Kosterlitz–Thouless transition in the quasi-two-dimensional Bose gas

Werner Krauth

Laboratoire de Physique Statistique
Ecole Normale Supérieure, Paris, France

Numerical approaches to Quantum Many-Body systems,
UCLA, 30 January 2009

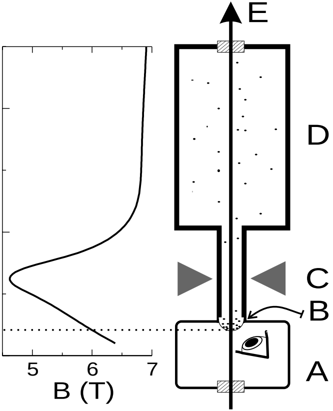
References

- M. Holzmann, W. Krauth "Kosterlitz–Thouless transition of the quasi two-dimensional trapped Bose gas" *PRL*, 2008
- M. Holzmann, M. Chevallier, W. Krauth "Semiclassical theory of the quasi two-dimensional trapped Bose gas" *EPL*, 2008

Early quest for BEC

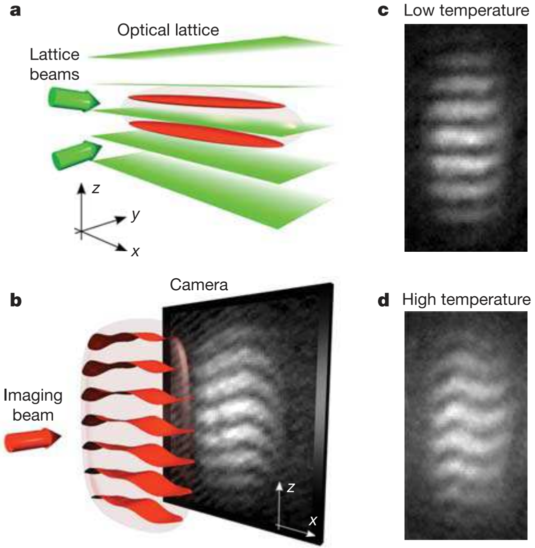
Efforts to make a dilute BEC in an atomic gas were sparked by a 1976 paper by Stwalley and Nosanow [8]. They argued that spin-polarized hydrogen had no bound states and hence would remain a gas down to zero temperature, and so it would be a good candidate for BEC. This stimulated a number of experimental groups [9–12] in the late 70s and early 80s to begin pursuing this

Early set-up of 2*d* BEC experiment

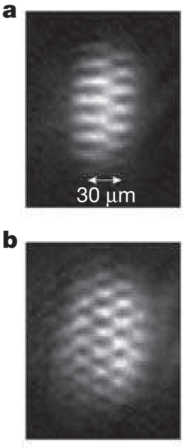


- Mosk et al (PRL, 1998)
- Quasi condensation reached by Safonov et al (PRL, 1998)

2*d* BEC experiment by Hadzibabic et al (Nature 2006)

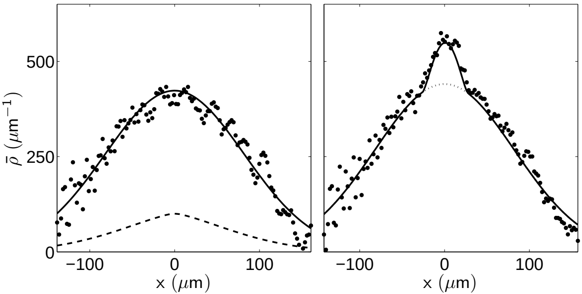


Direct imaging of vortices



- Hadzibabic et al, Nature (2006),

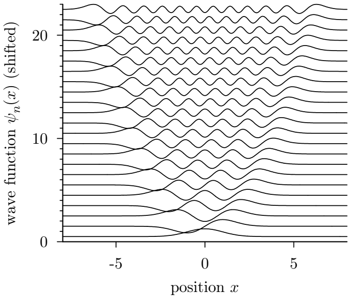
Density plots



- Krueger et al, PRL (2007),

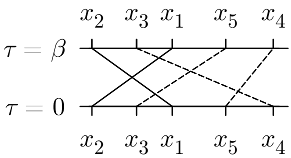
Two descriptions of Bosons...

