

Bose-Einstein condensation

- Ideal Bose gas
- Weakly interacting homogenous Bose gas
- Inhomogeneous Bose gas
- Superfluid hydrodynamics

Ideal BEC

See thermodynamics textbooks

To remember:

- (1) Whether BEC occurs or not depends on density of states:
Power law, depends on dimension and confinement
- (2) Even for interacting BEC, normal component is described as
ideal gas
 T_c
Condensate fraction

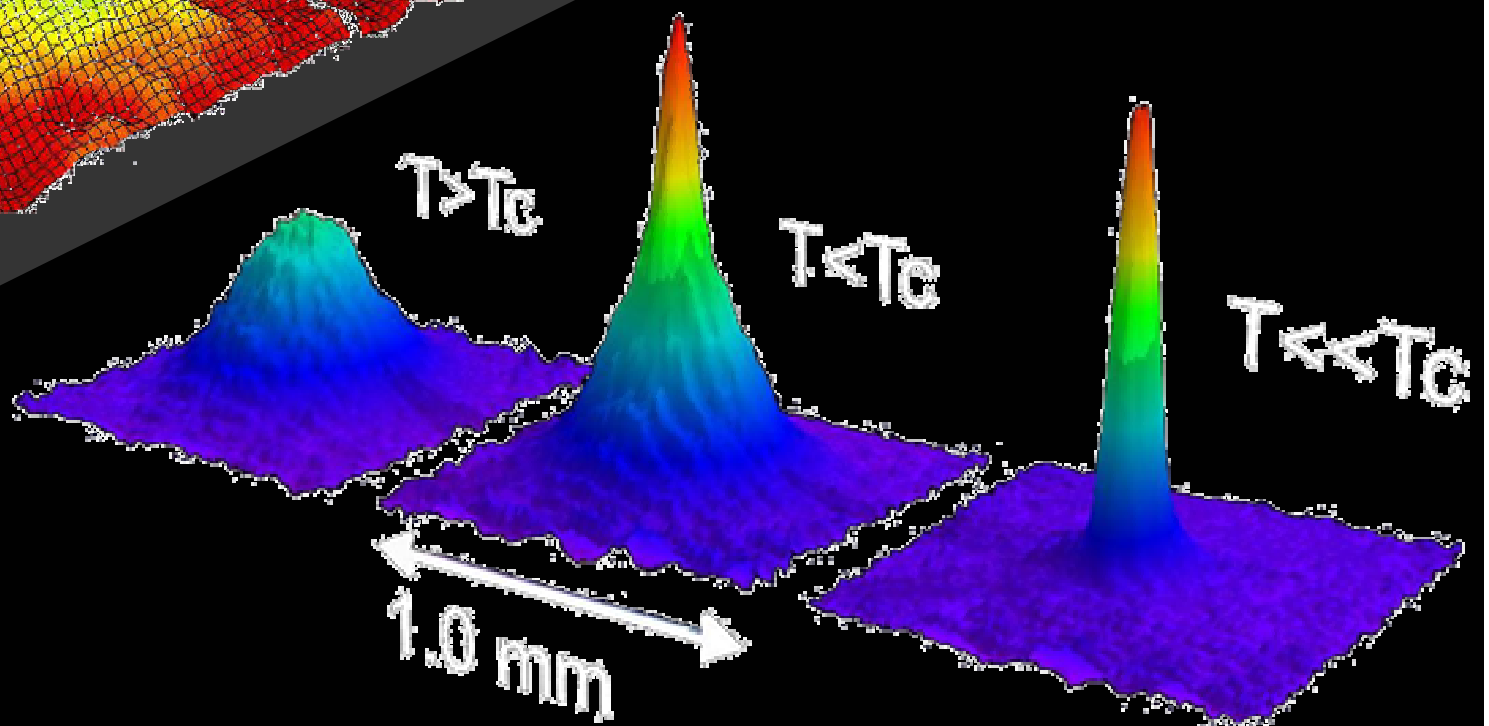
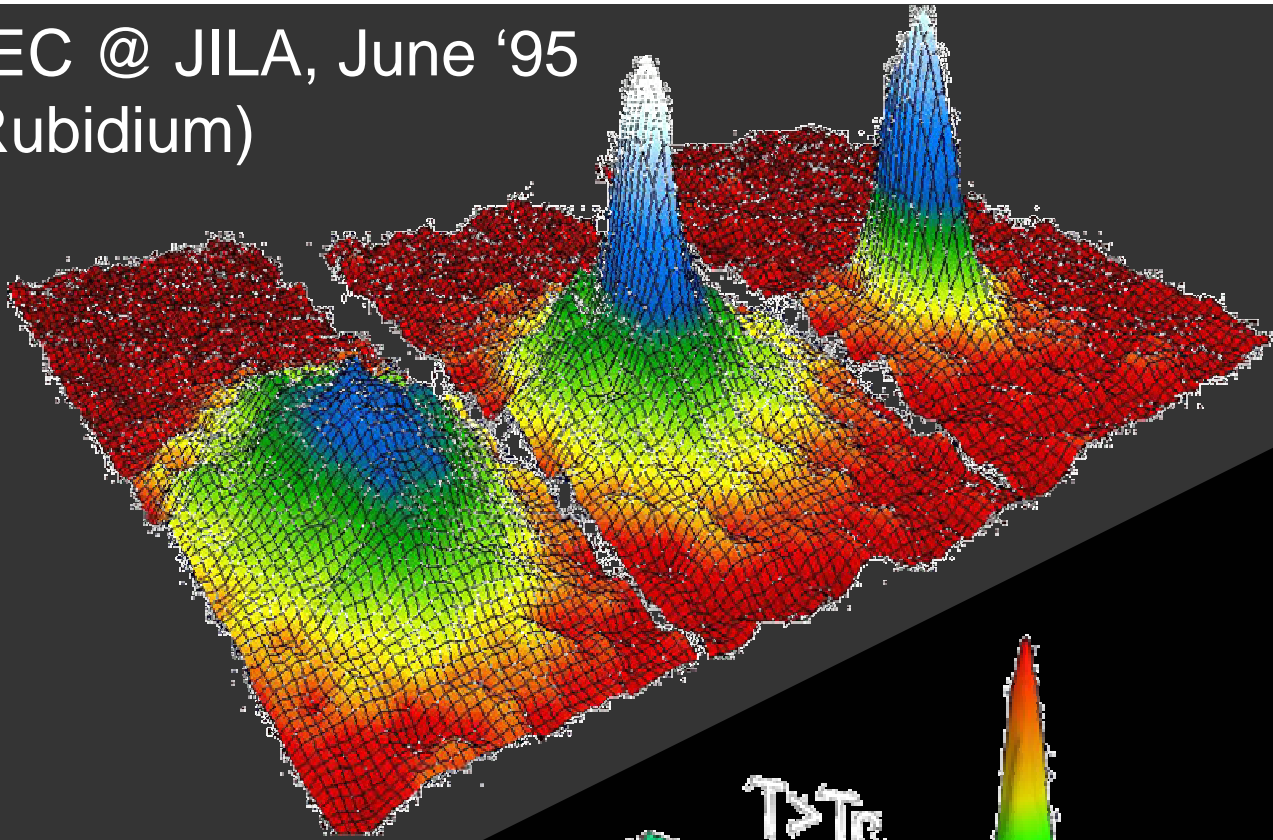
The shadow of a cloud of bosons
as the temperature is decreased

