	6.0 Gb	5.0 Gb

INNSBRUCK EXPERIMENT

Vol 466|29 July 2010|doi:10.1038/nature09259 nature

Pinning quantum phase transition for a Luttinger liquid of strongly interacting bosons

Elmar Haller[1], Russell Hart[1], Manfred J. Mark[1], Johann G. Danzl[1], Lukas Reichsöllner[1], Mattias Gustavsson[1], Marcello Dalmonte[2,3,4,5], Guido Pupillo[2,3] & Hanns-Christoph Nägerl[1]

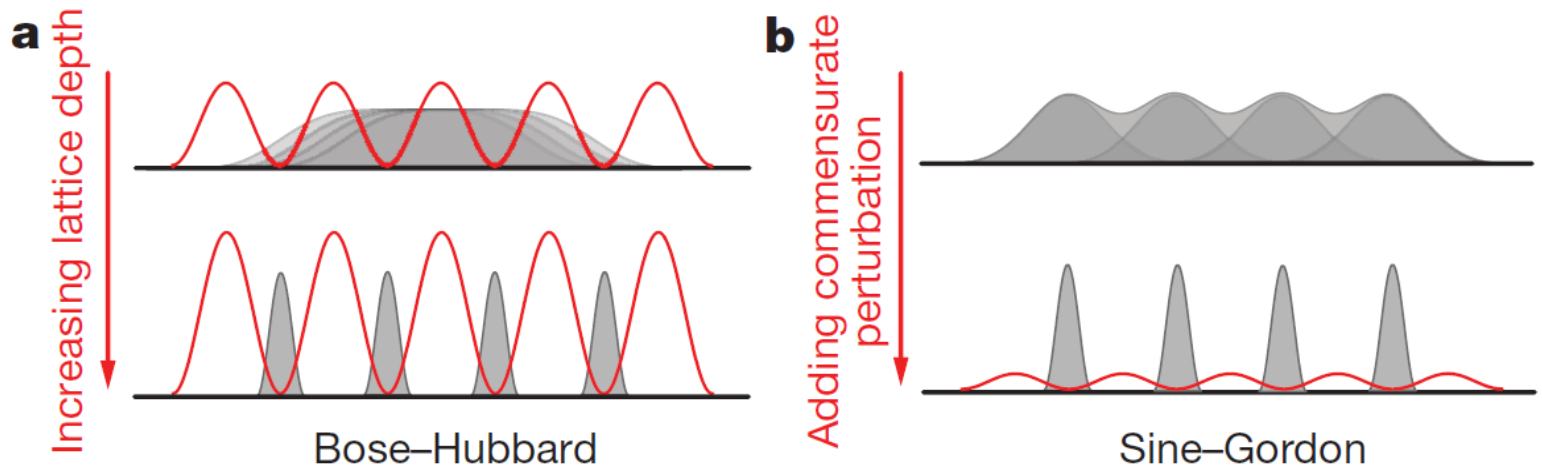

Figure 1 | Comparing two types of superfluid-to-Mott-insulator phase transition in one dimension. Schematic density distributions (grey) in the presence of a periodic potential (red solid line).

Superlfuid – Mott-Insulator phase transition observed in 1D system