I) Energy levels



- BEC $\equiv$ saturation . . .

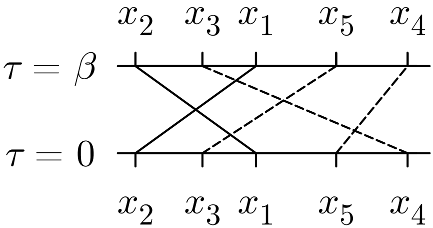
II) Density Matrices



- BEC $\equiv$ long cycles . . .

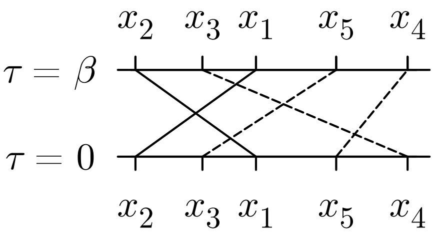
Quantum Monte Carlo I (free particle)

$$Z(\{x_1,\dots,x_N\}) =$$
$$\frac{1}{N!}\sum_P \int dx_1\,,\dots,dx_N\;\rho^{\text{free}}(\{x_1,\dots,x_N\};\{x_{P_1},\dots,x_{P_N}\};\beta)$$



- this is last week's 44-line program (see www.smac.lps.ens.fr)

Quantum Monte Carlo II (interacting bosons)



- Analytical reweighting of (free-particle) paths
- This is the perfect action approach.

Ideal 2*d* Bosons

- number dN of particles per phase-space element dk_xdk_ydxdy

$$\mathrm{d}N = \frac{1}{(2\pi)^2} \frac{\mathrm{d}k_x \mathrm{d}k_y \mathrm{d}x \mathrm{d}y}{\exp\left[\beta(\frac{\hbar^2 k^2}{2m} + v(r) - \mu)\right] - 1},$$

- ... yields

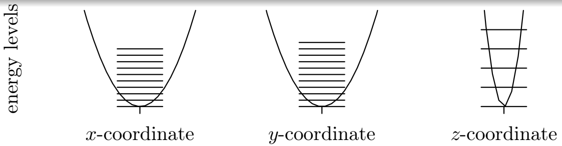
$$n(r) = -\frac{1}{\lambda^2} \ln\{1 - \exp\left[\beta(\mu - v(r))\right]\},$$

- ... and ...

$$N = -\frac{\pi}{\lambda^2} \sum_{\nu=0}^{\infty} \int_0^{\infty} \mathrm{d}(r^2) \ln\left[1 - e^{\beta(\mu - m\omega^2 r^2/2)}\right]$$

$$= \frac{T^2}{\hbar^2 \omega^2} F_2(-\mu\beta),$$

Quasi-two-dimensional gas (scaling with N)



- quasi-two-dimensional trap ...

$$\omega = \omega_x = \omega_y \ll \omega_z$$

- ... at temperatures comparable to the z-level spacing ...

$$T \simeq \hbar\omega_z$$

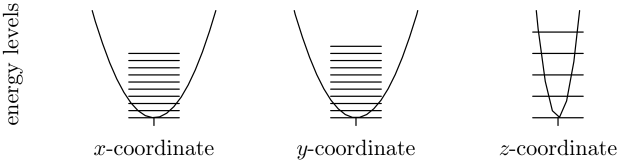
- ... and to the *2D* Bose–Einstein transition temperature

$$T \simeq T_{\text{BEC}}^{\text{2d}} = \frac{\sqrt{6N}\hbar\omega}{\pi}$$

- leads to:

$$\omega_z/\omega \propto \sqrt{N}$$

Quasi-two-dimensional gas (scaling of a_0)



