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Università di Camerino

Bose-Einstein condensation of quantum mixtures

Gabriele Spada

University of Camerino

Universal themes in Bose-Einstein Condensation
ECT* Trento, 2024-11-07

INFN PERUGIA
PROVINCIA AUTONOMA DI TRENTO
CNR-INO
ISTITUTO NAZIONALE DI OTTICA
CONSIGLIO NAZIONALE DELLE RICERCHE
CINECA

Based on:

- SG, Pilati & Giorgini. Attractive Solution of Binary Bose Mixtures: Liquid-Vapor Coexistence and Critical Point. *Phys. Rev. Lett.* **131,** 173404 (2023)

- SG, Pilati & Giorgini. Quantum Droplets in Two-Dimensional Bose Mixtures at Finite Temperature. *Phys. Rev. Lett.* **133,** 083401 (2024)

Sebastiano Pilati
University of Camerino

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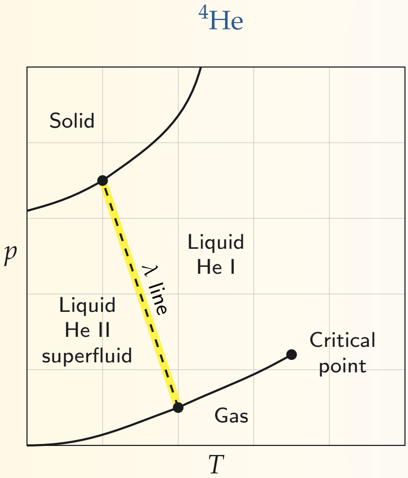
University of Trento

Introduction 1

States of matter for 3D quantum systems

States of matter for 3D quantum systems



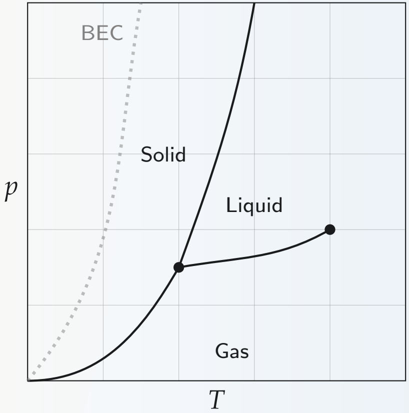
- Liquid at $T = 0$
- BEC phase is in true equilibrium *

* Another such case is obtained for H atoms in a strong magnetic field (parallel electronic spins)

States of matter for 3D quantum systems

- No thermodynamically stable BEC phase
  - Three-body recombination events
    Molecules ⇒ **Solid**

Other atomic systems



States of matter for 3D quantum systems

- No thermodynamically stable BEC phase
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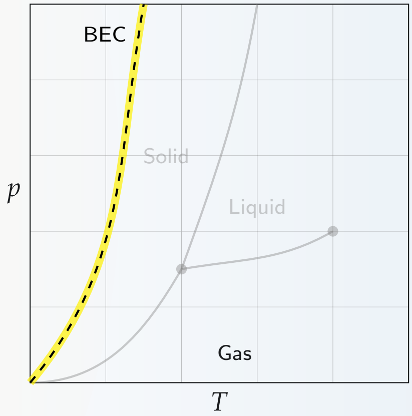
    Molecules ⇒ **Solid**
- BEC phase in **metastable** conditions
  - Low density (rare three-body collisions)
  - Gas distant from walls

Other atomic systems



States of matter for 3D quantum systems

- No thermodynamically stable BEC phase
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    Molecules ⇒ **Solid**
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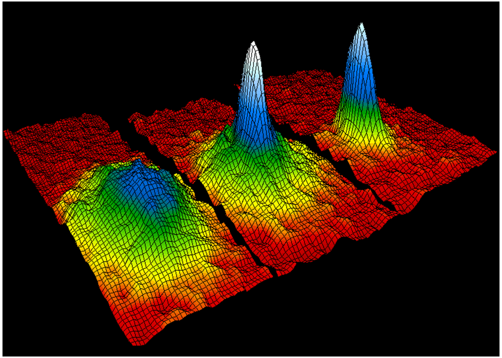
  - Gas distant from walls

  Very dilute, cold gas in magnetic trap

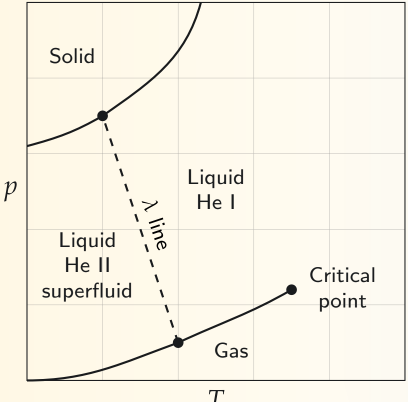
Other atomic systems



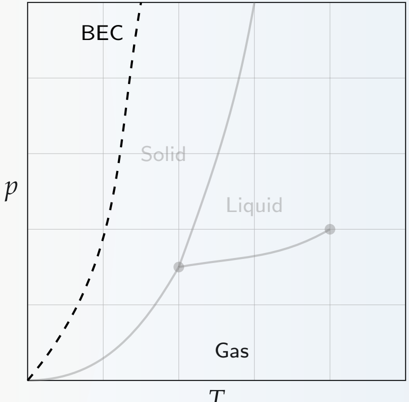
Velocity distribution of ^{87}Rb atoms (Anderson at. al., 1995)

States of matter for 3D quantum systems

^{4}He



Other atomic systems



Introduction 2

Mean-field analysis of Liquid-Gas transitions

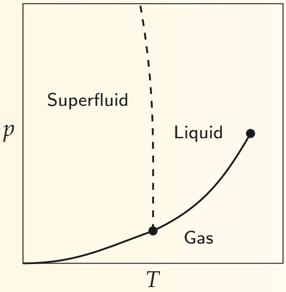
Mean-field analysis of quantum Liquid-Gas transitions

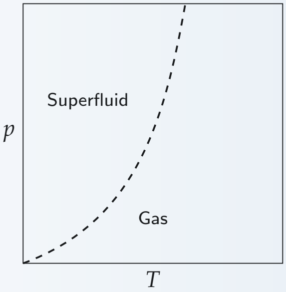
Landau's theory for helium-like system

liquid-gas order parameter (real), Z_2

$$\Omega(\phi, |\psi|) = \frac{t}{2}\phi^2 + \frac{u}{4}\phi^4 - h\phi + (t + \widetilde{m})|\psi|^2 + \frac{\lambda}{2}|\psi|^4 - \phi|\psi|^2$$

condensate order parameter (complex), $U(1)$





Son, Stephanov & Yee, *J. Stat. Mech* (2021)

