The phase transtions of a dilute Bose gas in two and three dimensions

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Gordon Baym, Jean-Paul Blaizot, Franck Laloë, Dominique Vautherin

Dilute Bose gas

$$H = -\frac{1}{2m}\sum_i \nabla_i^2 + \sum_{i<j} v(|\mathbf{r}_i - \mathbf{r}_j|)$$

- Finite temperature T>0 ($\beta=1/T$)
- Homogeneous systems
- Thermodynamic limit, constant density n=N/V
- Short range interaction described by scattering length a ($g=4\pi a/m$)
- Dilute Bosons: $na^3 \rightarrow 0$

Questions & Results (3D):

- Critical temperature shift (with respect to ideal gas T_C^0)?

$$\frac{\Delta T_c}{T_c^0} = c\, a n^{1/3} \left(1 + \tilde{c}\, a n^{1/3} \log a n^{1/3} + \dots\right)$$

Leading order:
linear in a, constant c>0 is “universal”

G. Baym, J.-P. Blaizot, M. H., F. Laloë, D. Vautherin,
Phys. Rev. Lett. 83, 1703 (1999)

Next-to-leading order: a^2 log a
restricts linear region drastically

M. H., G. Baym, J.-P. Blaizot, F. Laloë,
Phys. Rev. Lett. 87, 120403 (2001)

Perturbative calculation of $\bar{c}$:
P. Arnold, G. Moore, B. Tomasik,
Phys. Rev. A 65, 013606 (2001).

Best value for c from
classical field calculations on a lattice: c≈1.3

P. Arnold, G. Moore,
Phys. Rev. Lett. 87, 120401 (2001);
V. A. Kashurnikov, N.V. Prokof ’ev, B.V. Svistunov,
Phys. Rev. Lett. 87, 120402 (2001).

- Critical region, scaling behavior?

$$t \equiv \frac{|T - T_c|}{T_c} \lesssim a n^{1/3}$$

condensate/ superfluid fraction inside critical region:

$$\frac{n_0}{n} = c_0\, a n^{1/3} f_0\left(\frac{t}{a n^{1/3}}\right) \qquad \frac{n_s}{n} = c_s\, a n^{1/3} f_s\left(\frac{t}{a n^{1/3}}\right)$$

In particular: $\left.\frac{n_0}{n}\right|_{T=T_c^0} \sim a n^{1/3}$

M. H., G. Baym, Phys. Rev. Lett. 90, 040402 (2003)

- External, harmonic trap?

thermodynamic limit in trap

$$T_c(N) = T_0(N)\left[1 + c_1 \frac{a}{l} + \left(c_2' \ln\frac{a}{l} + c_2''\right)\left(\frac{a}{l}\right)^2 + \cdots\right]$$

$$l \sim \bar{n}^{-1/3} \sim N^{-1/6} a_{\mathrm{ho}}$$

(perturbative)

S. Giorgini, L. P. Pitaevskii, S. Stringari,
Phys. Rev. A 54, R4633 (1996)

P. Arnold, B. Tomášik
Phys. Rev. A 64, 053609 (2001)

Non-perturbative,
uses universal "c" result
of the homogeneous system

- Experiments (trap)?

Mean-field shift

F. Gerbier, J. H. Thywissen, S. Richard, M. Hugbart, P. Bouyer, A. Aspect, Phys. Rev. Lett. 92, 030405 (2004)

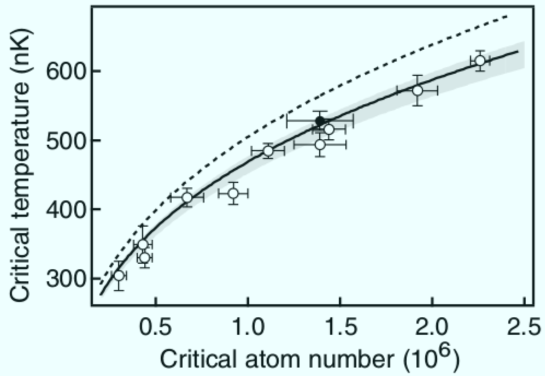


FIG. 3. Critical temperature as a function of atom number at the transition. The experimental points (circles) are lower than the ideal gas law Eq. (1) (dashed) by two standard deviations. The shaded area is the range of acceptable fits taking statistical and systematic errors into account. Our results are consistent with the shift due to the compressional effect given by Eq. (2), indicated by the solid line. The filled circle represents the data of Fig. 2.

Beyond Mean-field shift

R. Smith, R. Campbell, N. Tammuz, Z. Hadzibabic Phys. Rev. Lett. 106, 250403 (2011)

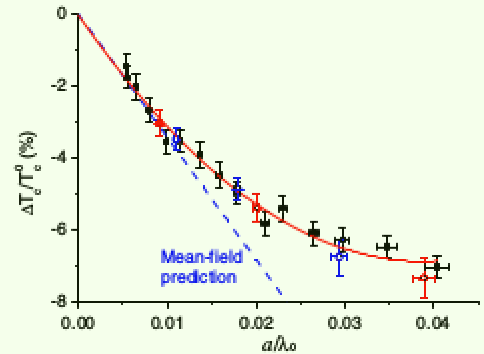


FIG. 3 (color online). Interaction shift of T_c. Data points were taken with $N \approx 2 \times 10^5$ (blue circles), 4×10^5 (black squares), and 8×10^5 (red triangles) atoms. The dashed line is the mean-field result $\Delta T_c/T_c^0 = -3.426a/\lambda_0$. The solid line shows a second-order polynomial fit to the data (see text). Vertical error

Condensate density shift:

R. Smith, N. Tammuz, R. Campbell, M. H., Z. Hadzibabic Phys. Rev. Lett. 107, 190403

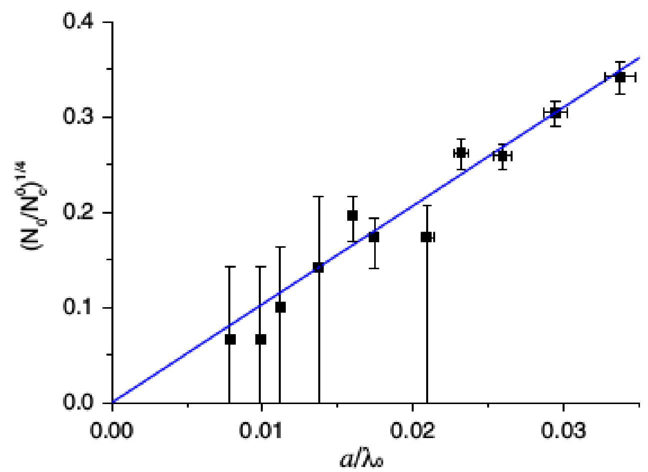


FIG. 3 (color online). Comparison with Monte Carlo calculations for a uniform system. To quantitatively compare our data with the MC simulations we plot $(N_0/N_c^0)^{1/4}$ versus a/λ_0 (see text). A linear fit gives a gradient of $\alpha_{exp} = 10.3 \pm 0.3$, in excellent agreement with the prediction $\alpha_{MC} = 10.4 \pm 0.4$.