- Life (QMC, experiment) is 3D, coupling constant

$$g_{3d} = 4\pi\hbar^2 a_0/m$$

- …integrating out the z-direction

$$g_{2d} = 4\pi\hbar^2 a_0/m \int \mathrm{d}z\,[\rho(z,z)]^2$$

- …supposing harmonic groundstate in z

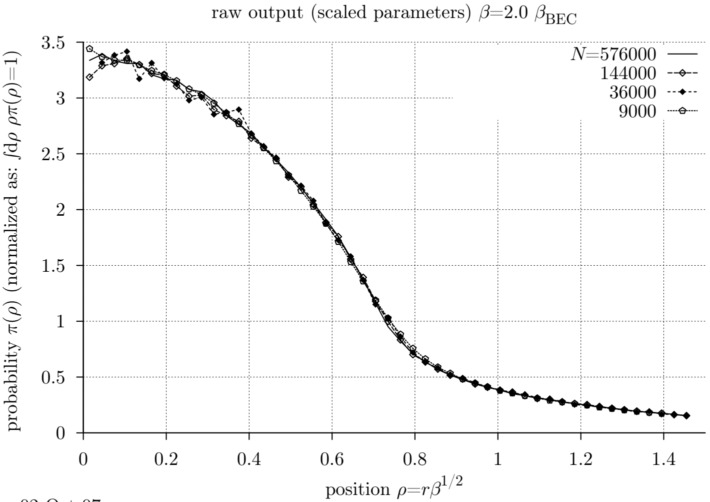
$$g_{2d} \simeq \tilde{g} = a_0\sqrt{8\pi\omega_z\hbar^3/m}$$

- leads to:

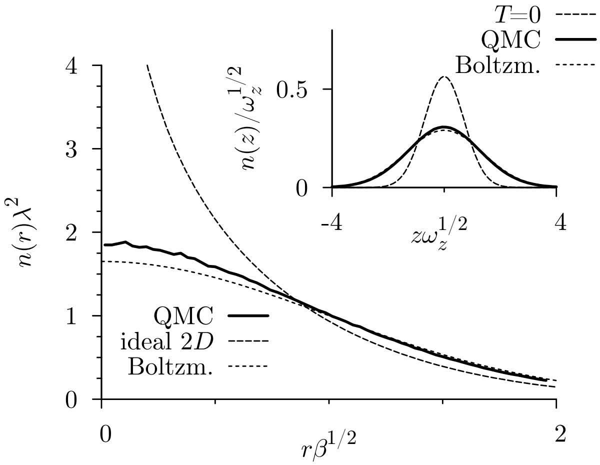
$$a_0(N) \propto 1/\sqrt{\omega_z} \propto 1/N^{1/4}$$

First check ...

- Initial simulation, with $\omega_z \propto \sqrt{N}$ and $a_0 \propto 1/N^{1/4}$
- experimental $\hbar\omega_z/T_{\text{BEC}}^{\text{2d}} = 0.55$ and $m\tilde{g}/\hbar^2 = 0.13$



Density profile at $T = T_{\text{BEC}}^{\text{2d}}$



- let's do the non-interacting case first.

Semiclassical theory I (no interaction)

- number dN of particles per element dk_xdk_ydxdy in the z-energy level ν

$$\mathrm{d}N = \frac{1}{(2\pi)^2} \frac{\mathrm{d}k_x \mathrm{d}k_y \mathrm{d}x \mathrm{d}y}{\exp\left[\beta(\frac{\hbar^2 k^2}{2m} + v(r) + \nu\hbar\omega_z - \mu)\right] - 1},$$

- ... yields density $n[v(r)] = n(r)$

$$n(r) = -\frac{1}{\lambda^2} \sum_{\nu=0}^{\infty} \ln\{1 - \exp\left[\beta(\mu - v(r) - \nu\hbar\omega_z)\right]\},$$