Mean-field analysis of quantum Liquid-Gas transitions

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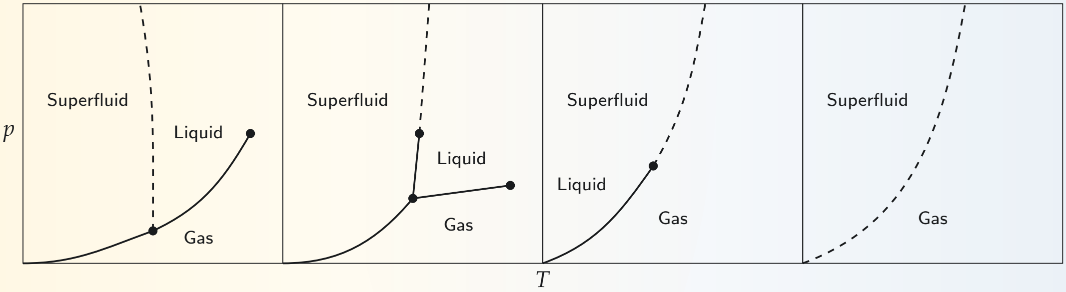


confirmed by numerical simulations Kora, Boninsegni, Son & Zhang, *PNAS* (2020)

Son, Stephanov & Yee, *J. Stat. Mech* (2021)

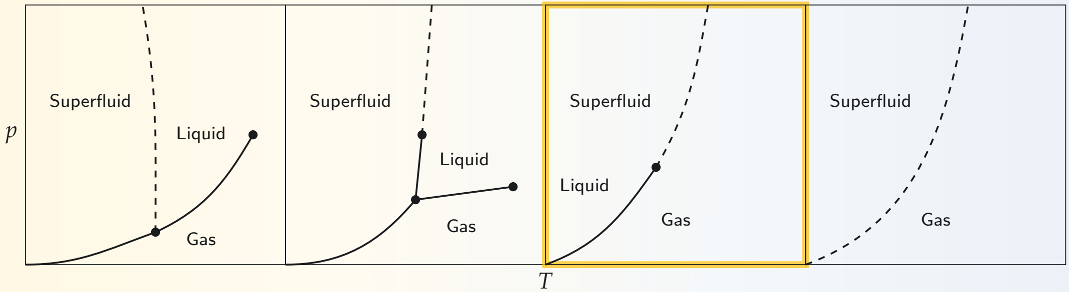
Mean-field analysis of quantum Liquid-Gas transitions

Landau's theory for helium-like system $\phi_0 = \sqrt{-t/u}$

effective potential for condensate

$$V_{\text{eff}}(\psi) = (\widetilde{m} + t - \phi_0)|\psi|^2 + \left(\frac{\lambda}{2} - \frac{1}{4(-t)}\right)|\psi|^4 + \frac{u\phi_0}{8(-t)^3}|\psi|^6 + O(|\psi|^8)$$

Tricritical point $t = -\frac{1}{2\lambda}$, $\widetilde{m}_1 = \frac{1}{\sqrt{2\lambda u}} + \frac{1}{2\lambda}$

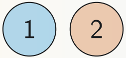


Son, Stephanov & Yee, *J. Stat. Mech* (2021)

Introduction 3

Binary Bose mixtures

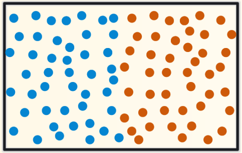
Binary Bose mixtures



$$H = \int d\mathbf{r} \left[\sum_{i=1,2} \left(-\frac{\hbar}{2m_i} \psi_i^\dagger \nabla_i^2 \psi_i + \frac{g_{ii}}{2} |\psi_i|^4 \right) + g_{12} |\psi_1|^2 |\psi_2|^2 \right]$$

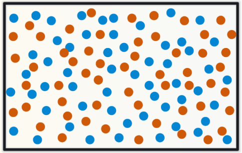
MF prediction

$g_{12} > \sqrt{g_{11} g_{22}}$



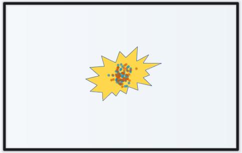
immiscible

$|g_{12}| < \sqrt{g_{11} g_{22}}$



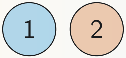
miscible

$g_{12} < -\sqrt{g_{11} g_{22}}$



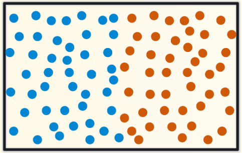
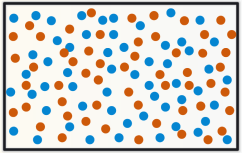
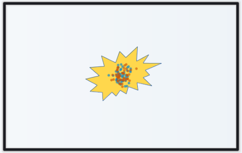
collapse

Binary Bose mixtures



$$H = \int d\mathbf{r} \left[\sum_{i=1,2} \left(-\frac{\hbar}{2m_i} \psi_i^\dagger \nabla_i^2 \psi_i + \frac{g_{ii}}{2} |\psi_i|^4 \right) + g_{12} |\psi_1|^2 |\psi_2|^2 \right]$$

MF prediction

$g_{12} > \sqrt{g_{11} g_{22}}$	$\lvert g_{12} \rvert < \sqrt{g_{11} g_{22}}$	$g_{12} < -\sqrt{g_{11} g_{22}}$
		
immiscible	miscible	collapse

Stabilization of attractive mixtures: $T = 0$

Symmetric

$$\begin{cases} \text{couplings} \\ g_{11} = g_{22} = g \\ \text{masses} \\ m_1 = m_2 = m \\ \text{densities} \\ n_1 = n_2 = n/2 \end{cases}$$

