Title: Superfluid to normal phase transition in strongly interacting bosons in two and three dimensions.

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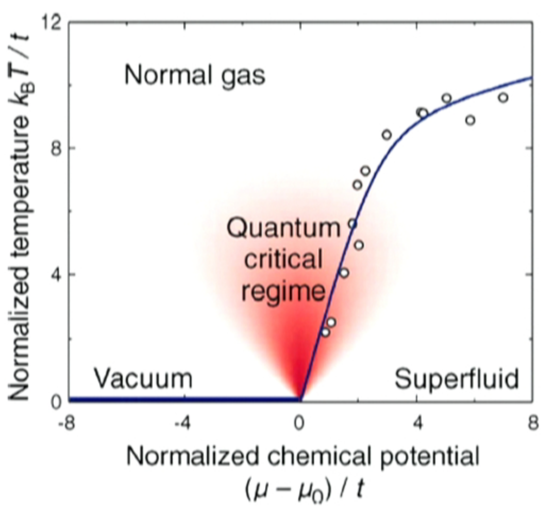
URL: http://www.pirsa.org/13010107

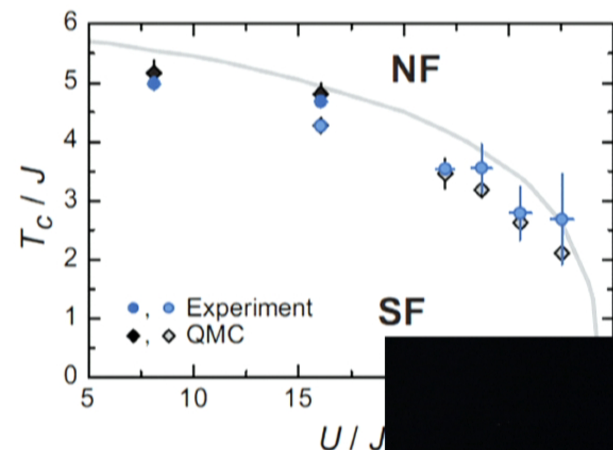
Abstract: Using quantum Monte Carlo simulations, we investigate the finite-temperature phase diagram of hard-core bosons (XY model) in

two- and three-dimensional square lattices. To determine the phase boundaries, we perform a finite-size scaling analysis of the condensate fraction and/or the superfluid stiffness. We then discuss how this diagrams can be measured in experiments with trapped ultracold gases, where the systems are inhomogeneous. For that, we introduce a method based on the measurement of the zero-momentum occupation, which is adequate for experiments dealing with both homogeneous and trapped systems. Finally, we provide an analytical argument that demonstrates that the Bose-Hubbard model does not exhibit ï¬•nite-temperature BEC in two dimensions, provided that density remains finite across the entire system in the thermodynamic limit.

Two dimensions (BKT)



Three dimensions (3D XY)



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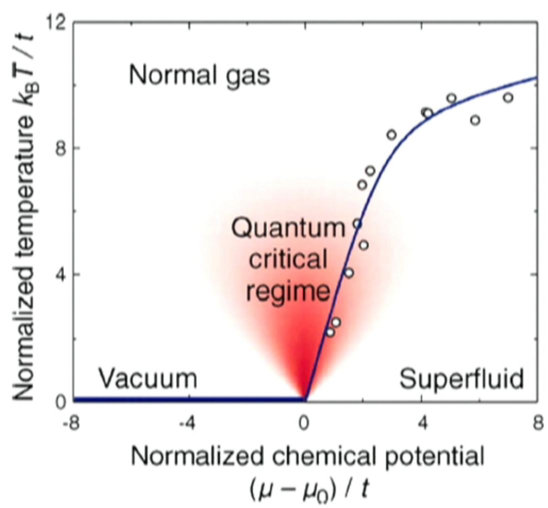

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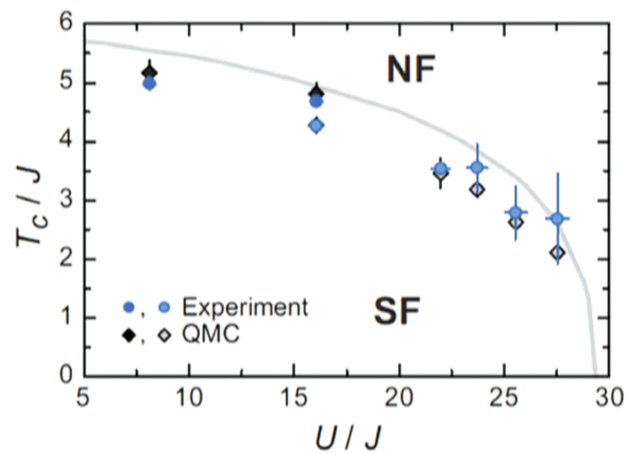