(Ballistic expansion for a fixed time-of-flight)

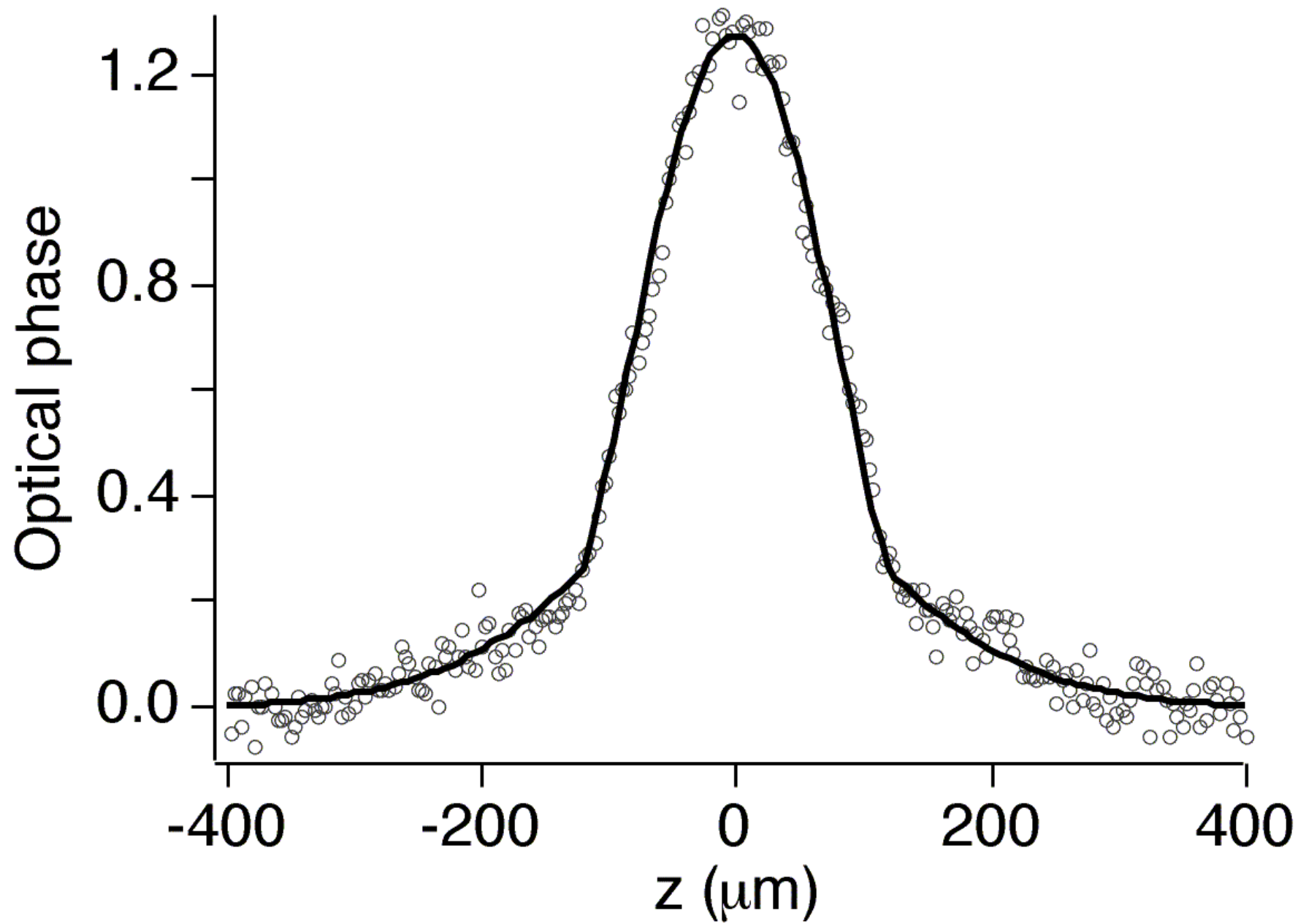


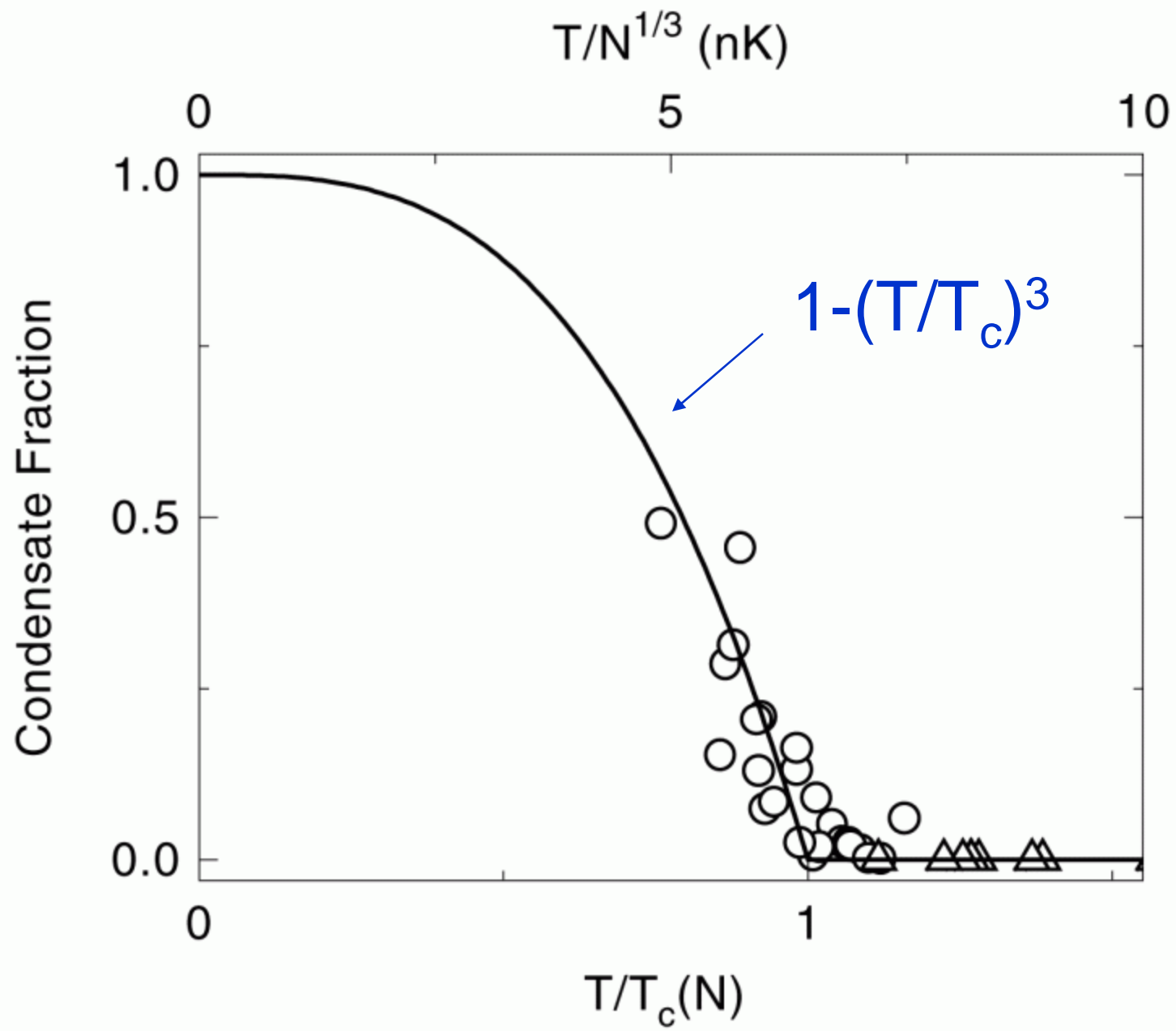
Temperature is linearly related to the rf frequency
which controls the evaporation