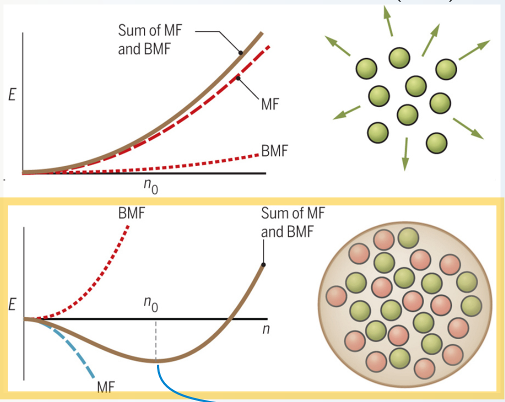
Attractive $g_{12} < 0$

$$\frac{E}{N} = \frac{1}{4} n \left(g + g_{12} \right) + \frac{8}{15\pi^2} \frac{m^{3/2} g^{3/2}}{\hbar^3} n^{3/2}$$

Credits: Ferrier-Barbut & Pfau, *Science* (2018)

$|g_{12}| < g$

$|g_{12}| > g$

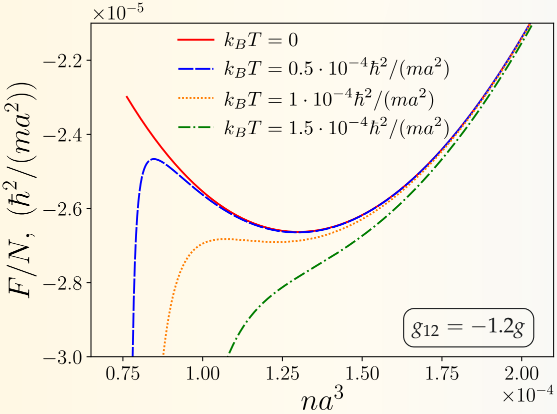


Stable finite-density state ⇒ **Liquid**

Petrov, *Phys. Rev. Lett.* (2015)

Liquid droplets at low T

- BMF theories: imaginary dispersion of density waves $\longrightarrow$ *thermodynamics?*



Low T description

$$\frac{F}{N} = \frac{E}{N} - \frac{\pi^2}{90} \frac{(k_B T)^4}{n \hbar^3} \left(\frac{1}{c_d^3} + \frac{1}{c_s^3} \right)$$

$$c_d^2 \simeq \frac{n}{2m} \left[\delta g + g \sqrt{na^3} \frac{4\sqrt{2}}{\sqrt{\pi}} \left(1 - \frac{g_{12}}{g} \right)^{5/2} \right]$$

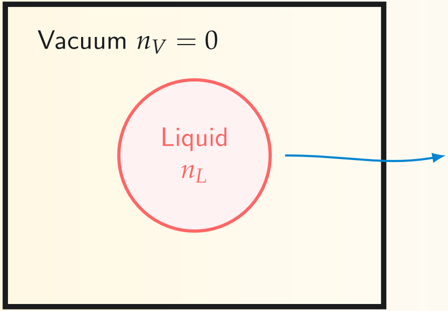
$$c_s^2 \simeq \frac{n}{2m} (g - g_{12}) \left[1 - \frac{\delta g}{g_{12}} \sqrt{na^3} \frac{8\sqrt{2}}{3\sqrt{\pi}} \left(1 - \frac{g_{12}}{g} \right)^{3/2} \right]$$

$$\delta g = g + g_{12}$$

Droplet destabilized by temperature

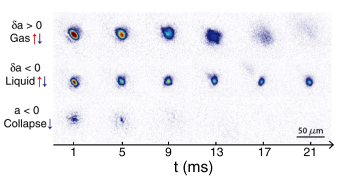
Ota & Astrakharchik, *SciPost Phys.* (2020)
Wang, Hu & Liu, *New Journal of Physics* (2020)

Summary: droplets at low temperature



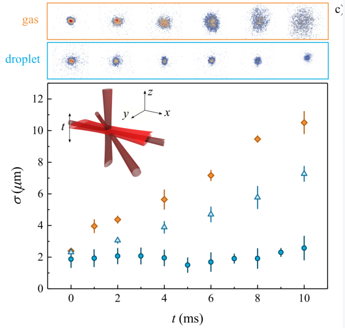
Droplet in equilibrium at $p = 0$
- stable at $T = 0$
- metastable at $0 < T < T^\star$

Experiments



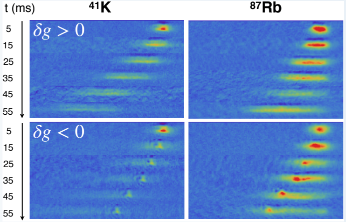
ICFO

homonuclear ^{39}K



LENS

homonuclear ^{39}K



LENS

heteronuclear $^{41}\mathrm{K} + {}^{87}\mathrm{Rb}$

Cabrera, Tanzi, Sanz, *et al.*, *Science* (2018)
Semeghini, Ferioli, Masi, *et al.*, *Phys. Rev. Lett.* (2018)
D'Errico, Burchianti, Prevedelli, *et al.*, *Phys. Rev. Res.* (2019)

3D Bose mixtures at finite temperature

Bose mixtures at $T > 0$

Path Integral Monte Carlo (PIMC) simulations from microscopic Hamiltonian

$$H = -\frac{\hbar^2}{2m}\sum_{i=1}^{N_1}\nabla_i^2 - \frac{\hbar^2}{2m}\sum_{i'=1}^{N_2}\nabla_{i'}^2 + \sum_{i<j}^{N_1} v(|\mathbf{r}_i - \mathbf{r}_j|) + \sum_{i'<j'}^{N_2} v(|\mathbf{r}_{i'} - \mathbf{r}_{j'}|) + \sum_{i,i'}^{N_1,N_2} v_{12}(|\mathbf{r}_i - \mathbf{r}_{i'}|)$$

Hard sphere with range a

Zero-range with scattering length $a_{12} < 0$

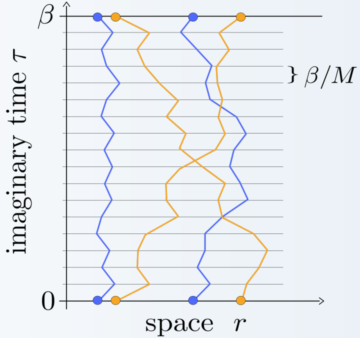
Partition function: high-T expansion

$$Z = \operatorname{tr} e^{-\beta H} = \frac{1}{N!}\sum_P \int d\mathbf{R}\, \rho(\mathbf{R}, P\mathbf{R}, \beta)$$

$$= \frac{1}{N!}\sum_P \int d\mathbf{R}\, d\mathbf{R}_2 \cdots d\mathbf{R}_M\, \rho(\mathbf{R}, \mathbf{R}_2, \frac{\beta}{M}) \cdots \rho(\mathbf{R}_M, P\mathbf{R}, \frac{\beta}{M})$$