Model and phase diagram

We study on the superfluid-to-normal transition in a system of hard-core bosons (limit $U \gg t$ in the Bose-Hubbard model) in two- and three-dimensional lattices

Model

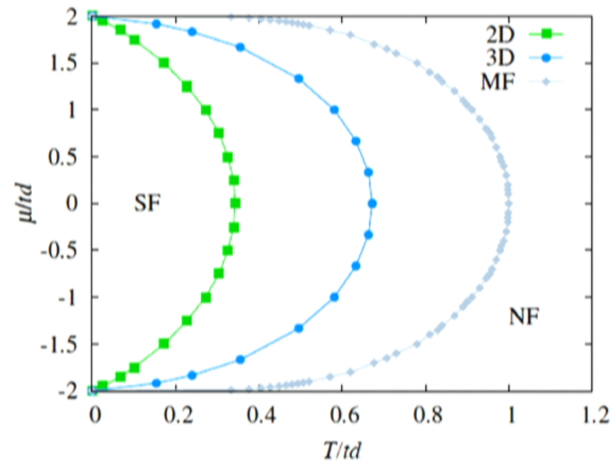
$$\hat{H} = -t \sum_{\langle i,j \rangle} \left(\hat{a}_i^\dagger \hat{a}_j + \mathrm{H.c.} \right) - \sum_i \mu_i \hat{n}_i \ ,$$

where the operators $\hat{a}_i^{\dagger 2} = \hat{a}_i^2 = 0$. The model can be mapped to the extensively studied XY model:

$$\hat{H} = -2t \sum_{\langle i,j \rangle} (S_i^x S_j^x + S_i^y S_j^y) - \sum_i \mu_i S_i^z \ ,$$

where S_i^α is the αth component of the spin-1/2 spin operator

Phase diagram



Juan Carrasquilla and Marcos Rigol, Phys. Rev. A 86, 043629 (2012).

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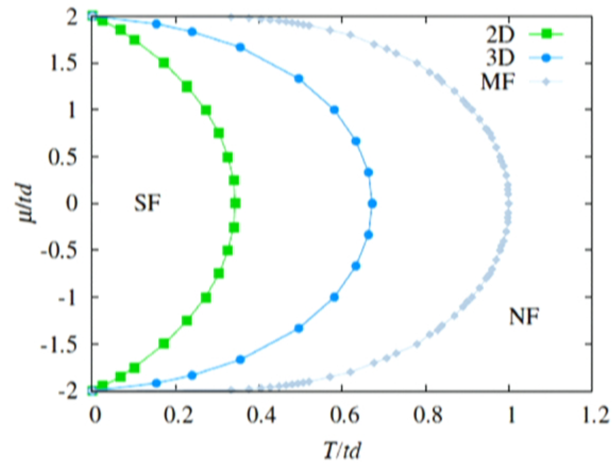

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Site-decoupled mean field

Site decoupling of the kinetic energy term:

$$\hat{a}_i^\dagger \hat{a}_j \simeq \hat{a}_i^\dagger \Phi_j + \hat{a}_j \Phi_i^* - \Phi_i^* \Phi_j,$$

with $\Phi_j = \langle \hat{a}_j \rangle$, for homogeneous systems, leads to

$$\hat{h}_{\mathrm{MF}} = -2dt\,\Phi\left(\hat{a}^\dagger + \hat{a}\right) - \mu\hat{n}.$$

Partition function

$$Z = 2e^{-\beta\frac{\mu}{2}} \cosh \beta\sqrt{\frac{\mu^2}{4} + (2dt\,\Phi)^2}.$$

Equation for the order parameter

$$\sqrt{\frac{\mu^2}{4} + (2dt\,\Phi)^2} = dt \tanh \beta\sqrt{\frac{\mu^2}{4} + (2dt\,\Phi)^2}.$$

It is then solved numerically.

How did we determine the phase diagrams?