BEC @ JILA, June '95
(Rubidium)



BEC @ MIT, Sept. '95 (Sodium)





Homogeneous BEC

Weakly interacting Bose gas at $T=0$

6

$$\hat{H}_I = \frac{1}{2V} \sum u_q a_{p+q}^\dagger a_{k-q}^\dagger a_k a_p$$

$$\left[u_q = u_0 \Rightarrow u(r) = u_0 \delta(r) \right]$$

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$$\left[U_q = U_0 \Rightarrow U(r) = U_0 \delta(r) \right]$$

$$U_0 = \frac{4\pi \hbar^2}{m} a$$

a scattering length

$$a = \lim_{k \rightarrow 0} \left(-\frac{\delta_0}{k} \right) = -4$$

$$\hat{H}_I = \frac{4\pi a \hbar^2}{m} \sum_{i < j} \delta(\tau_i - \tau_j) \cdot \underbrace{\frac{\partial}{\partial \tau_{ij}} r_{ij}}_{=1 \text{ in first order perturbation theory}}$$

$= 1$ in first order perturbation theory

Homogeneous interacting gas

$$H = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} + \frac{u_0}{2V} \sum_{\mathbf{k}, \mathbf{k}', \mathbf{q}} a_{\mathbf{k}+\mathbf{q}}^{\dagger} a_{\mathbf{k}'-\mathbf{q}}^{\dagger} a_{\mathbf{k}'} a_{\mathbf{k}}$$

BEC in $\mathbf{k}=0$ state

$$a_0^{\dagger} |N_0\rangle = \sqrt{N_0+1} |N_0+1\rangle$$

$$a_0 |N_0\rangle = \sqrt{N_0} |N_0-1\rangle$$

$$N_0 \text{ (large)} \quad N_0 \approx N_0 + 1,$$

$$a_0 = a_0^{\dagger} = \sqrt{N_0} \\ \text{(Bogoliubov)}$$

Homogeneous interacting gas

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N_0 (large) $N_0 \approx N_0+1$, $a_0 = a_0^{\dagger} = \sqrt{N_0}$
(Bogoliubov)

$$H = \frac{U_0 N_0^2}{2V} + \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} + \frac{U_0 N_0}{2V} \sum_{\mathbf{k} \neq 0} a_{\mathbf{k}}^{\dagger} a_{-\mathbf{k}}^{\dagger} + a_{\mathbf{k}} a_{-\mathbf{k}} + 2 a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} + 2 a_{-\mathbf{k}}^{\dagger} a_{-\mathbf{k}}$$

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Introduce $N = N_0 + \frac{1}{2} \sum_{\mathbf{k} \neq 0} a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} + a_{-\mathbf{k}}^{\dagger} a_{-\mathbf{k}}$

$$H = \frac{U_0 N^2}{2V} + \frac{1}{2} \sum_{k \neq 0} \left(\epsilon_k + \frac{NU_0}{V} \right) (a_k^\dagger a_k + a_{-k}^\dagger a_{-k}) + \frac{NU_0}{V} (a_k^\dagger a_{-k}^\dagger + a_k a_{-k})$$

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Structure of H :

With $a = a_k, b = a_{-k}$

H has only terms of $\mathcal{H} = \epsilon_0 (a^\dagger a + b^\dagger b) + \epsilon_1 (a^\dagger b^\dagger + b a)$
with $[a, a^\dagger] = [b, b^\dagger] = 1$

$$H = \frac{u_0 N^2}{2v} + \frac{1}{2} \sum_{k \neq 0} \left(\epsilon_k + \frac{N u_0}{v} \right) (a_k^\dagger a_k + a_{-k}^\dagger a_{-k}) + \frac{N u_0}{v} (a_k^\dagger a_{-k}^\dagger + a_k a_{-k})$$

Structure of H :

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H has only terms of $\mathcal{H} = E_0 (a^\dagger a + b^\dagger b) + E_1 (a^\dagger b^\dagger + b a)$
with $[a, a^\dagger] = [b, b^\dagger] = 1$

bilinear expression solved by Bogoliubov transformation

$$a = u \alpha - v \beta^\dagger \quad b = u \beta - v \alpha^\dagger$$

$u^2 - v^2 = 1$ ensures $[\alpha, \alpha^\dagger] = [\beta, \beta^\dagger] = 1$

Canonical transformation

$$H = \frac{u_0 N^2}{2v} + \frac{1}{2} \sum_{k \neq 0} \left(\epsilon_k + \frac{N u_0}{v} \right) (a_k^\dagger a_k + a_{-k}^\dagger a_{-k}) + \frac{N u_0}{v} (a_k^\dagger a_{-k}^\dagger + a_k a_{-k})$$