Expectation values

$$\langle O \rangle = \frac{1}{Z}\frac{1}{N!}\sum_P \int d\mathbf{R}\, O(\mathbf{R})\rho(\mathbf{R}, P\mathbf{R}, \beta)$$

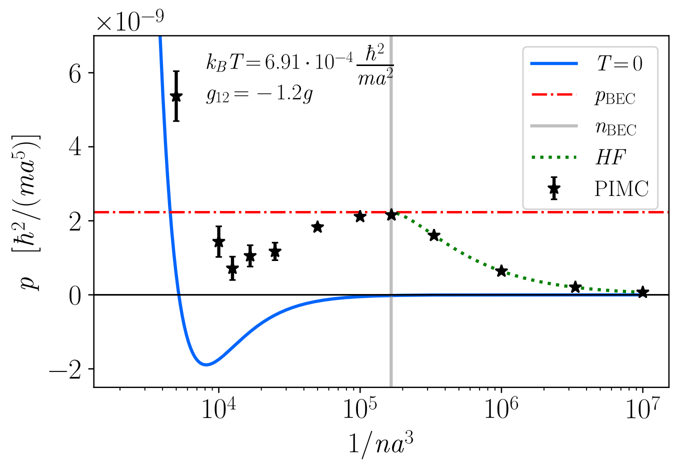


Ceperley, *Rev. Mod. Phys.* (1995), Boninsegni, Prokof'ev & Svistunov, *Phys. Rev. E* (2006)
SG, Giorgini & Pilati, *Condensed Matter* (2022)

Pressure along isothermal lines ($T = \text{const}$)

pressure $p = -\left(\frac{\partial F}{\partial V}\right)_T = k_B T \left(\frac{\partial \log Z}{\partial V}\right)_T$

compressibility $\kappa_T = -\left[V\left(\frac{\partial p}{\partial V}\right)_T\right]^{-1}$



SG, Pilati & Giorgini, *Phys. Rev. Lett.* (2023)

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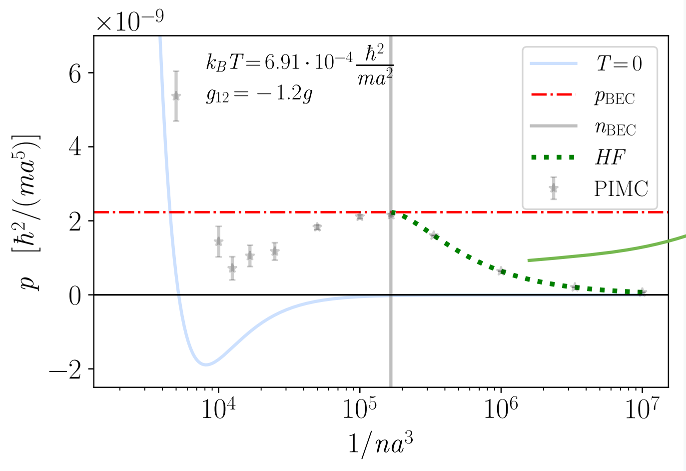

Normal phase ($n < n_{\text{BEC}}$)

$$p_{HF} = \frac{m^{3/2}(k_B T)^{5/2}}{\sqrt{2}\pi^{3/2}\hbar^3} g_{5/2}(e^{\beta\tilde{\mu}}) + \frac{1}{4} n^2 (2g + g_{12})$$

SG, Pilati & Giorgini, *Phys. Rev. Lett.* (2023)

Pressure along isothermal lines ($T = \text{const}$)

pressure $p = -\left(\frac{\partial F}{\partial V}\right)_T = k_B T \left(\frac{\partial \log Z}{\partial V}\right)_T$

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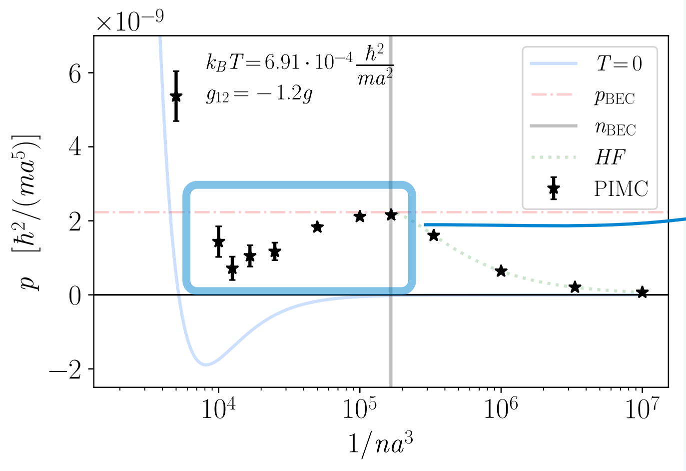
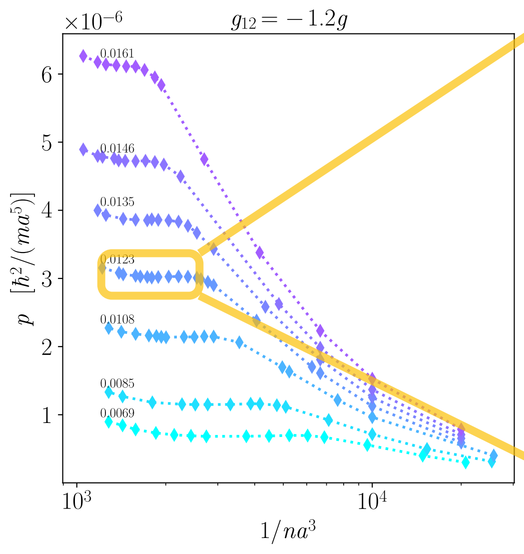
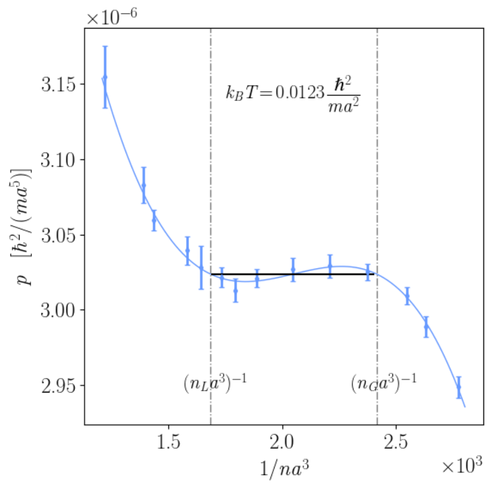