Superfluid stiffness using QMC + finite-size scaling

BKT scenario for ρ_s

Finite-size scaling relation for ρ_s based on the BKT renormalization group equations:

$$\frac{\rho_s(T,L)\,\pi}{T} - 2 = \frac{1}{\ln L + l_0} F\left[(\ln L + l_0)^2 (T - T_c)\right]$$

where $F(x) = 1 - (4/3)x$

They predict a jump in ρ_s at T_c

$$\rho_s(T_c) = 2T_c/\pi$$

$$\rho_s(T,L)^* = \rho_s(T,L)\left(1 + \frac{1}{2[\ln L + l_0]}\right)^{-1}$$

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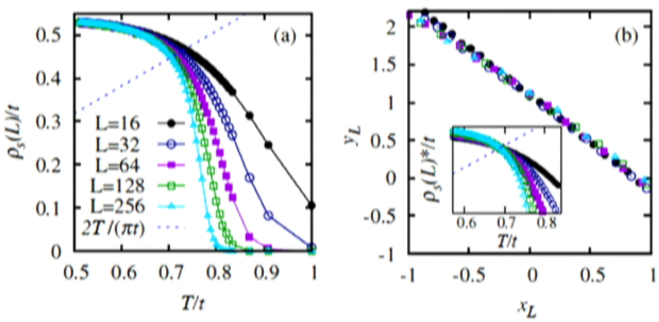

$T_c/t = 0.685 \pm 0.001$ for $\mu/t = 0$

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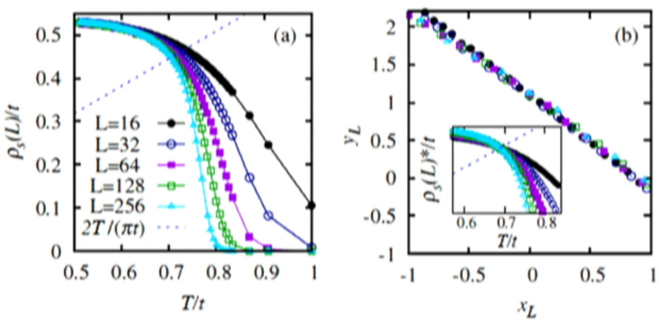

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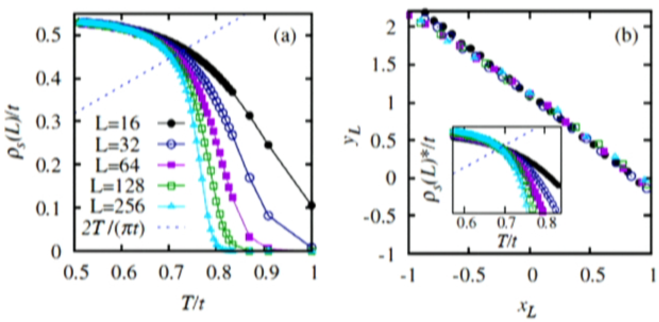

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3*d XY*

Correlation length:

$$\xi \sim |T - T_c|^{-\nu}$$

Superfluid stiffness (infinite system):

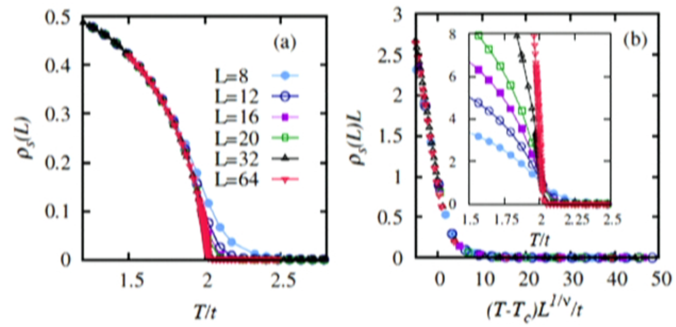
$$\rho_s \sim (T_c - T)^{(d-2)\nu}$$

Finite-size scaling relation:

$$\rho_s L^{d-2} = F\left(|T - T_c| L^{1/\nu}\right),$$

J. Phys. A: Math. Gen **32** 6361 (1999)

Three dimensions (3*d XY*)



$T_c/t = 2.0169 \pm 0.0005$ for $\mu/t = 0$

Recent calculation
$T_c/t = 2.016 \pm 0.004$
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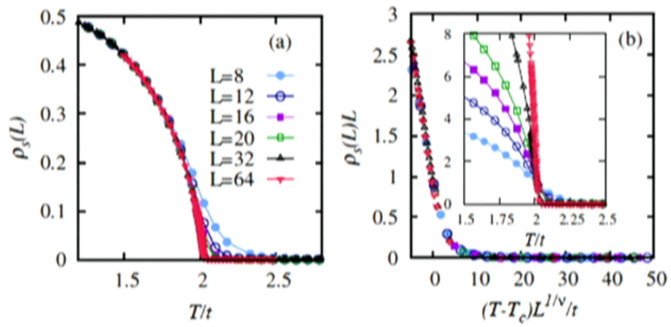