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Canonical transformation

$$\mathcal{H} = () + () (\alpha^\dagger \alpha + \beta^\dagger \beta) + () (\alpha \beta + \beta^\dagger \alpha^\dagger)$$

for choice of $u, v = 0 \leftarrow$

$$H = \lambda (\alpha^\dagger \alpha + \beta^\dagger \beta) + \text{Const}$$

H_0 with quanta created by $\alpha^\dagger, \beta^\dagger$

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Elementary excitations

$$H = \sum_{\mathbf{k}} E_{\mathbf{k}} a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + \text{Const}$$

$$E_{\mathbf{k}} = \sqrt{\epsilon_{\mathbf{k}}^2 + 2 \epsilon_{\mathbf{k}} N u_0 / V}$$

$$H = \lambda (\alpha^\dagger \alpha + \beta^\dagger \beta) + \text{Const}$$

H_0 with quanta created by $\alpha^\dagger, \beta^\dagger$

Elementary excitations

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$$c = \sqrt{U_0 N / V m}$$

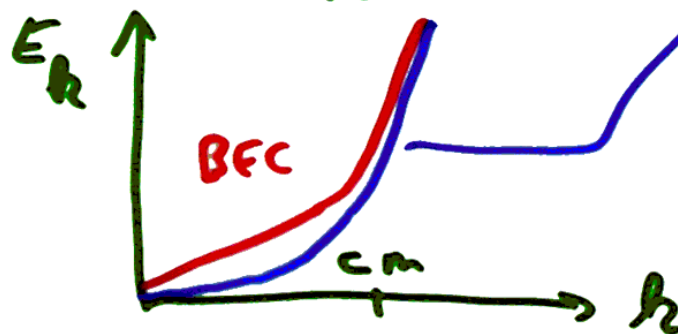
Speed of sound

$$E_{\mathbf{k}} = \sqrt{\left(\frac{\hbar^2 k^2}{2m}\right)^2 + (\hbar c k)^2}$$

$$= \begin{cases} \hbar c k & k \rightarrow 0 \\ \hbar^2 k^2 / 2m & k \rightarrow \infty \end{cases}$$

phonon, sound

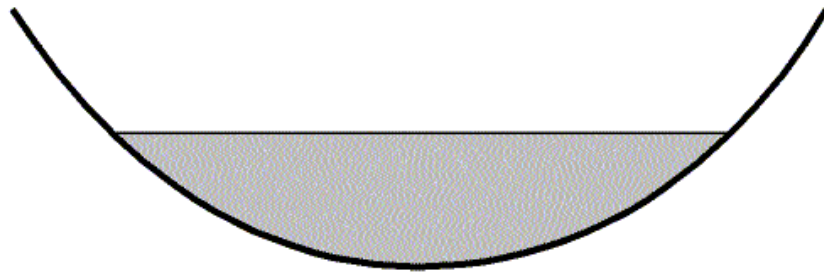
Free particle



Propagation of sound

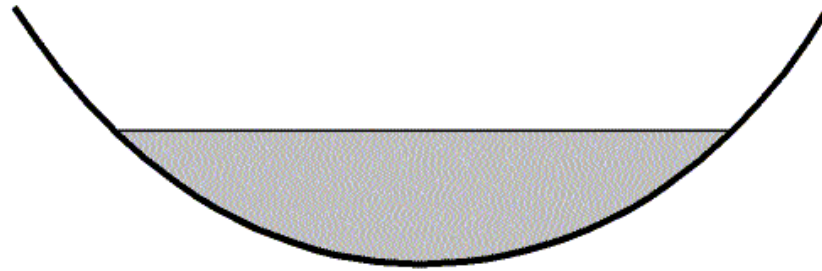
Excitation of sound

$t < 0$

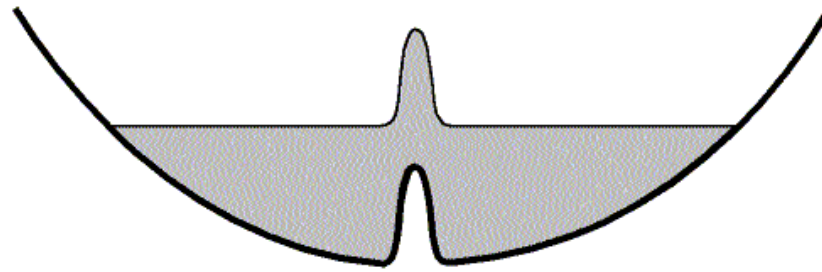


Excitation of sound

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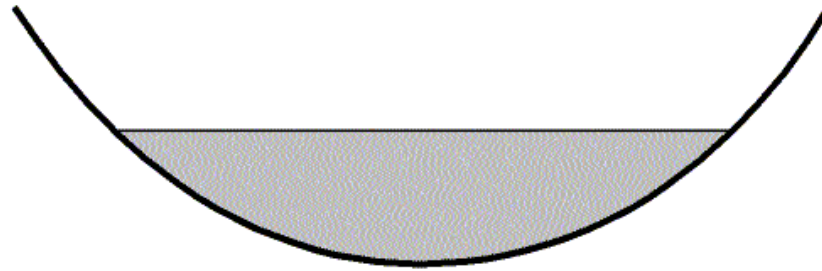