Homogeneous Bose gas: linear shift

- Critical temperature shift vs critical density shift:

$$\frac{\Delta T_c}{T_c^0} = -\frac{2}{3}\frac{n_c - n_c^0}{n_c^0}$$

Ideal gas BEC:

$$n\left(\frac{2\pi}{mT}\right)^{3/2}\Big|_c = 2.61\ldots$$

- Density expressed in finite temperature Green's function

$$n = \int \frac{d^3k}{(2\pi)^3}\langle a_{\mathbf{k}}^\dagger a_{\mathbf{k}}\rangle = -T\sum_\nu \int \frac{d^3k}{(2\pi)^3} G(k, i\omega_\nu)$$

$$\omega_\nu = 2\pi\nu T,$$

$$\nu = 0, \pm 1, \pm 2, \ldots$$

$$G^{-1}(k,z) = z + \mu - \frac{k^2}{2m} - \Sigma(k,z)$$

Self-energy
(contains all interaction effects)

- BEC transition point (for chemical potential, T and a fixed):

$$\mu_c = \Sigma_\mu(0,0)$$

$$n_c - n_c^0 \simeq T_c^0 \int \frac{d^3k}{(2\pi)^3}\left[G(k,0) - G^0(k,0)\right]$$

$$\frac{\Delta T_c}{T_c} \sim \int dk \frac{U(k)}{k^2 + U(k)} \qquad U(k) = 2m\left[\Sigma(k,0) - \Sigma(0,0)\right]$$

Self-energy: diagramatic analysis

- Diagrams linear in a => mean field $\Sigma_{mf} = 2gn$ $g = 4\pi a/m$

$$\Sigma_{mf} - \mu_c = 0$$

No shift in T_c !

$$\Delta T_c\Big|_{mf} = 0$$

- a^2: second order diagram

$$\Sigma_2(k, i\omega_\nu) = 2g^2T^2 \sum_{\mu\mu'} \int \frac{d^3q}{(2\pi)^3}\frac{d^3p}{(2\pi)^3} G_{mf}(p, i\omega_{\mu'})G_{mf}(\mathbf{p}+\mathbf{q}, i\omega_{\mu'+\mu})G_{mf}(\mathbf{k}-\mathbf{q}, i\omega_{\nu-\mu})$$

dominant contribution for small wavevectors:

$$2m\Sigma_2(k,0) \simeq -2(2mg)^2(2mT)^2 \int \frac{d^3q}{(2\pi)^3}\frac{d^3p}{(2\pi)^3} \frac{1}{(\mathbf{p})^2+\xi^{-2}} \frac{1}{(\mathbf{p}+\mathbf{q})^2+\xi^{-2}} \frac{1}{(\mathbf{k}-\mathbf{q})^2+\xi^{-2}}$$

$$U_2(k) = a^2(mT)^2 f(k\xi) \qquad \frac{1}{2m\xi^2} = \mu_{mf} - \mu$$

If we have at critical point: $\mu_{mf} - \mu_c \sim a^2$ $\xi_c \sim a^{-1}$

then
$$\frac{\Delta T_c}{T_c} \sim \int dk \frac{U(k)}{k^2 + U(k)} \sim a$$

M. H., P. Grüter, F. Laloë,
Eur. Phys. J. B10, 739 (1999)

- Higher order diagrams:

Power counting of infrarouge: $$\Sigma_n \sim T\left(\frac{a}{\lambda}\right)^2\left(\frac{a\zeta}{\lambda^2}\right)^{n-2}.$$

at criticality we have $\xi_c \sim a^{-1}$

All orders are relevant!!!

- Classical phi^4 field theory is sufficient to get linearity, prefactor universal

$$p\left\{\Phi(\mathbf{r})\right\} \sim \exp\left[-S\left\{\Phi(\mathbf{r})\right\}\right]$$
$$S\left\{\Phi(\mathbf{r})\right\} = \frac{1}{2mT}\int d\mathbf{r}\left[\left|\nabla\Phi(\mathbf{r})\right|^2 + \frac{1}{\xi^2}\left|\Phi(\mathbf{r})\right|^2 + 2\pi a\left(\left|\Phi(\mathbf{r})\right|^2 - \langle\left|\Phi(\mathbf{r})\right|^2\rangle\right)^2\right]$$

use UV cutoff Λ (lattice) to regularize
and simple 2nd order counter-term to
separate IR and UV (no mixing of logs!)

$-128(a/\lambda^2)^2 \ln(\Lambda\zeta)$ to $2m\Sigma$

Universal behavior in critical region

- Scaling behavior of self energy

$$\beta[\Sigma(k,0) - \Sigma_{mf} - \Sigma^*] = \frac{a^2}{\lambda^2} u(k\xi, J) \qquad \xi^{-1} = \frac{\beta\left(\Sigma_{mf} + \Sigma^* - \mu\right)}{a} \sim \frac{a}{\lambda^2}$$

$$u(0, J_c) = \frac{\lambda^2}{a\xi_c} = J_c^{-1} \qquad \lambda = \sqrt{\frac{2\pi}{mT}}$$

counter term needed to renormalize 2nd order UV divergence:

$$2m\Sigma^* = -128a^2/\lambda^4 \log(\Lambda a/\lambda^2)$$

- Scaling function u(x) "dominates" inside critical region

$$u(x, J_c) \sim x^{2-\eta}, \quad x \to 0$$

Matching with "real world"

- Strategy:
  - calculate non-perturbative contributions numerically (classical field, lattice)
  - tabulate scaled functions
  - add perturbative contributions with mean-field
  - use local density approximation for smooth external potentials

density, condensate density…:

classical field contribution
calculate numerically f

$$(n - n_c)\,\lambda^3 = \frac{a}{\lambda} f\left(\frac{\beta(\mu - \mu_c)}{(a/\lambda)^2}\right)$$

add quantum/UV contributions perturbatively, e.g. mean-field

$$n\lambda^3 = (n - n_c)\lambda^3\Big|_{mf}(\beta\mu) + \frac{a}{\lambda} f\left(\frac{\beta(\mu - \mu_c)}{(a/\lambda)^2}\right)$$

use local density approximation (LDA) to account for trap potential:

$$\mu(r) = \mu - u(r) = \mu - m\omega^2 r^2/2$$

2D: Berenzinskii-Kosterlitz-Thouless transition

- Perturbative analysis:
  close to transition IR divergencies, classical phi^4 theory dominates
- Classical phi^4 “easier”: mean-field terms are enough for renormalization
- transition point as in 3D, but structure below is different:
  no condensate density in the thermodynamic limit but
  finite superfluid density (use Josephson’s relation to relate them with G(k)
- calculate classical \phi^4 contributions numerically match with mean-field
- Typically: classical field contributions dominate over broad region,
  matching relatively simple, works quantitatively well….

QMC simulations of Bosons: A successful story

based on Feynman's path integral representation of the N-particle density matrix

$$\rho(\mathbf{R},\mathbf{R}') = \frac{1}{Z}\langle \mathbf{R}|e^{-\beta H}|\mathbf{R}'\rangle \qquad \langle \mathbf{R}|e^{-\beta H}|\mathbf{R}'\rangle \equiv \int d\mathbf{R}_2\, \langle \mathbf{R}|e^{-\beta H/2}|\mathbf{R}_2\rangle\langle \mathbf{R}_2|e^{-\beta H/2}|\mathbf{R}'\rangle$$

Bosons: $\rho_B(\mathbf{R},\mathbf{R}') = \frac{1}{Z_B}\frac{1}{N!}\sum_P (+1)^P \rho(\mathbf{R}, P(\mathbf{R}'))$ $\quad \mathbf{R} \equiv (\mathbf{r}_1, \mathbf{r}_2, \ldots \mathbf{r}_N)$

Path Integral Monte Carlo:

use M>>1 discretizations («time slices»): $\tau = \beta/M \to 0$

use of high temperature approximation, e.g. :
(position representation → positive!) $\langle R|e^{-\tau H}|R'\rangle \simeq \langle R|e^{-\tau T}|R'\rangle\, e^{-\tau V(R')}$

Do random walk in extended position space (M x d x N coordinates) and permutation space (N! permutations)

Zero temperature variants:
Ground State Path Intetgral, Diffusion, Reptation,... Monte Carlo

Quasi2D Bose gases

direct comparison between experiment and exact QMC calculations possible

S.P. Rath, T. Yefsah, K.J. Günter, M. Cheneau, R. Desbuquois, M.H., W. Krauth, J. Dalibard,
Phys. Rev. A 82, 013609 (2010)