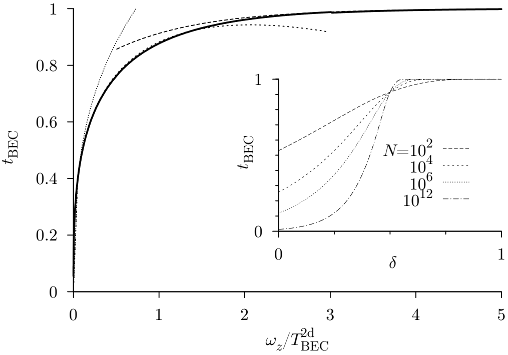
- ... and also $N(\mu, \omega_z)$ if potential $v(r) = m\omega^2 r^2/2$

$$N = -\frac{\pi}{\lambda^2} \sum_{\nu=0}^{\infty} \int_0^{\infty} \mathrm{d}(r^2) \ln\left[1 - e^{\beta(\mu - \nu\hbar\omega_z - m\omega^2 r^2/2)}\right]$$

$$= \frac{T^2}{\hbar^2\omega^2} \sum_{\nu=0}^{\infty} F_2(-\mu\beta + \nu\beta\hbar\omega_z),$$

T_c for the ideal quasi-2D trapped Bose gas

- Critical temperature $t = T^{\text{q2d}}_{\text{BEC}} / T^{\text{2d}}_{\text{BEC}}$ vs. $\tilde{\omega}_z = \omega_z / T^{\text{2d}}_{\text{BEC}}$ at chemical potential $\tilde{\mu} = \beta\mu = 0$:



- Critical temperature $t_{\text{BEC}} = 0.78$ for $\tilde{\omega}_z = 0.55$ (experimental value).

Semiclassical theory II (contact interaction)

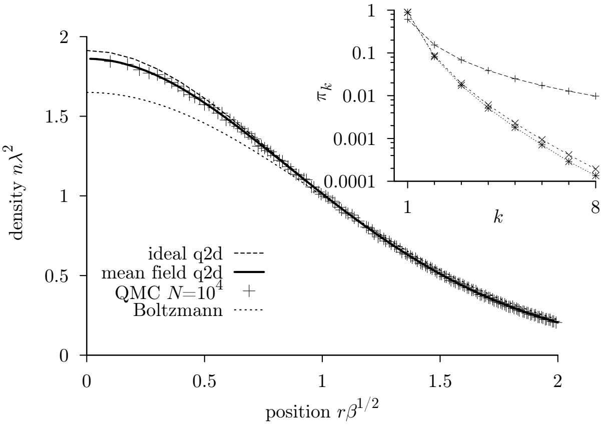
- introduce contact interaction

$$v(r) = m\omega^2 r^2/2 + 2g[n(r) - n(0)].$$

- yields total density

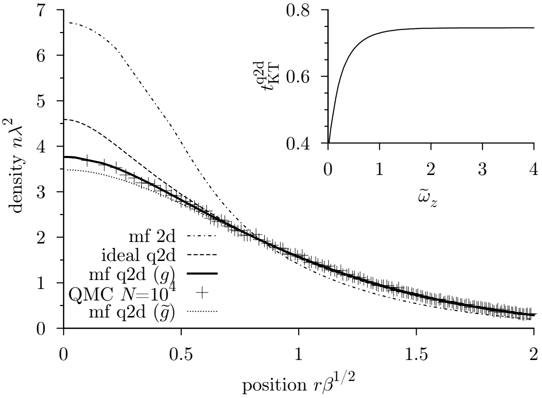
$$N = \pi \int_0^\infty \mathrm{d}(r^2)\, n(r) = \pi \int_0^\infty \mathrm{d}v \,\left[\frac{\partial(r^2)}{\partial v}\right] n(v)$$
$$= \cdots =$$
$$= \frac{T^2}{\hbar^2\omega^2}\left(\sum_{\nu=0}^{\infty} F_2(-\tilde{\mu} + \nu\beta\hbar\omega_z) + \frac{mg}{2\pi\hbar^2}\left[n(0)\lambda^2\right]^2\right),$$

density profile at $T = T_{\text{BEC}}^{\text{2d}}$ (exp. parameters)



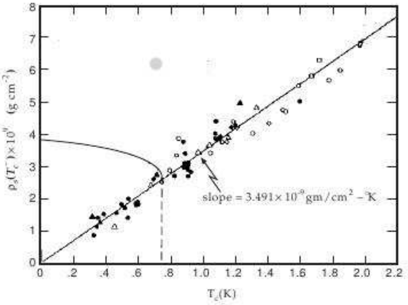
- excellent agreement of semiclassical theory with QMC.
- interaction g (not $\tilde{g}$), contact term $2g$.

density profile at $T = 0.8 T_{\text{BEC}}^{\text{2d}}$ (exp. parameters)



- central density much higher than at $T = T_{\text{BEC}}^{\text{2d}}$
- no phase transition within semiclassical theory.