$t = 0$

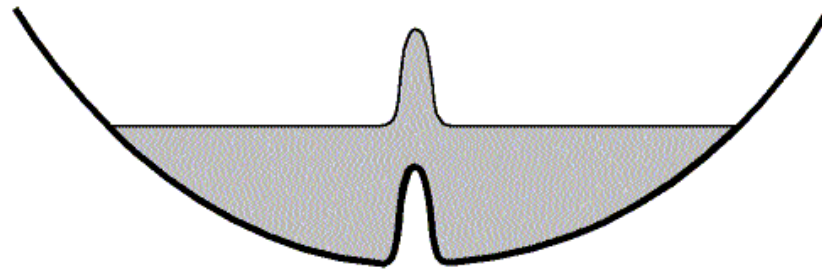


Excitation of sound

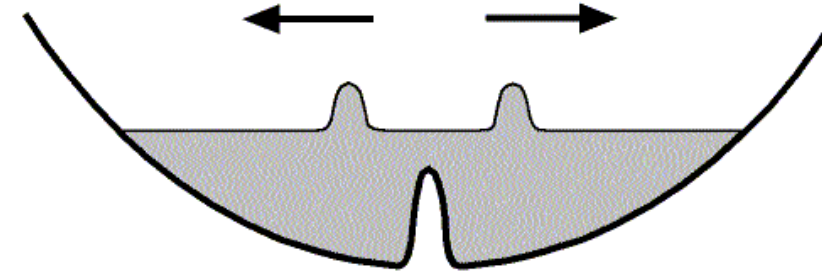
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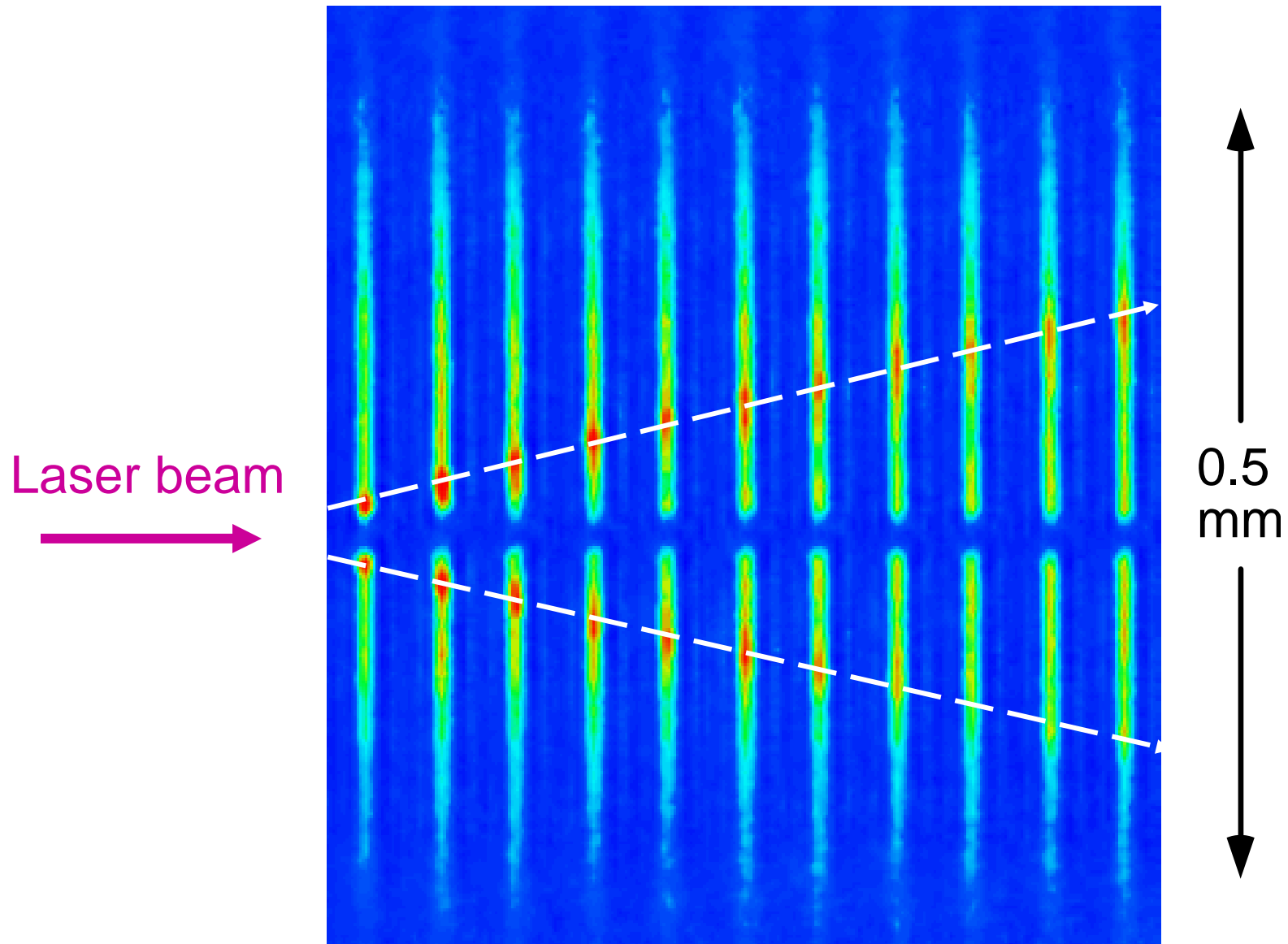
$t = 0$



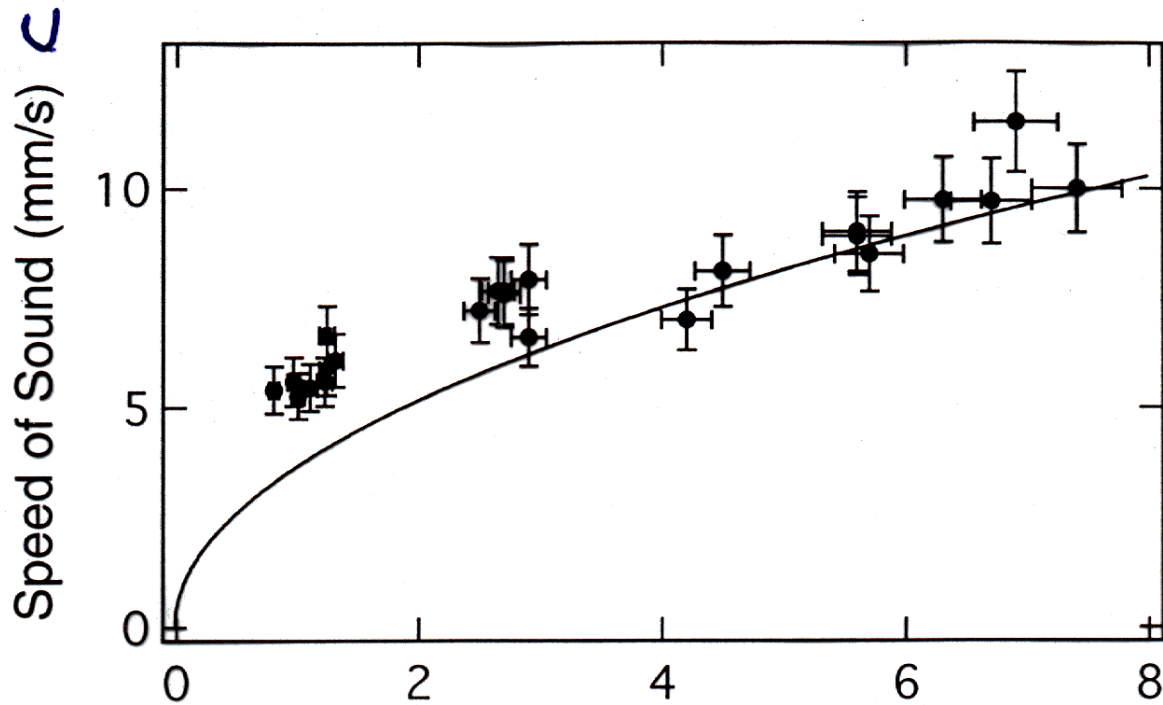
$t > 0$



Sound = propagating density perturbations



1.3 ms per frame



Peak Density (10^{14} cm^{-3}) n_0

$$c = (4\pi \hbar^2 a / m^2)^{1/2} \sqrt{n_0} / \sqrt{2}$$

Bogoliubov 1947

Lee, Huang, Yang 1957

(M. Andrews, D.M. Kurn, H.-J. Miesner, D.S. Durfee, C.G. Townsend, S. Inouye, W.K., PRL 79, 549 (1997))