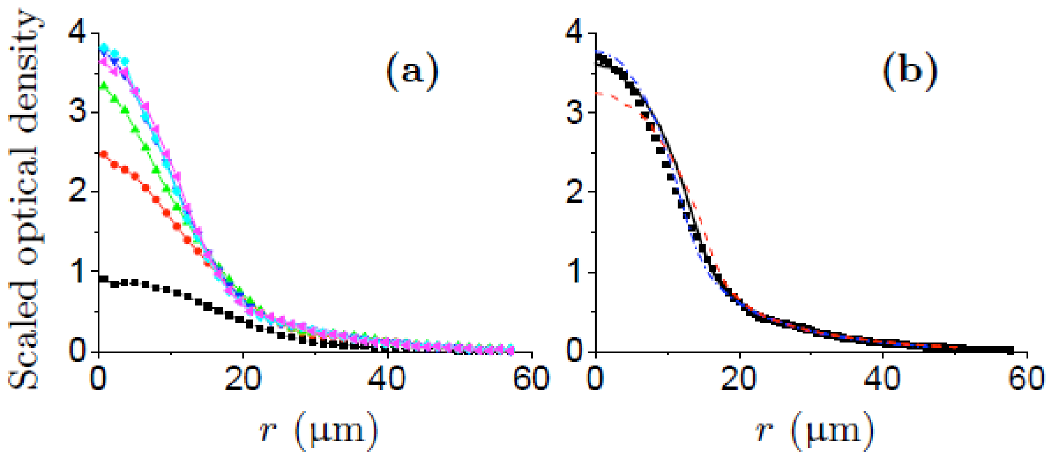


FIG. 4: (Color online) (a) Optical density profiles obtained for a TOF duration $t = 0$ (black), 3 (red), 6 (green), 10 (blue), 12 (cyan), 14 (magenta) ms and rescaled to their in-situ value according to (1). (b) Squares: Optical density profile obtained by averaging the results of (a) for $10 \leq t \leq 14$ ms, yielding fit parameters $T = 94$ nK, $\alpha = 0.36$ for $\xi = 0.63$. Lines: QMC results for the same fit parameters (continuous, $N = 42000$), and for those deduced assuming $\xi = 0.47$ [dashed red, $(T \text{ (nK)}, \alpha, N) = (104, 0.39, 57600)$] and $\xi = 0.79$ [dash-dotted blue, $(87, 0.33, 32100)$].

density profiles compared using scale invariance in 2D time-of-flight exapnsion

density profile after 2D time-of-flight given by scaling transform

$$n(\mathbf{r}, t) = \nu_t^2 n(\nu_t \mathbf{r})$$

$$\nu_t = (1 + \omega^2 t^2)^{-1/2}$$

Quasi2D: true 2D or anisotropic 3D?

- pure 2D bosons:

Correlation effects are quantitatively described by classical field theory

Universal expression for Equation of State (EOS) in 2D
for weak interactions ($g \to 0$)

mean-field energy
$\mu_{mf} = 2gn$

$$\Delta n \lambda^2 \equiv (n - n_{mf})\lambda^2 \quad \text{is a unique function of} \quad \Delta_{mf}/\tilde{g} \equiv \frac{\mu - \mu_{mf}}{mgT}$$

mean-field EOS

Universal function calculated and tabulated

N. Prokof'ev, B. Svistunov PRA 66, 043608 (2002).

- quasi 2D bosons:

only mean-field EOS and mean-field energy μ_{mf} are adapted to
external trapping potential, correlations remain pure 2D

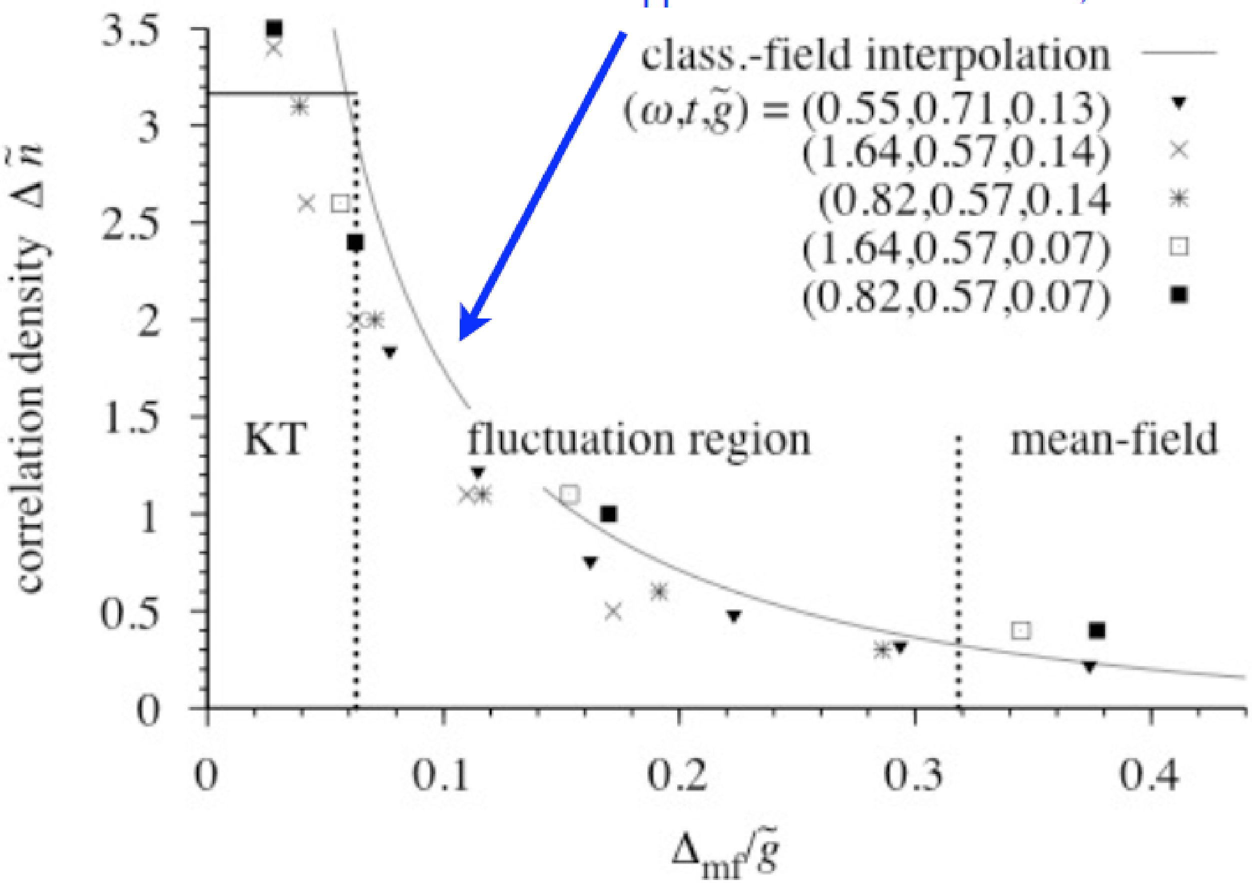
Is the quasi 2D picture quantitativly correct?

Analysis of QMC density profiles in local density approximation (LDA):

correlation density $_\Delta n\lambda^2 = (n-n_{mf})\lambda^2$ vs LDA-gap Δ_{mf}
from many systems with different ω_z, T, g

$_\Delta n\lambda^2 = (n-n_{mf})\lambda^2$

classical field approximation: N. Prokof'ev, B. Svistunov PRA 66, 043608 (2002).