- PIMC $p > 0$
  $\Rightarrow$ no minimum in F/N
- Finite N
  $\Rightarrow$ S-like shape in the coexistence region

SG, Pilati & Giorgini, *Phys. Rev. Lett.* (2023)

Liquid-gas coexistence region





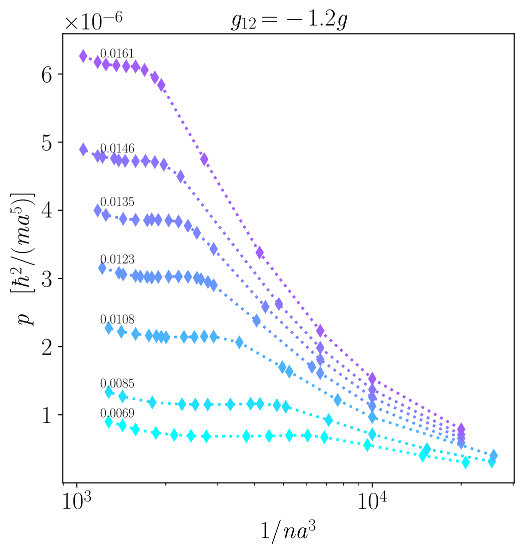
Maxwell construction

Equilibrium

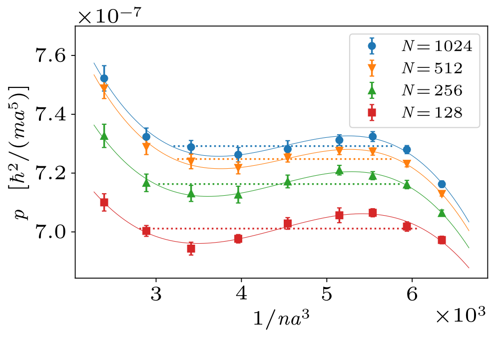
$$p(n_L) = p(n_G), \quad \mu(n_L) = \mu(n_G)$$

$$\int_{n_G^{-1}}^{n_L^{-1}} p\, \mathrm{d}(1/n) = 0$$

Liquid-gas coexistence region



Scaling with N



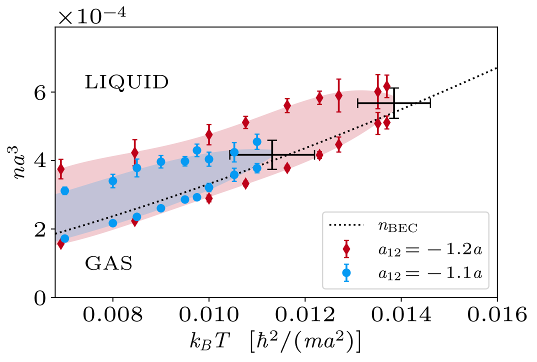
Equilibrium

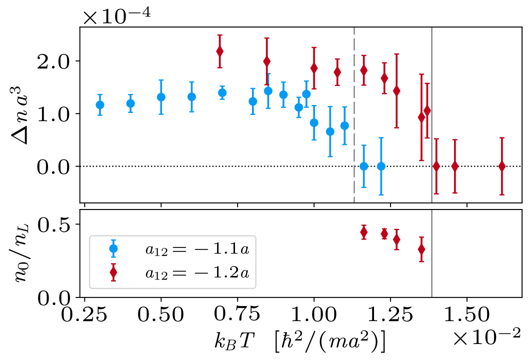
$$p(n_L) = p(n_G), \quad \mu(n_L) = \mu(n_G)$$

Maxwell construction

$$\int_{n_G^{-1}}^{n_L^{-1}} p \, \mathrm{d}(1/n) = 0$$

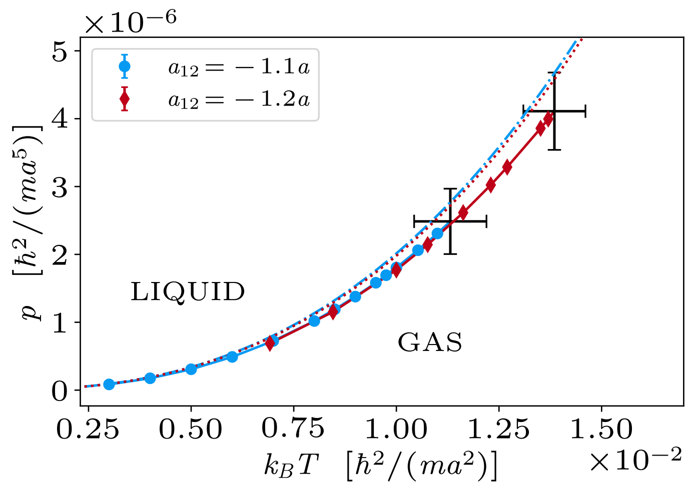
Phase diagram and critical point

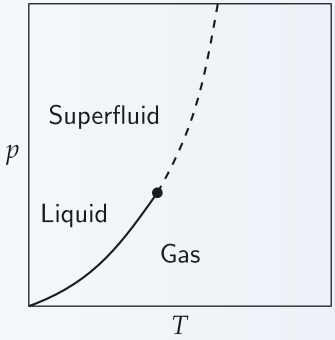




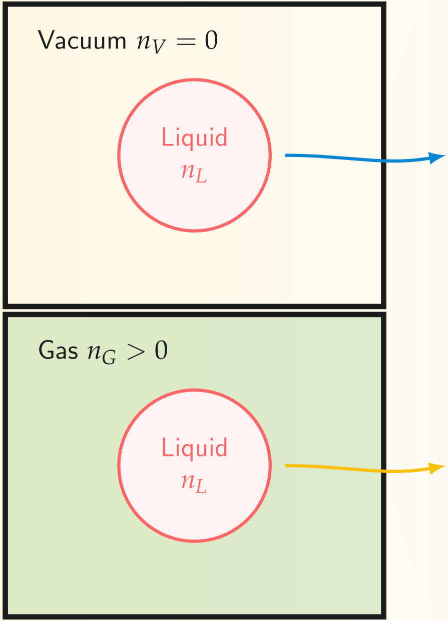
- Jump in the condensate fraction (first-order transition)
- Tricritical point estimated from $\Delta n = n_L - n_G \to 0$