Bogoliubov solution

→ E_k elementary excitation

Bogoliubov solution

→ $E_{\mathbf{k}}$ elementary excitation

→ ground state energy

$$E_0 = \frac{U_0 n}{2} \left(1 + \frac{128}{15} \sqrt{na^3/\pi} \right)$$

Bogoliubov solution

→ E_k elementary excitation

→ ground state energy

$$E_0 = \frac{U_0 n}{2} \left(1 + \frac{128}{15} \sqrt{na^3/\pi} \right)$$

→ ground state wavefunction

$$\langle n_k \rangle = \frac{v_k^2}{1 - v_k^2}$$

$$\langle n_0 \rangle = N - \sum \langle n_k \rangle = N \left[1 - \frac{8}{3} \sqrt{na^3/\pi} \right]$$

$$| \psi_0 \rangle = (| 0 \rangle)^N + \epsilon$$

Quantum depletion

90% He

1% alkalis

Quantum depletion
or
How to observe the transition from a
quantum gas to a quantum liquid

In 1D: Zürich

K. Xu, Y. Liu, D.E. Miller, J.K. Chin, W. Setiawan, W.K., PRL 96, 180405 (2006).

What is the wavefunction of a condensate?

Ideal gas:

$$\Psi = \left(|q = 0\rangle \right)^N$$

Interacting gas:

$$H' = U_0 \delta(r)$$

$$H' = U_0 \sum a_p^\dagger a_q^\dagger a_r a_s$$

$$H' = U_0 a_0 a_0 \sum a_p^\dagger a_{-p}^\dagger$$

$$\Psi = \left(|q = 0\rangle \right)^N + \alpha \left(|q = 0\rangle \right)^{N-2} |q = p\rangle |q = -p\rangle + \dots$$

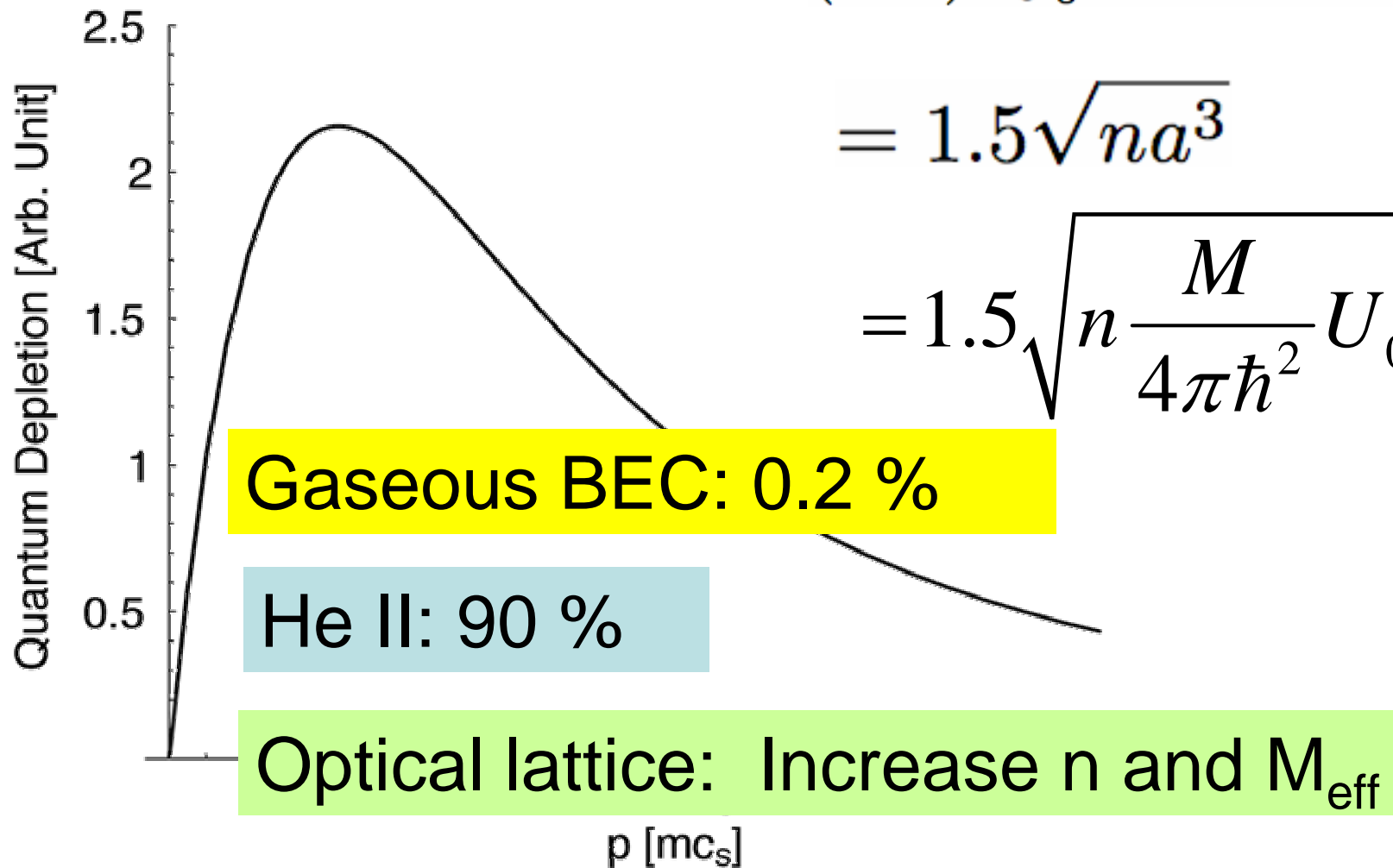
Quantum depletion

Quantum depletion in 3-dimensional free space

$$\frac{V}{(2\pi\hbar)^3} \int_0^\infty v_p^2 (4\pi p^2) dp$$

$$= 1.5\sqrt{na^3}$$

$$= 1.5\sqrt{n \frac{M}{4\pi\hbar^2} U_0}$$



Quantum Depletion

$$v_p^2 = \frac{T(p) + \mu - \sqrt{T^2(p) + 2\mu T(p)}}{2\sqrt{T^2(p) + 2\mu T(p)}}$$

Free space

$$T(p) = \frac{p^2}{2M}$$

$$\mu = \frac{4\pi\hbar^2 a}{M} n = Mc_s^2$$

Lattice

$$4J \sin^2\left(\frac{\lambda_L}{4\hbar} p\right)$$

$$n_0 U$$

J : tunneling rate

U : on-site interaction

As one increases the depth of the optical lattice, the quantum depletion is dramatically increased

Finally, the condensate fraction becomes zero - a quantum phase transition to an insulator is taking place.