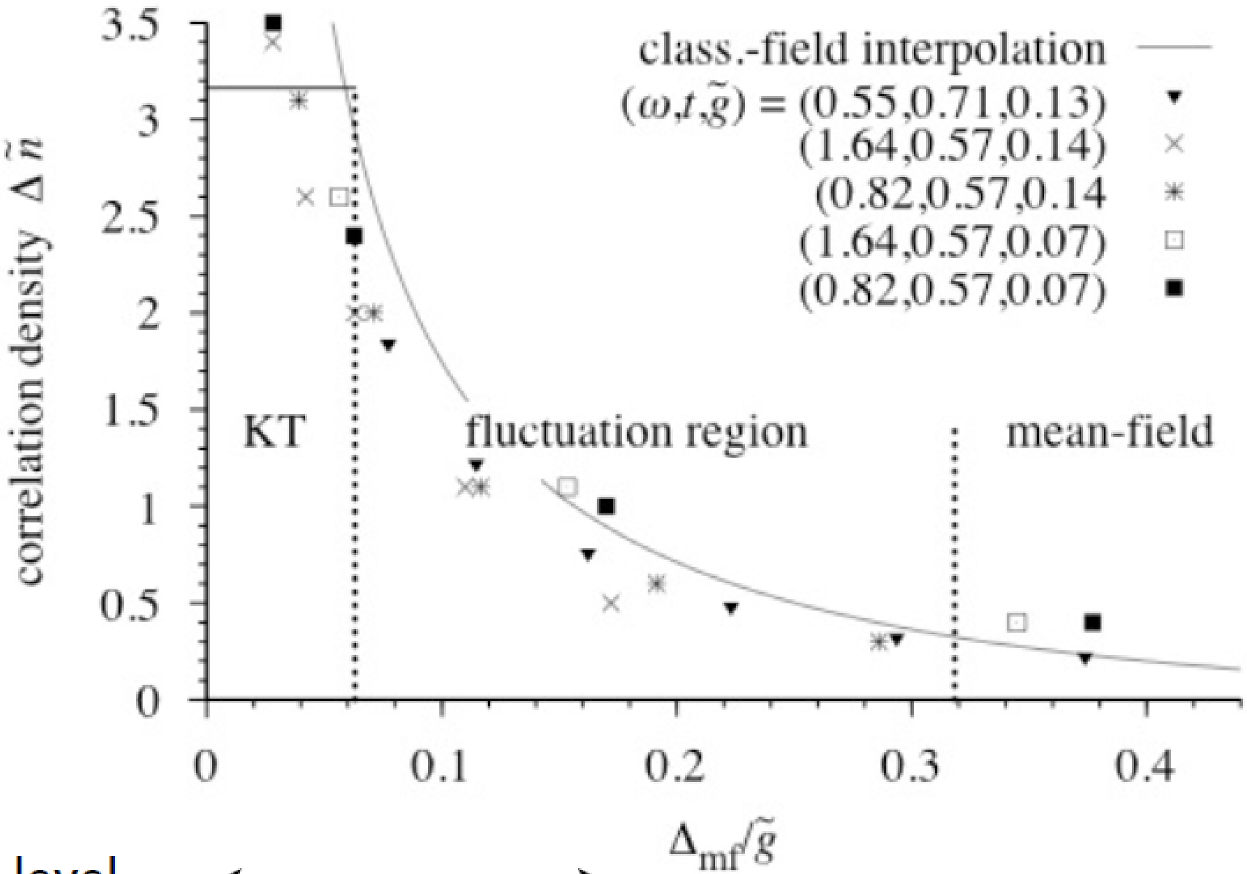


full QMC calculations in quasi2D trap

Δ_{mf} /g

M. H., M. Chevallier, W. Krauth, Phys. Rev. A 81, 043622 (2010)

Finite size effects: Cross-over to BEC for small N



finite system: level spacing in trap: ω

$\omega/(gT)$

at T_{BEC}: $\omega/T_{BEC} = \pi\,(6\,N)^{-1/2}$

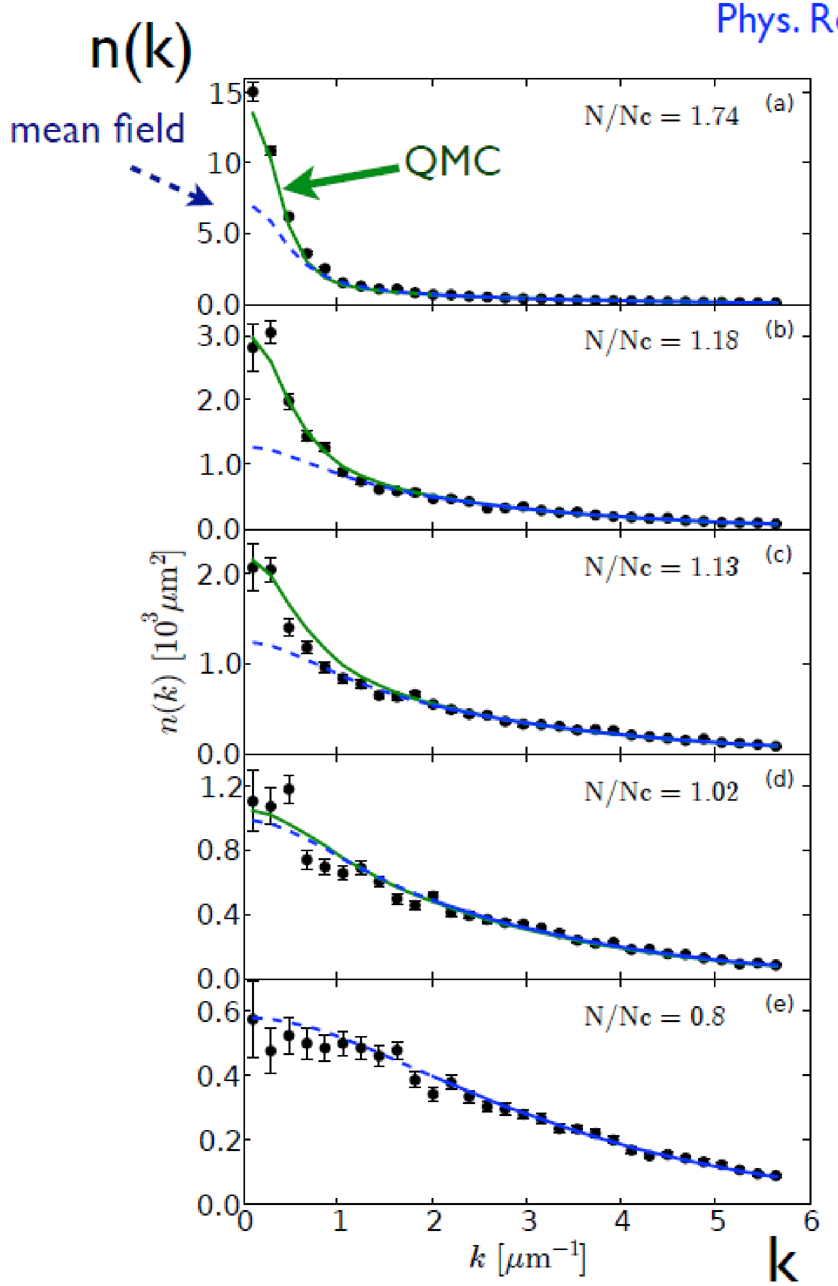
Cross-over to mean-field physics for $\omega/T_{BEC} > g/\pi$

mean-field (with BEC) for $N < \pi^4/(6\,g^2)$

M. H., M. Chevallier, W. Krauth, Phys. Rev. A 81, 043622 (2010)

Non-local probe for: Momentum profile n(k)

T. Plisson, B. Allard, M. H., G. Salomon, A. Aspect, P. Bouyer, and T. Bourdel
Phys. Rev. A 84, 061606(R) (2011)



3D Time of flight expansion (TOF):

- time evolution of the density operator

$$\rho(t) = e^{-iHt/\hbar} \rho(t=0) e^{iHt/\hbar}$$

- strong confinement in z (quasi 2D)
  - ⇒ large initial momentum in z
  - ⇒ rapid expansion in z
- slow expansion for in-plane density x/y