Phase diagram and critical point





Liquid-gas coexistence



Droplet in equilibrium at $p = 0$

- stable at $T = 0$
- metastable at $0 < T < T^\star$

Liquid and gas in equilibrium at $p > 0$
$T^\star < T < T_C$

Experimental signatures

Trapping potential (e.g. harmonic $V_{\text{ext}}(\mathbf{r}) = m\omega^2\mathbf{r}^2/2$)

Local Density Approximation

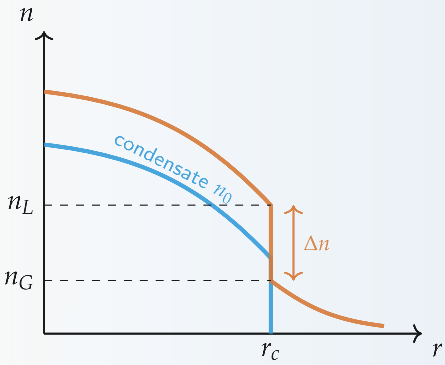
$$\mu_{\text{local}}(\mathbf{r}) + V_{\text{ext}}(\mathbf{r}) = \mu$$

Jump $\Delta n = n_L - n_G$ at the critical chemical potential

$$\mu_c = \mu_L(n_L) = \mu_G(n_G)$$

Observed at the position $\mathbf{r}_c$

$$\mu_c + V_{\text{ext}}(\mathbf{r}_c) = \mu$$



Landau's functional

Qualitative description near the tricritical point

$$\mathcal{L}(|\psi|) = \alpha|\psi|^2 + \beta|\psi|^4 + \gamma|\psi|^6$$

Three-body interaction terms

- Gn_i^3 for $i = 1, 2$
- $\widetilde{G}(n_1 n_2^2 + n_1^2 n_2)$

- Irrelevant at $T = 0$
- Small shift of n_L
- Dominant at large n

$$\begin{aligned} \mathrm{H} &= \sum_{i=1,2} \left(-\frac{\hbar^2}{2m_i} \psi_i^\dagger \nabla^2 \psi_i - \mu_i \psi_i^\dagger \psi_i \right) + \frac{1}{2} \sum_{i,j} g_{ij} \psi_i^\dagger \psi_j^\dagger \psi_j \psi_i \\ &+ \frac{1}{6} \sum_{i=1,2} G_{ii} \psi_i^\dagger \psi_i^\dagger \psi_i^\dagger \psi_i \psi_i \psi_i + \frac{1}{2} \sum_{i \neq j} G_{ij} \psi_i^\dagger \psi_i^\dagger \psi_j^\dagger \psi_j \psi_i \psi_i \end{aligned}$$

2D Bose mixtures at finite temperature

Berezinskii-Kosterlitz-Thouless transition

Mermin-Wagner Theorem

No spontaneous breaking of continuous symmetries in 2D at finite temperature

- thermal fluctuations destroy BEC
- one-body density matrix vanishes according to a power law $n^{(1)}(r) \propto r^{-\nu}$

Berezinskii-Kosterlitz-Thouless (BKT) transition

From bound vortex-antivortex pairs at low temperatures to unpaired vortices and anti-vortices above the critical temperature

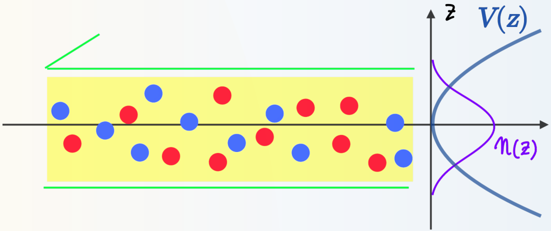
$$T_{\mathrm{BKT}} = \frac{\pi}{2k_B}\rho_s\frac{\hbar^2}{m^2}$$

$$n_{\mathrm{BKT}} = \frac{mk_BT}{2\pi\hbar^2}\log\frac{\xi}{g_0}, \qquad \xi \approx 380$$

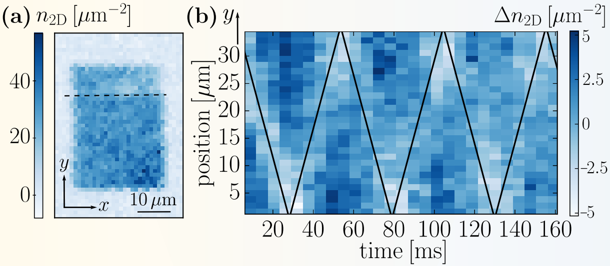
Strong transverse confinement: from 3D to 2D

Harmonic confinement

$$V(z) = \sum_i \frac{1}{2} m\omega_z^2 z_i^2$$



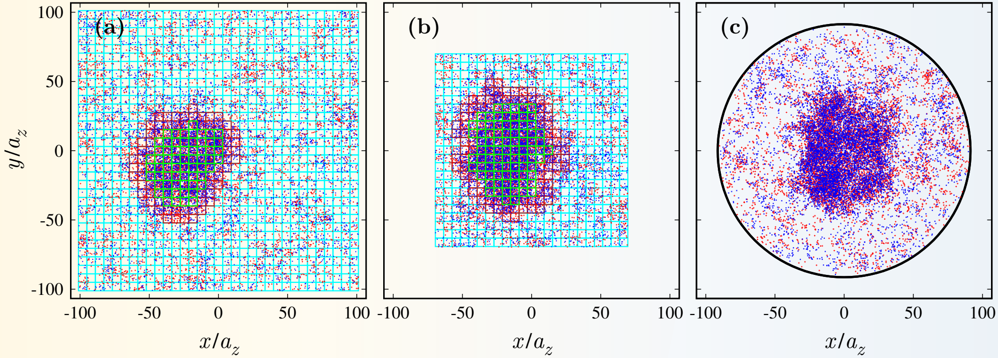
Quasi-2D kinematic conditions $k_B T \ll \hbar\omega_z, \quad a_{3D} \ll a_z = \sqrt{\hbar/m\omega_z}$



Ville, Saint-Jalm, Le Cerf, *et al.*, *Phys. Rev. Lett.* (2018)