Dispersion relation

Elementary excitations

$$H = \sum_{\mathbf{k}} E_{\mathbf{k}} a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} + \text{const}$$

$$E_{\mathbf{k}} = \sqrt{\epsilon_{\mathbf{k}}^2 + 2 \epsilon_{\mathbf{k}} \underbrace{N U_0 / V}_{= c^2 m}}$$

$$c = \sqrt{U_0 N / V m}$$

Speed of sound

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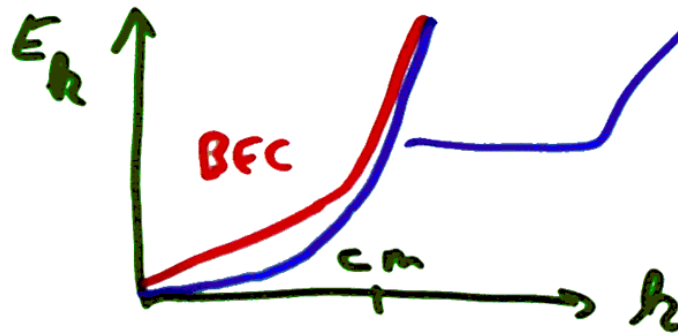
$$= \begin{cases} \hbar c k & \hbar \rightarrow 0 \\ \hbar^2 k^2 / 2m & \hbar \rightarrow \infty \end{cases}$$

$\hbar \rightarrow 0$

phonon, sound

$\hbar \rightarrow \infty$

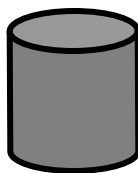
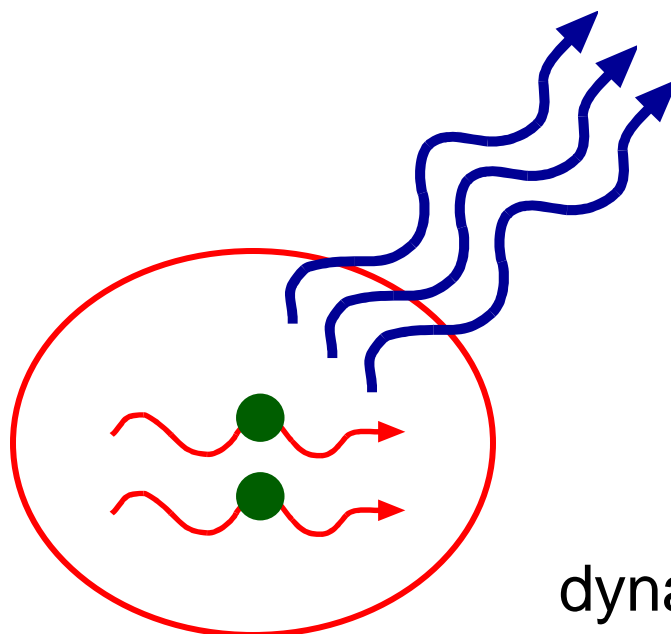
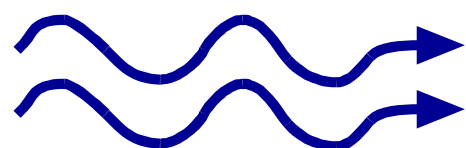
Free particle