$$H_{TOF} \approx \sum_i \frac{p_{ix}^2 + p_{iy}^2}{2m}$$

⇒ TOF density ≅ momentum dist., n(k),

for long TOF-time t

Theory (QMC) ↔ Experiment: Coherence properties

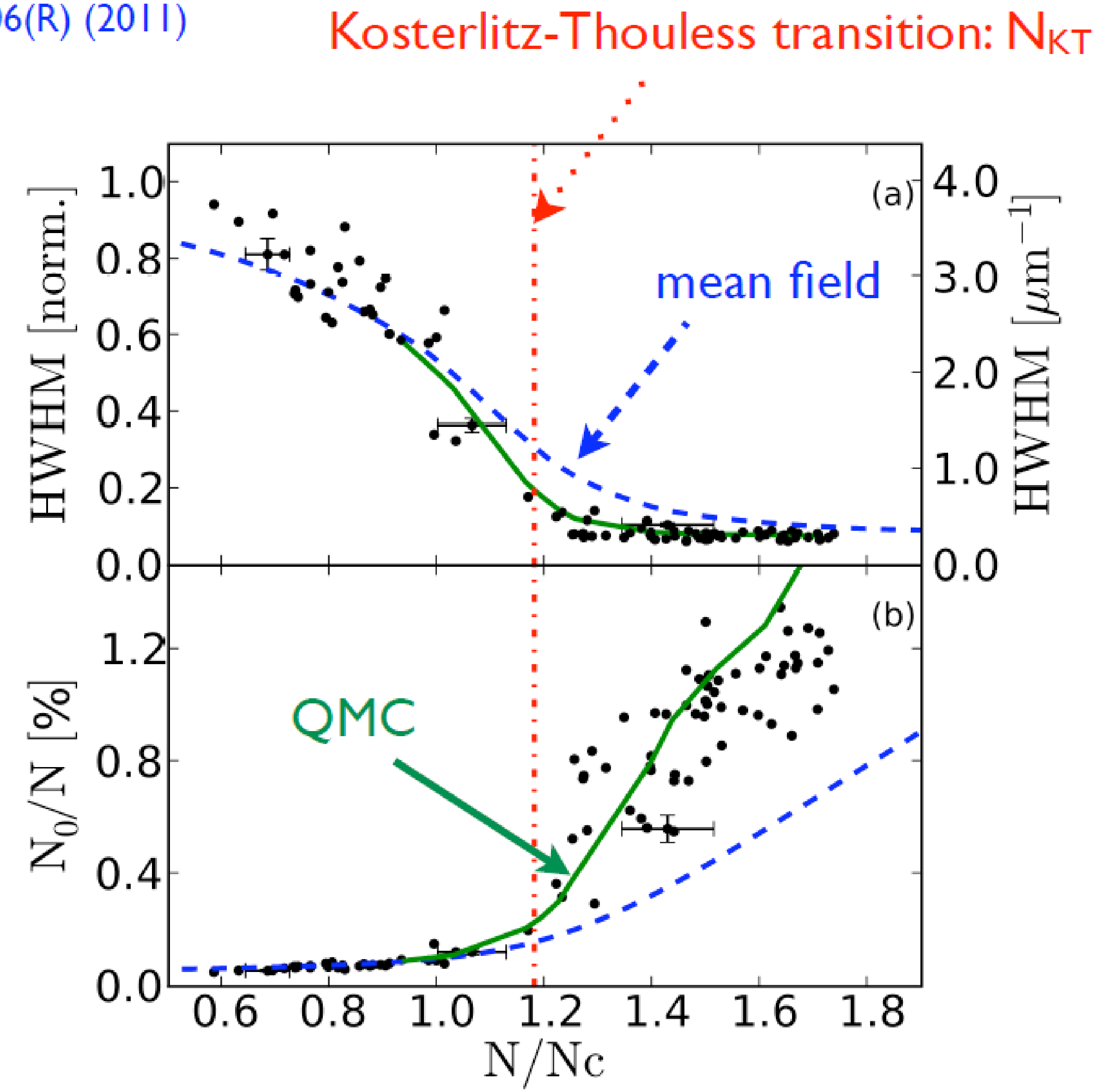
T. Plisson, B. Allard, M. H., G. Salomon, A. Aspect, P. Bouyer, and T. Bourdel
Phys. Rev. A 84, 061606(R) (2011)

Characterization of Coherence (Peak around k=0):

Width of the peak: HWHM

Height of the peak:

Fraction of particles in k=0 peak: N_0/N



$N/N_c = (T/T_c)^{-2}$

Critical temperature/ particle number

T_c: Change of slope of zero momentum peak

R.J. Fletcher, M. Robert-de-Saint-Vincent, J. Man, N. Navon, R.P. Smith, K.G.H. Viebahn, Z. Hadzibabic,
Phys. Rev. Lett. 114, 255302 (2015).

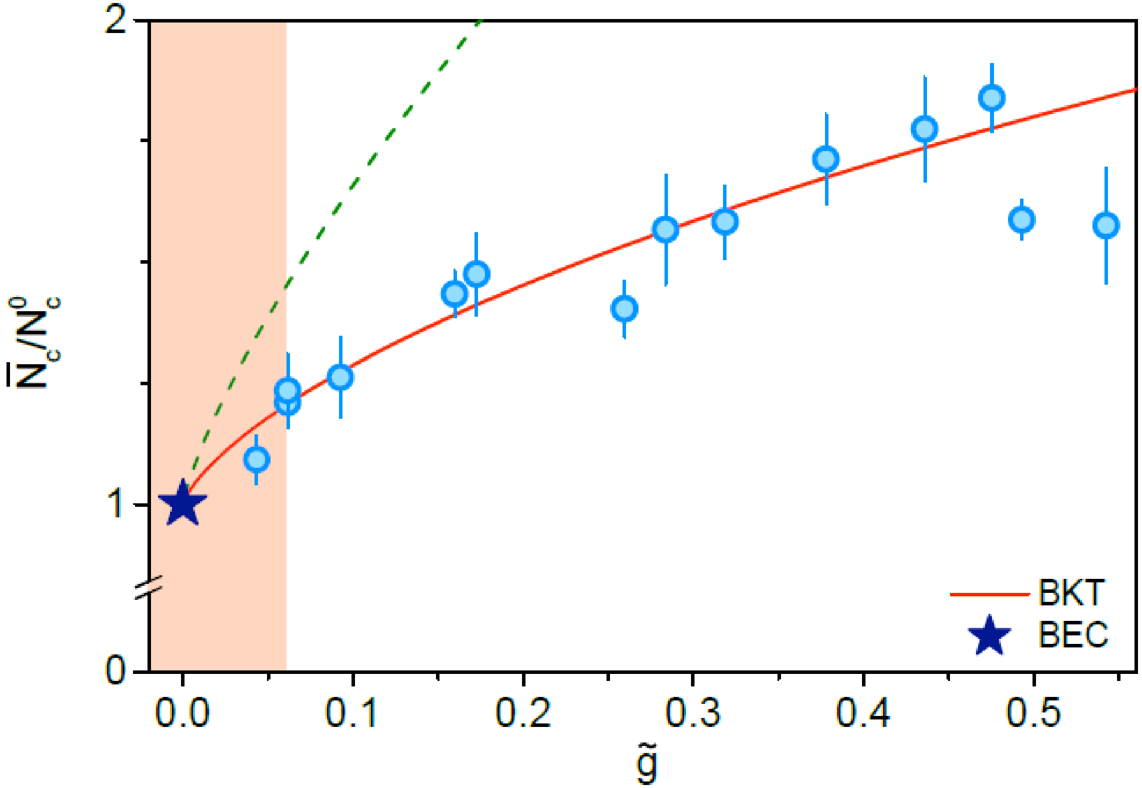


FIG. 2. (color online) Critical atom number as a function of the interaction strength $\tilde{g}$. All numbers are scaled to the ideal-gas BEC critical number N_c^0, defined in Eq. (1). Solid line is the BKT prediction of Eq. (2), without any free parameters. Dashed line is an approximation which neglects suppression of density fluctuations in the normal state. The star ($\star$) denotes the critical point for BEC, which only occurs in the ideal-gas limit. The shaded region, $\tilde{g} < 0.06$, indicates the regime in which our measurements stop being reliable (see text). Error bars are statistical.

Quantitative agreement with critical particle number in trap:

$$\frac{N_c^{\mathrm{BKT}}}{N_c^0} \approx 1 + \frac{3\tilde{g}}{\pi^3}\ln^2\left(\frac{\tilde{g}}{16}\right) + \frac{6\tilde{g}}{16\pi^2}\left[15 + \ln\left(\frac{\tilde{g}}{16}\right)\right]$$