Universal jump of ρ_s (Nelson, Kosterlitz)



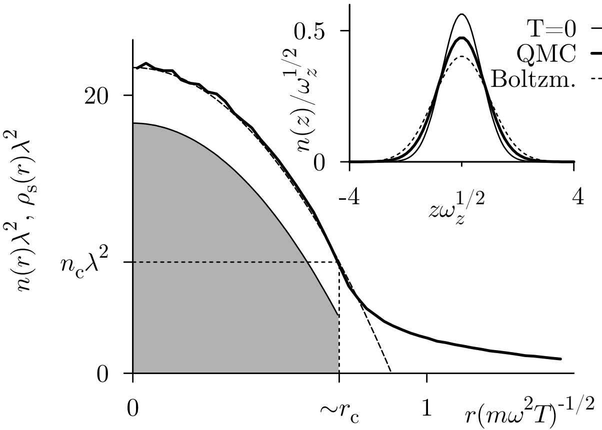
- Universal jump of superfluid density

$$\Delta\rho_s = \frac{2mT}{\pi\hbar^2}$$

- leads in our case to a jump of superfluid density

$$\frac{\Delta\rho_s}{n(r_c)} = \frac{2mT\lambda^2}{8\pi\hbar^2} \simeq \frac{1}{2}$$

Density profile at $T/T_{\mathrm{BEC}}^{2d} = 0.5$



- density for $r < r_c$: Thomas–Fermi profile
- superfluid density for $r < r_c$: again Thomas–Fermi
- interaction g from QMC, or $g \simeq \tilde{g}\sqrt{\tanh[\tilde{\omega}_z/(2t)]}$

Thomas–Fermi approximation

The Thomas–Fermi approximation neglects the kinetic energy in the Gross-Pitaevski equation ...

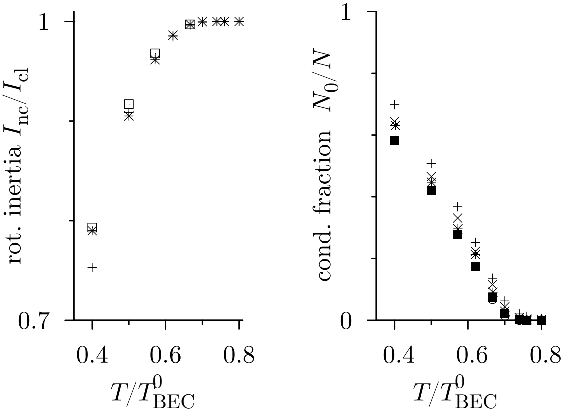
$$\mu\Psi(r) = \left[-\cancel{\frac{\hbar^2}{2m}\nabla^2} + V(r) + g|\Psi(r)|^2\right]\Psi(r)$$

... which leads to ...

$$n(r) = n(0) - \frac{1}{2}\frac{m\omega^2 r^2}{g}$$

- we must use the correct interaction g from QMC, or $g \simeq \tilde{g}\sqrt{\tanh[\tilde{\omega}_z/(2t)]}$.

Moment of inertia – condensate fraction



- moment of inertia I_{nc} from QMC, agrees excellently with ansatz □
- condensate fraction from QMC (separate calculation), finite-size behavior compatible with $N_0/N \sim N^{-\eta(T)/2}$, with $\eta(T_c) = 1/4$.

Conclusion

- Quasi-two-dimensional regime for Bose gas.
- Semi-classical description is fun, and so is QMC.
- Close relation with experiments.