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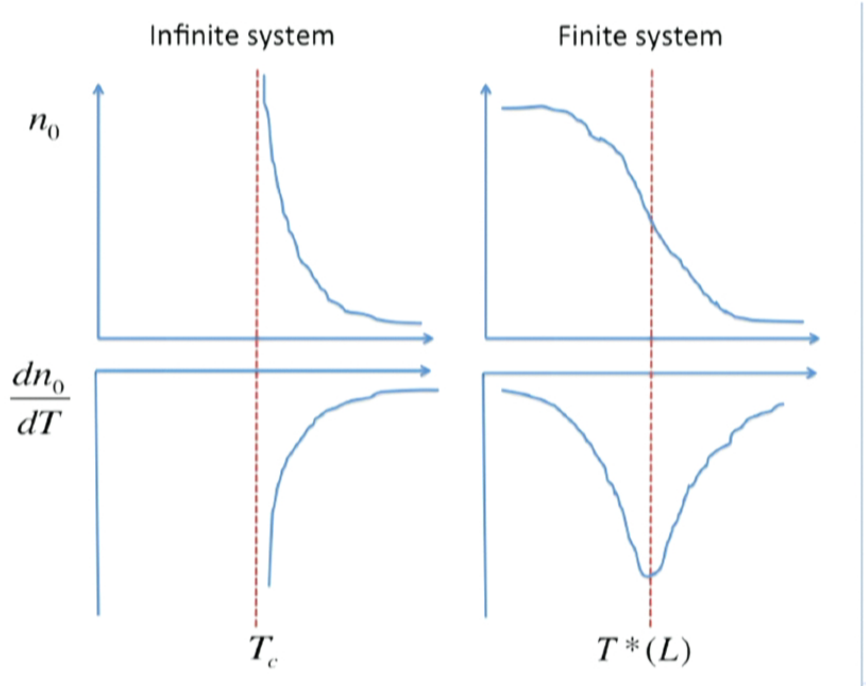
The zero-momentum occupation

The derivative dn_0/dT contains useful information about the transition in two and three dimensions! Good for finite-size systems



$T^*(L) = T_c +$ *size corrections*

$\left.\frac{dn_0}{dT}\right|_{T^*(L)} =$ *diverges with size*

Derivative of the zero-momentum occupation dn_0/dT + finite-size scaling

Size scaling

Zero-momentum occupation:

$$n_0 \sim \xi^{7/4}.$$

Derivative of n_0

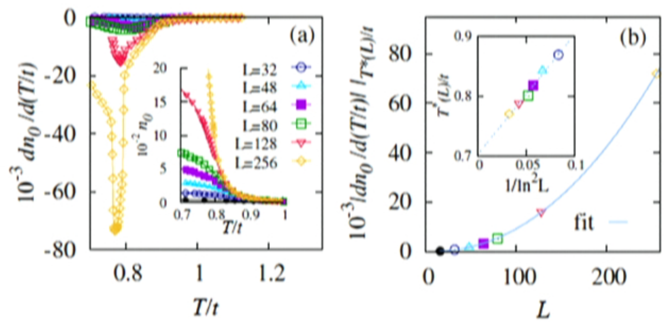
$$\frac{dn_0}{dT} \sim -\frac{\xi^{7/4} \ln^3 \xi}{b^2}$$

Finite-size scaling relations

$$T^*(L) = T_c + b'/\ln^2 L,$$

$$\left.\frac{dn_0}{dT}\right|_{T^*(L)} \sim -\frac{L^{7/4} \ln^3 L}{b^2}.$$

Two dimensions (BKT)



$T_c/t = 0.701 \pm 0.007$ for $\mu/t = 0$

Superfluid stiffness ρ_s
$T_c/t = 0.685 \pm 0.001$ for $\mu/t = 0$

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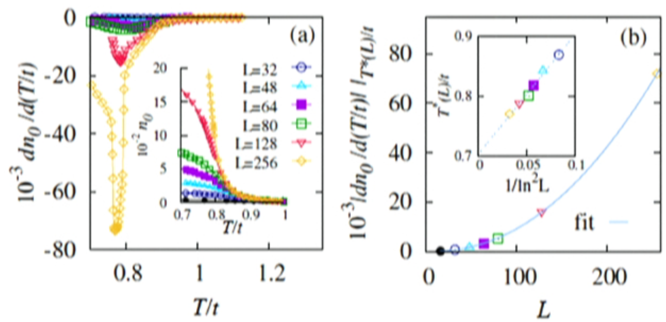