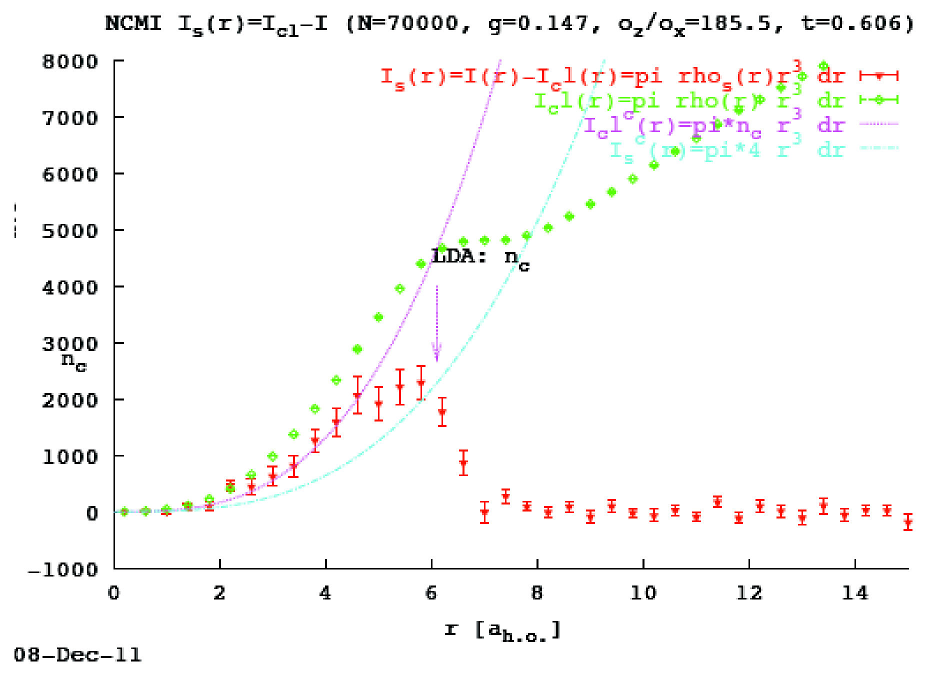
M. H., M. Chevallier, W. Krauth, Phys. Rev. A 81, 043622 (2010)

Local superfluid density: QMC

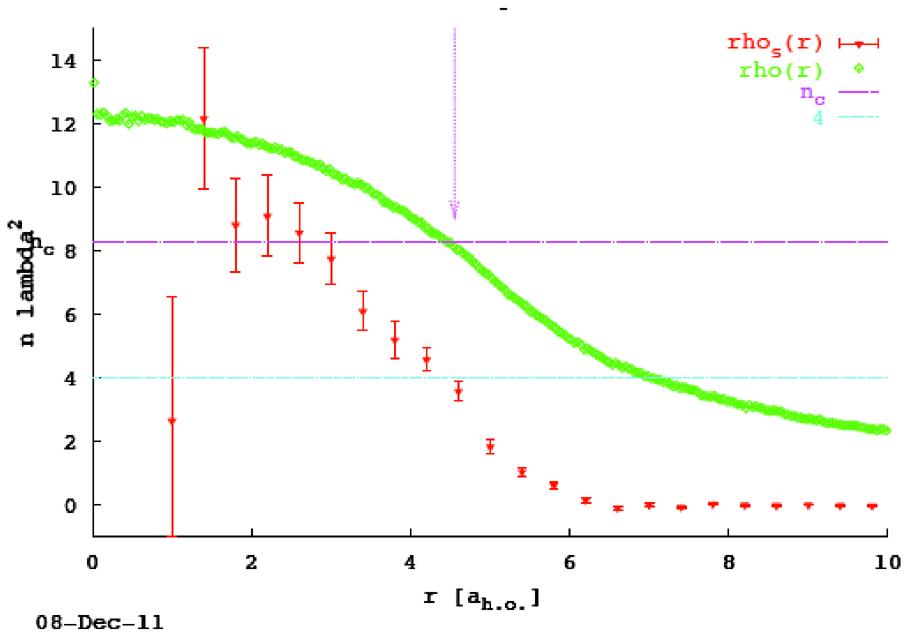
«local» moment of inertia I(r)
from linear response to local field coupled to momentum density