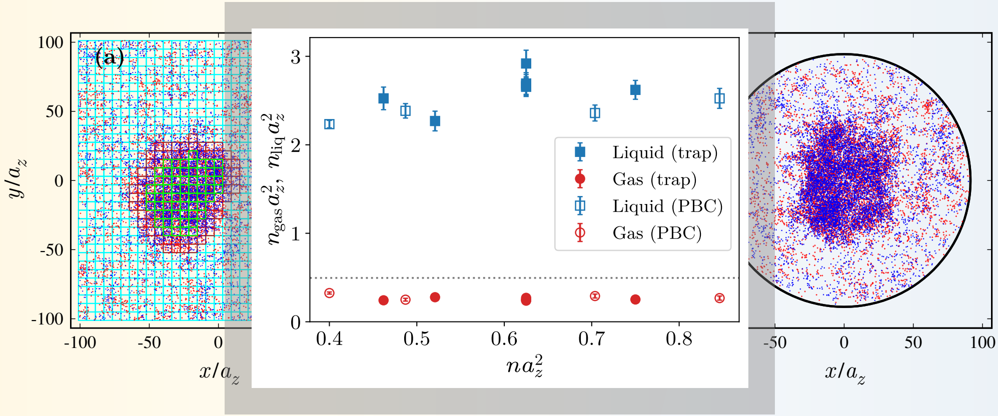
Bose mixtures: from 3D to 2D

3D simulations with harmonic confinement: Attractive mixtures form droplets



Bose mixtures: from 3D to 2D

3D simulations with harmonic confinement: Attractive mixtures form droplets

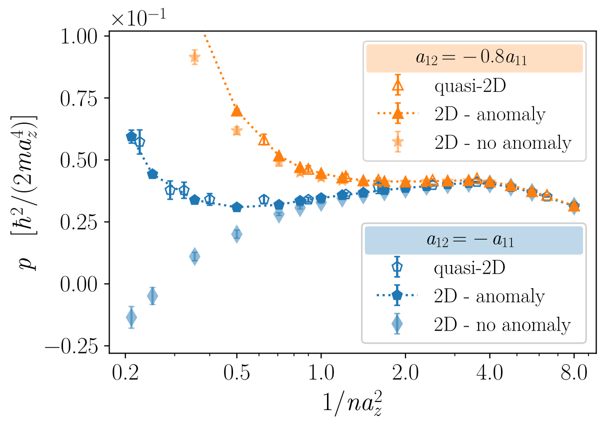


Bose mixtures: from 3D to 2D

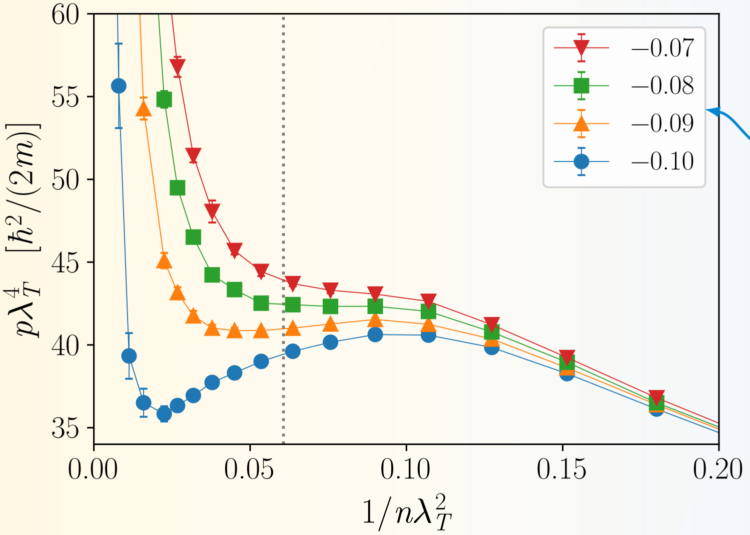
Pure 2D simulations: the role of quantum anomaly

Density-dependent 2D interaction

$$g = \frac{g_0}{1 + \frac{g_0}{4\pi} \log(A/na_z^2)}, \qquad g_0 = \sqrt{8\pi} a_{3D}/a_z\,, \quad A \approx 0.2284$$



Pure-2D mixtures at $T > 0$



Repulsive **intra**-species coupling $g_0 = 0.1$

Scan in the **inter**-species coupling $(g_{12})_0$

weak breaking of the **scale invariance**

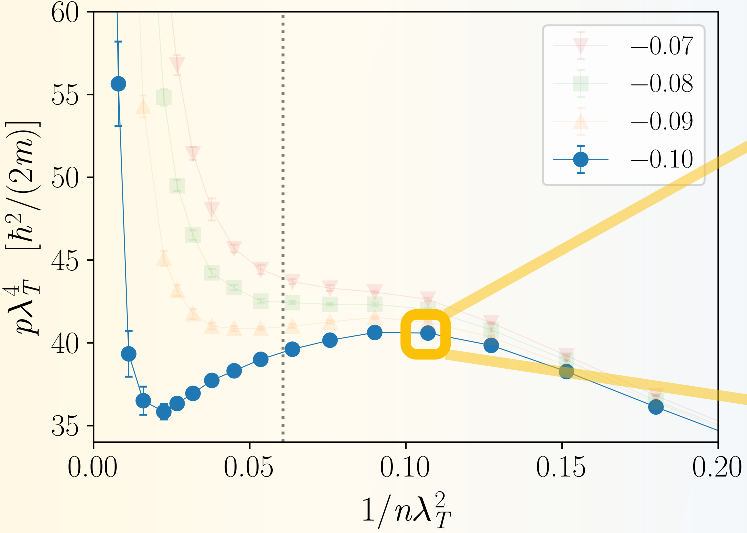
$\Downarrow$

almost universal scaling with T

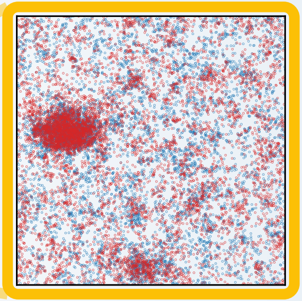
$$\lambda_T = \sqrt{2\pi\hbar^2/(mk_BT)}$$

SG, Pilati & Giorgini, *Phys. Rev. Lett.* (2024)