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Derivative of the zero-momentum occupation dn_0/dT + finite-size scaling

Size scaling relations

Zero-momentum occupation

$$n_0 \sim \xi^{2-\eta}$$

Derivative of n_0

$$\frac{dn_0}{dT} \sim -\xi^{2-\eta+1/\nu}.$$

Finite-size scaling relations

$$T^*(L) = T_c + c'/L^{1/\nu},$$

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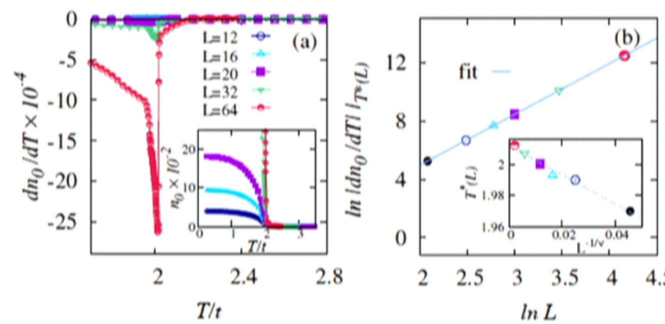
Three dimensions



$T_c/t = 2.012 \pm 0.002$ for $\mu/t = 0$
Superfluid fraction ρ_s

$T_c/t = 2.0169 \pm 0.0005$ for $\mu/t = 0$

Absence of BEC in interacting 2D systems

Facts:

- Thermal fluctuations destroy order at finite temperatures:
- No BEC in homogeneous non-interacting bosons.
- No BEC in homogeneous interacting bosons.
- Harmonically confined non-interacting bosons undergo BEC at finite temperature.
- Do interactions preclude BEC in harmonically confined bosons?

Absence of BEC in trapped interacting 2D systems

Bose-Einstein condensation occurs if the condensate fraction,

$$f_0 = n_M / N_b$$

remains finite after taking the appropriate thermodyanmic limit. n_M is the largest eigenvalue of the one-body density matrix $\rho_{ij} = \langle \hat{a}_i^\dagger \hat{a}_j \rangle$

An equivalent criterion for BEC

$$A_1 = \left(N_b L^d\right)^{-1} \sum_{i,j} |\rho_{ij}|$$

A_1 remains finite in the thermodynamic limit only if f_0 remains finite so long as the density ρ_{ii} remains finite everywhere in the system.

Penrose and Onsager. Phys. Rev. 104, 576584 (1956)

Fraction of particles in the $\vec{k} = 0$ state

$$A_0 = \frac{n_0}{N_b} = \left(N_b L^d\right)^{-1} \sum_{i,j} \rho_{ij}$$

If a system has $\rho_{i,j} \geq 0$, then $A_0 = A_1$.

Can we use A_1 to know if BEC occurs for trapped bosons described by the Bose-Hubbard model?

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Can we use A_1 to know if BEC occurs for trapped bosons described by the Bose-Hubbard model?

For the Bose-Hubbard model:

- Interaction prevents the divergence of the density (Criterion based on A_1 applies)
- In thermal equilibrium $\rho_{ij} \geq 0$.

Which means that A_1 coincides with the fraction of particles in the zero-momentum state A_0, which should be zero because of Mermin-Wagner theorem. $\Rightarrow$ There is no BEC in interacting 2-d inhomogeneous systems.

Weak link for non-interacting bosons: the density diverges at the center of the trap and A_1 is NOT equivalent to A_0

Condensation to a generic state in interacting systems is connected to condensation to the $\vec{k} = 0$ state

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Conclusions

- We determined the finite temperature phase diagram of bosons in the hard-core limit (or the XY model) in two and three dimensions.
- Measurements of the derivative dn_0/dT together with finite-size scaling relations can be used to determine critical temperatures.
- This last approach can be applied to systems that exhibit a diverging zero-momentum occupation in any dimension and universality class.
- We provided an argument against the possibility to have BEC for interacting trapped systems.
- The approach based on dn_0/dT can also can be extended to trapped atomic gases.