classical «local» moment of intertia $I_{cl}(r)$ from local total density

non-classical «local» moment of intertia $I_{ncmi}(r)=I_{cl}(r)-I(r)$

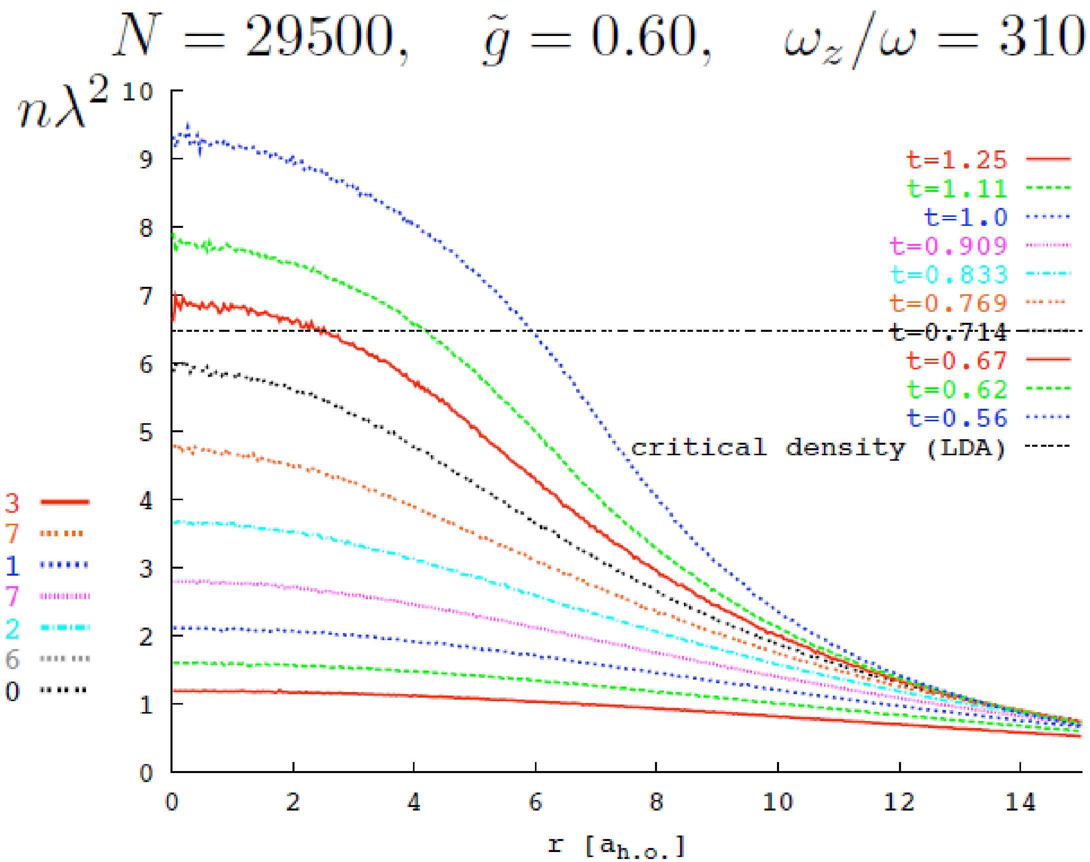


«local» superfluid density
from $I_{ncmi}(r)= n_s(r)\ r^2$

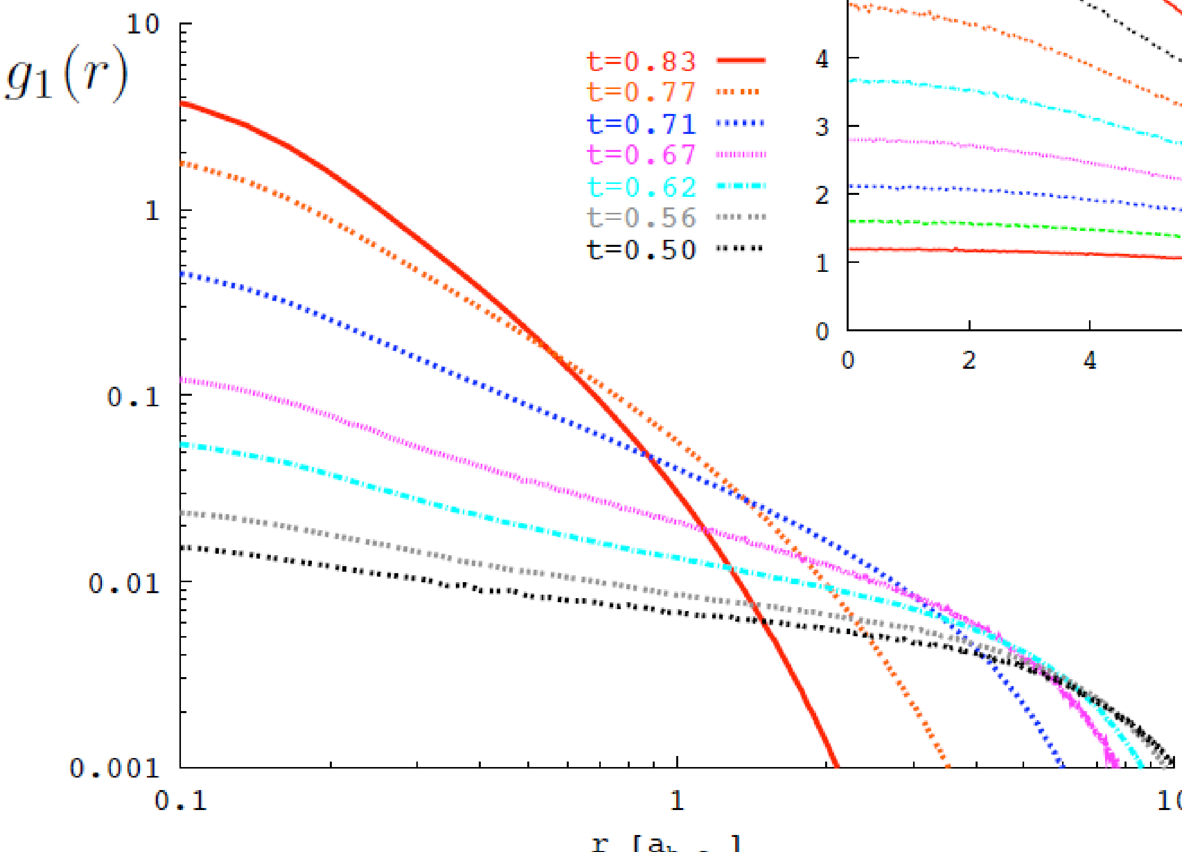


Kosterlitz-Thouless: algebraic order

- density profile: T_{KT} from phase space density + LDA



- one-body coherence (trap averaged)



Algebraic Decay of correlations?

Experimental Measurements:

P.A. Murphy, I. Boettcher, L. Bayha, M.H., D. Kedar, M. Neidig, M.G. Ries A.N. Wenz, G. Zürn, S. Jochim, Phys. Rev. Lett. 115, 010401 (2015).

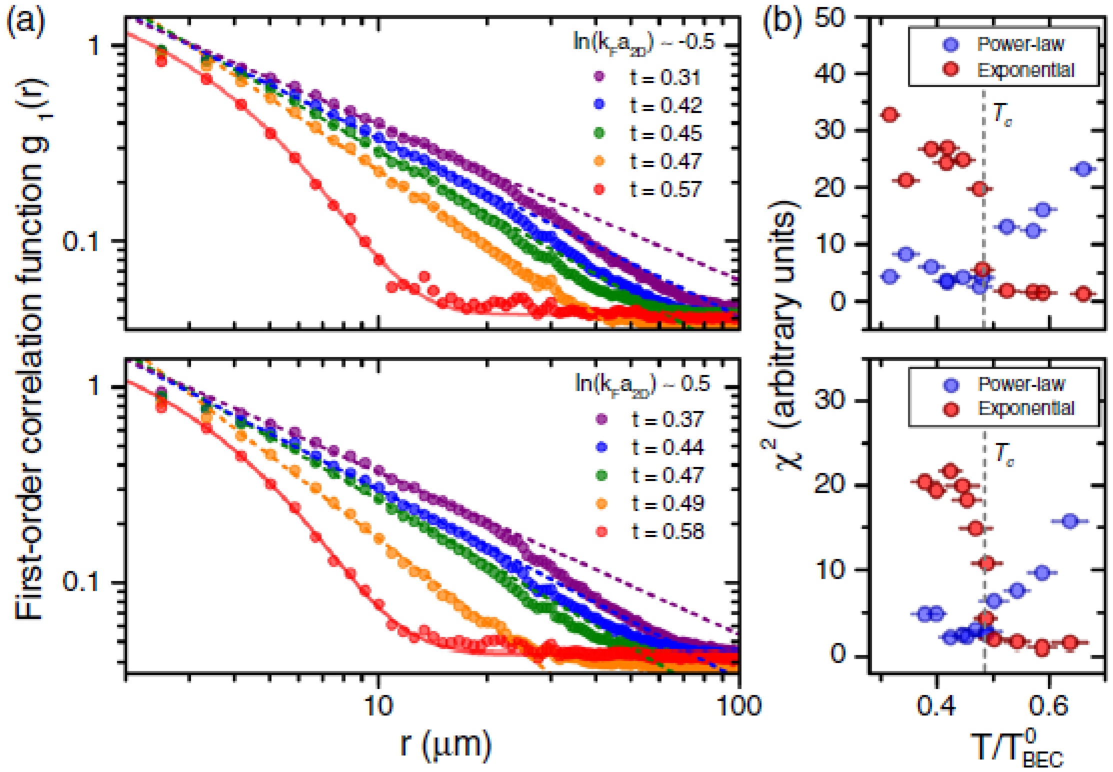
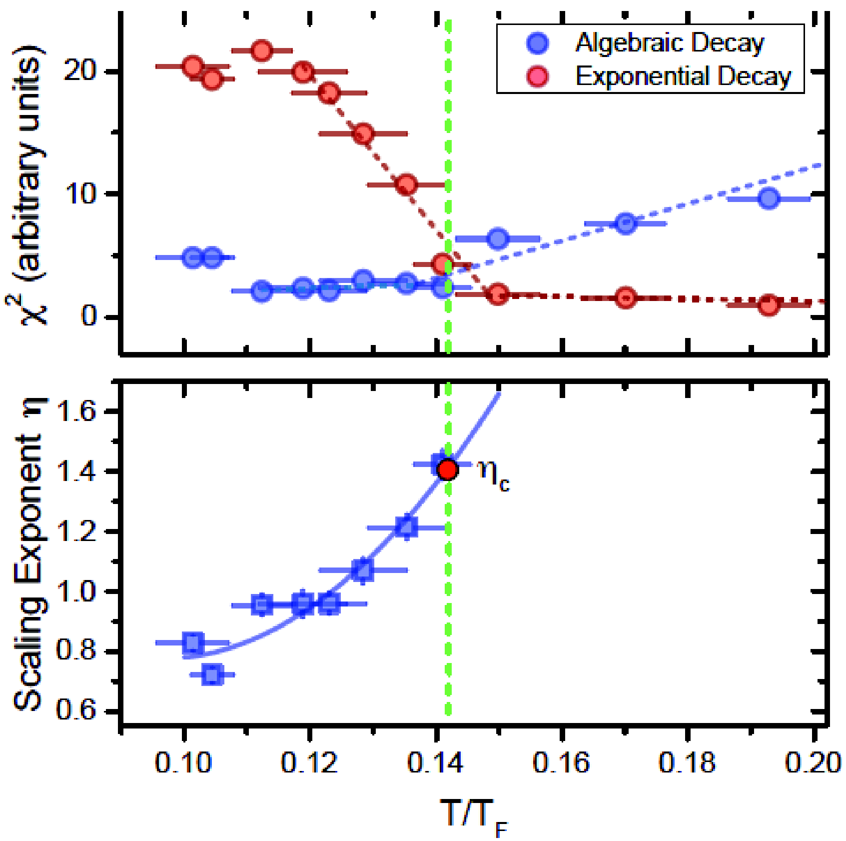


FIG. 1 (color online). First-order correlation function $g_1(r)$ for different temperatures at $\ln(k_F a_{2D}) \simeq -0.5$ (upper left panel) and $\ln(k_F a_{2D}) \simeq 0.5$ (lower left panel). The temperature scale used here is $t = T/T^0_{BEC}$. (a) At high temperatures, correlations decay exponentially as expected for a gas in the normal phase. At low temperatures, we observe algebraic correlations $[g_1(r) \propto r^{-\eta(T)}]$ with a temperature-dependent scaling exponent $\eta(T)$. (b) This qualitative change of behavior is clearly visible in the χ^2 for both exponential and algebraic fits (right panel), where a small value signals a good fit. In particular, this allows for an accurate determination of the transition temperature T_c (vertical dashed lines) [31].