Pure-2D mixtures at $T > 0$

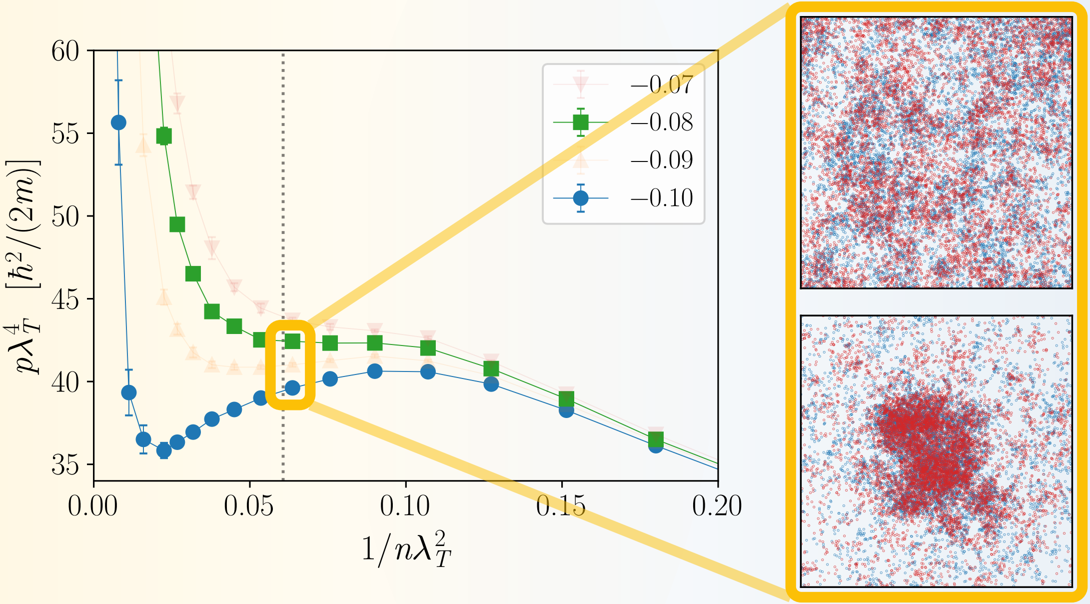


Droplet in **large-scale** PIMC simulations



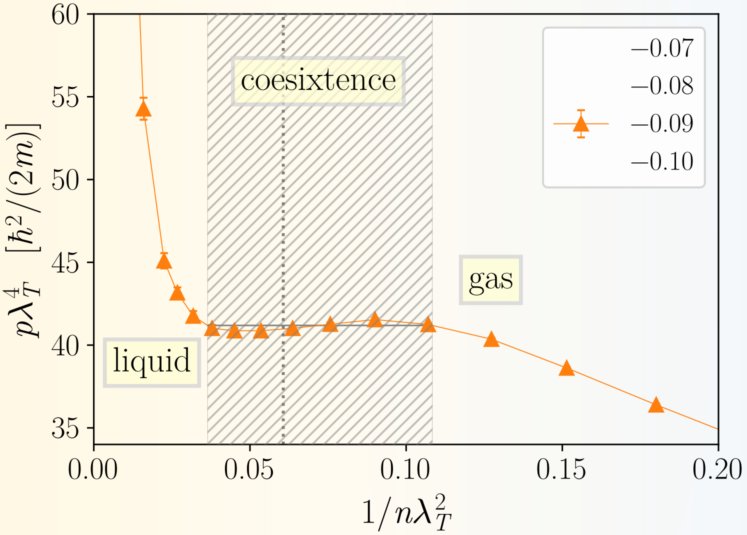
SG, Pilati & Giorgini, *Phys. Rev. Lett.* (2024)

Pure-2D mixtures at $T > 0$



SG, Pilati & Giorgini, *Phys. Rev. Lett.* (2024)

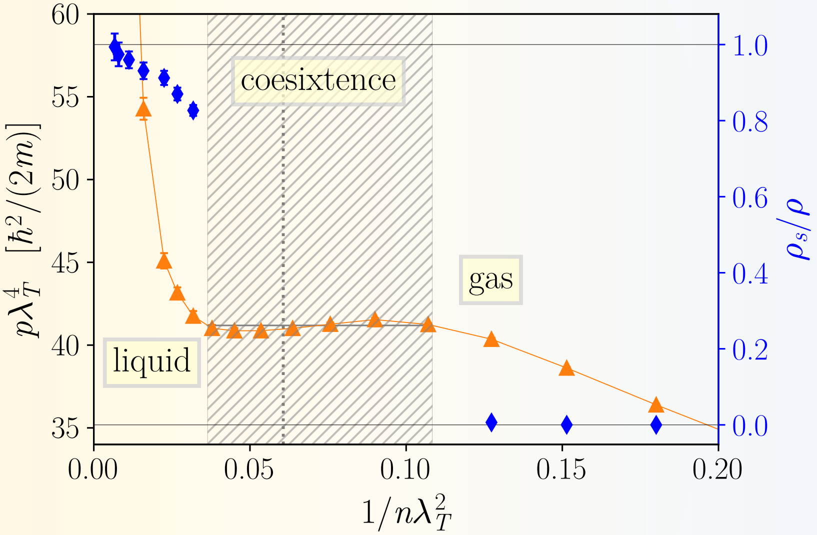
Pure-2D mixtures at $T > 0$



Coexistence region
from
Maxwell construction

SG, Pilati & Giorgini, *Phys. Rev. Lett.* (2024)

Pure-2D mixtures at $T > 0$



Superfluid fraction

$$\frac{\rho_s}{\rho} = \frac{mk_BT}{2N\hbar^2}\langle \mathbf{W}^2 \rangle$$

from winding

$$\mathbf{W} = \sum_{i=1}^{N}[\mathbf{r}_i(\beta) - \mathbf{r}_i(0)]$$

SG, Pilati & Giorgini, *Phys. Rev. Lett.* (2024)

CQM-Unicam

Complex Quantum Matter @ UNICAM

Left to right: Giovanni Midei, Victor Velasco, Luis Ardila, Sebastiano Pilati, Andrea Perali, Nicola Pinto, Simone Cantori, Luca Brodoloni, Andrea Della Valle and Verdiana Piselli. CQM-Unicam, May 30 2024.
Not Included: Carlo Lucheroni, Filippo Pascucci, Meenakshi Sharma and Gabriele Spada.

ME!

https://cqm.unicam.it/

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Thank you

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