Algebraic decay in trap

P.A. Murthy, I. Boettcher, L. Bayha, M.H., D. Kedar, M. Neidig, M.G. Ries, A.N. Wenz, G. Zürn, S. Jochim,
Phys. Rev. Lett. 115, 010401 (2015).



apparent exponent of algebraic decay in trap

$$\eta_c(trap) \simeq 1.4 \gg 1/4$$

analytical description based on phase fluctuations (spin-wave approximation):

I. Boettcher, M.H.,
Phys. Rev. A 94, 011602(R) (2016).

From Bosons to Fermions

experiment:

Universal behavior at the transition

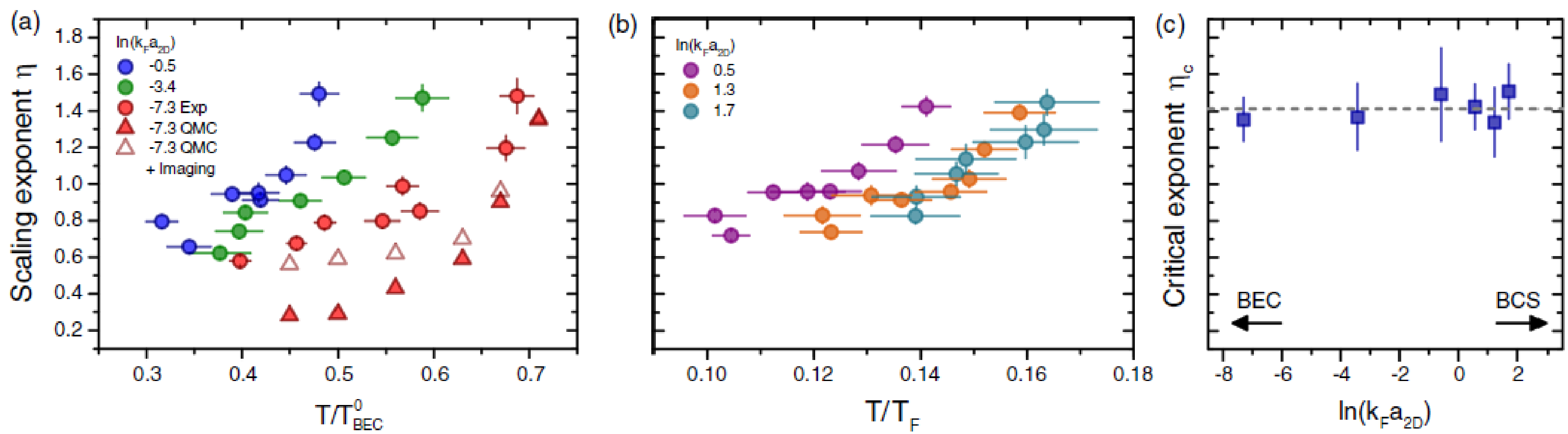


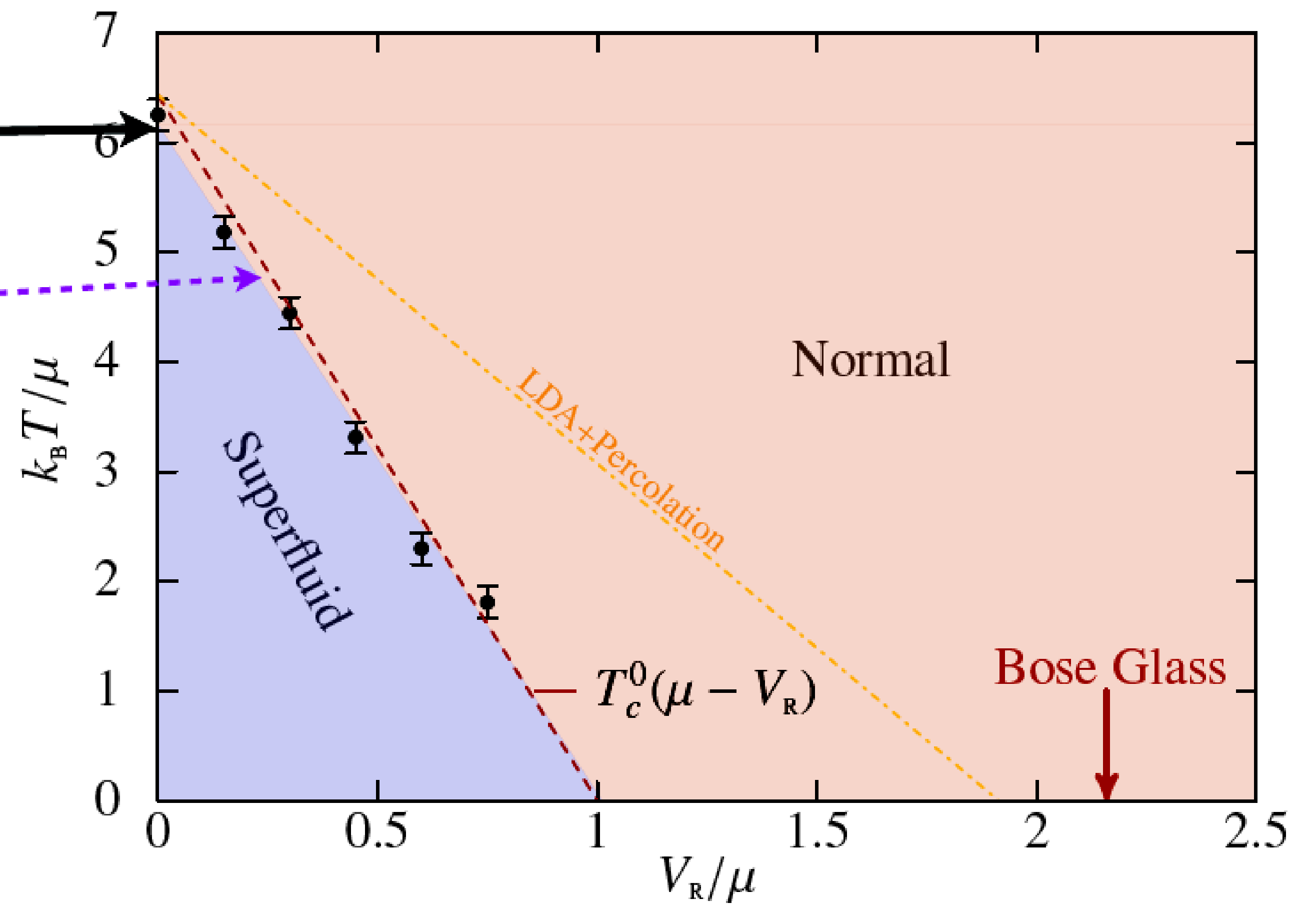
FIG. 2 (color online). Power-law scaling exponents across the two-dimensional BEC-BCS crossover. The temperature-dependent scaling exponent $\eta(T)$ in (a) the bosonic limit and (b) the crossover regime is shown. The relevant temperature scales in these cases are given by T^0_{BEC} and T_F, respectively. The crossover parameter $\ln(k_F a_{2\mathrm{D}})$ is mildly temperature dependent. For reference, we display the value at the critical temperature. For $\tilde{g} = 0.60$ [$\ln(k_F a_{2\mathrm{D}}) \simeq -7.3$], we show the prediction from QMC calculations for a Bose gas (filled red triangles) and an estimate of the effect of the finite imaging resolution present in the measured data (open red triangles) [31]. We find an exponent which increases with temperature in agreement with the BKT theory. The power-law decay eventually ceases at T_c, where a maximal exponent η_c is reached. (c) The value of η_c is approximately constant for all $\ln(k_F a_{2\mathrm{D}})$ where we have previously observed condensation of pairs [24]. This strongly suggests that the associated phase transitions are within one universality class.

Dirty Bosons in two dimensions: Phase diagram

Phase diagram as a function of temperature T and disorder amplitude V_R

$2m\sigma^2\mu=5$ fixed

$T_c^0(\mu)$



Kosterlitz-Thouless universality class

(different from Percolation transition!)

$$T_c(V_R) \approx T_c^0(V_R - \mu)$$

renormalization of μ compared to clean system

Berezinskii-Kosterlitz-Thouless cross-over in a trapped exciton gas (GaAs)

S. Dang, R. Anankine, C. Gomez, A. Lemaître, M. H., F. Dubin, Phys. Rev. Lett. 122, 17402 (2019)

GaAs Bilayer excitons:

- Low mass $M_X \approx 0.22\ m_{electron}$ T=340mK...2K
- 4 almost degenerate states (dark & bright excitons)
- Dipolar interaction => large effective coupling g=3...7