Laser light

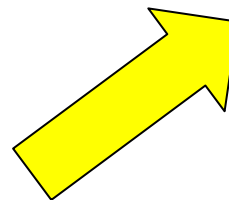
Condensate

Optical stimulation



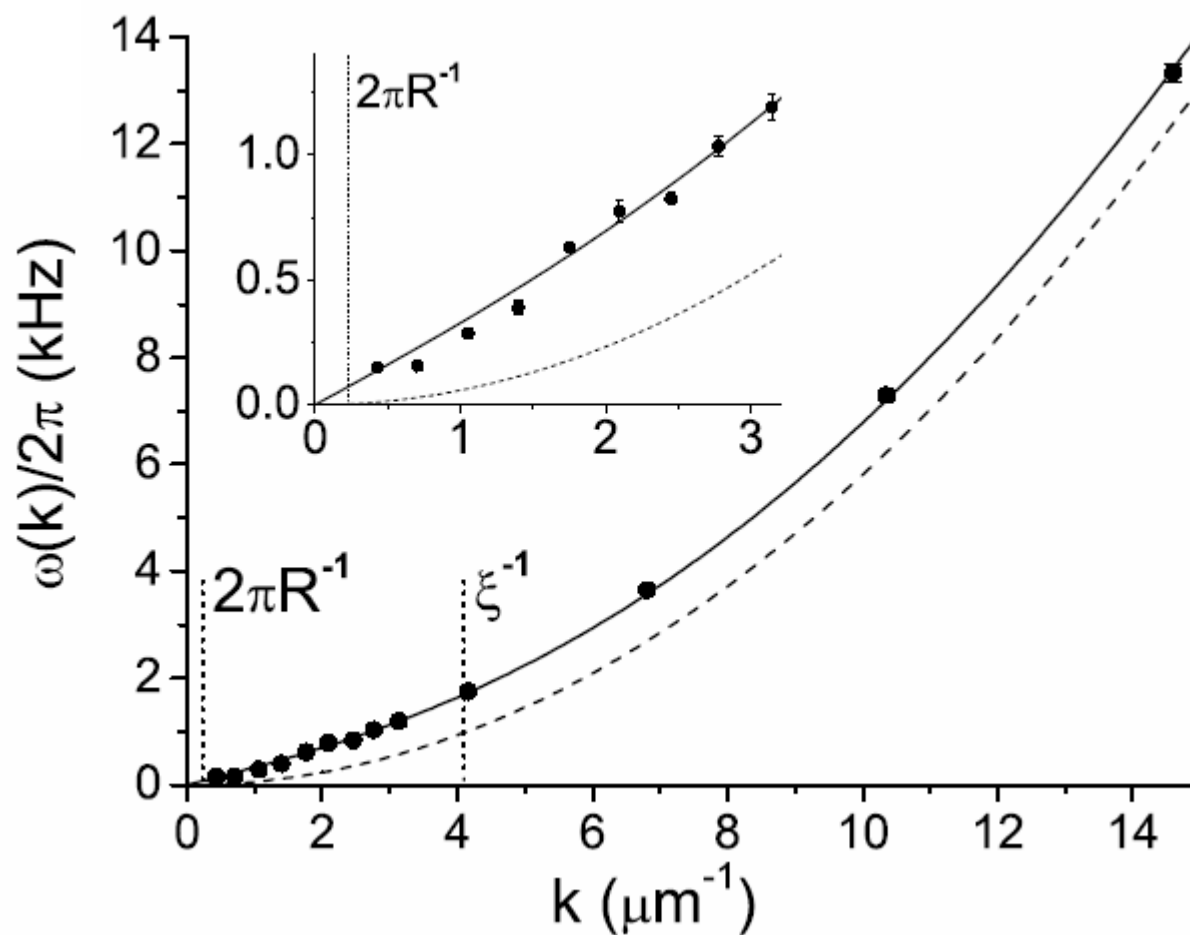
dynamic structure factor

$S(\mathbf{q}, \nu)$



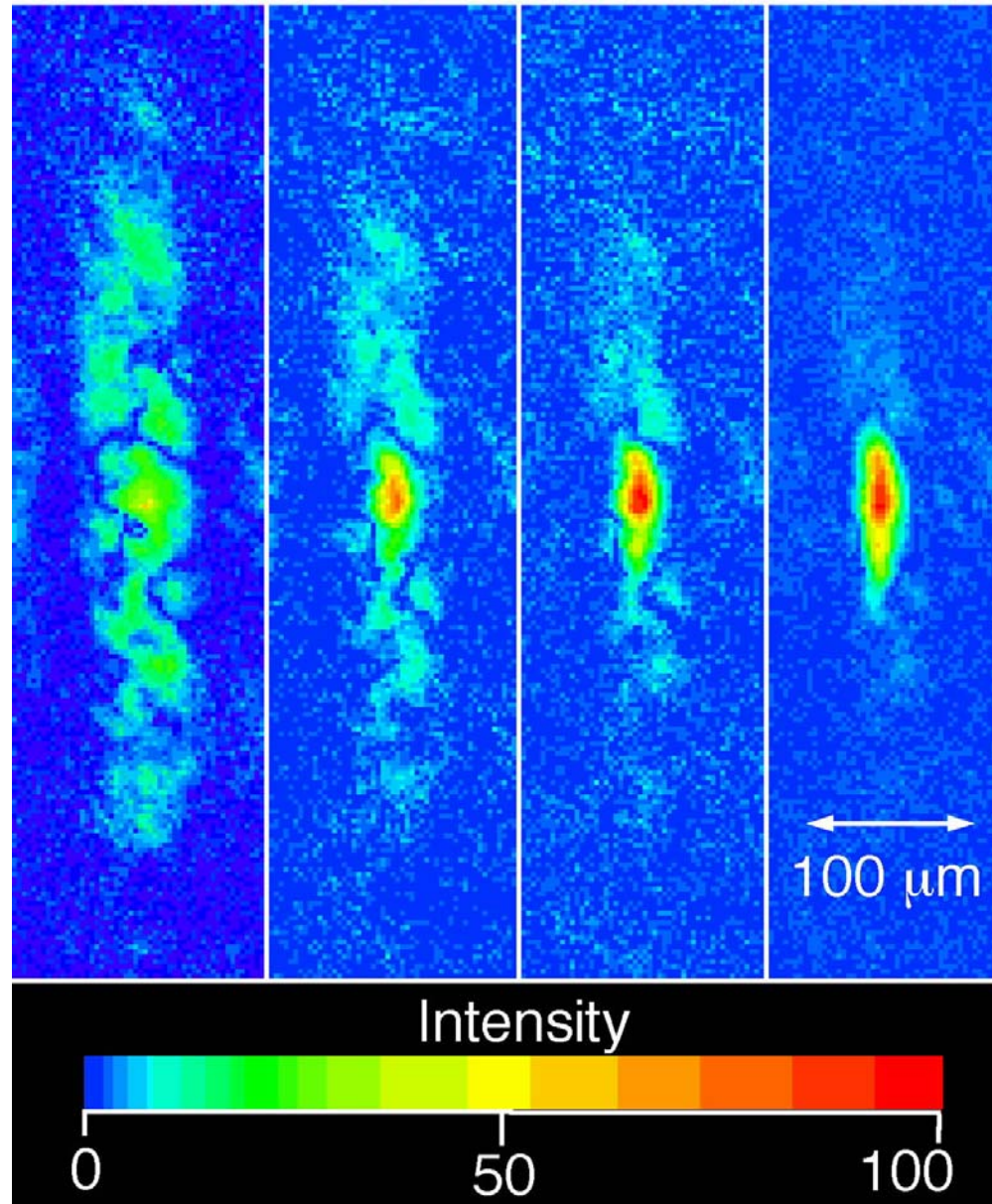
Excitation Spectrum of a Bose-Einstein Condensate

J. Steinhauer, R. Ozeri, N. Katz, and N. Davidson



Inhomogeneous BEC

A live condensate in the magnetic trap (seen by dark-ground imaging)



The inhomogeneous Bose gas

"

New Feature: trapping potential



→ go to \vec{r} space

$$\hat{H} = \int d^3r \hat{\psi}^\dagger(\mathbf{r}) \left[-\frac{\hbar^2}{2m} \nabla^2 + V_{\text{trap}} \right] \hat{\psi}(\mathbf{r}) \\ + \frac{1}{2} \int d^3r \int d^3r' \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}^\dagger(\mathbf{r}') U(\mathbf{r}-\mathbf{r}') \hat{\psi}(\mathbf{r}') \hat{\psi}(\mathbf{r})$$

The inhomogeneous Bose gas

11

New Feature: trapping potential



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$$+ \frac{1}{2} \int d^3r \int d^3r' \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}^\dagger(\mathbf{r}') \underbrace{U(\mathbf{r}-\mathbf{r}')}_{U_0 \delta(\mathbf{r}-\mathbf{r}')} \hat{\psi}(\mathbf{r}') \hat{\psi}(\mathbf{r})$$

$$\frac{U_0}{2} \int d^3r \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}(\mathbf{r}) \hat{\psi}(\mathbf{r})$$

The inhomogeneous Bose gas

11

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$$\frac{U_0}{2} \int d^3r \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}(\mathbf{r}) \hat{\psi}(\mathbf{r})$$

Heisenberg equation of motion for $\hat{\psi}$

$$i\hbar \frac{\partial \hat{\psi}(\mathbf{r}, t)}{\partial t} = [\hat{\psi}, \hat{H}] \quad \text{cannot be solved}$$

Bogoliubov: Condensate Operator \rightarrow C-number

$$\hat{\psi}(\tau, t) = \psi(\tau, t) + \tilde{\psi}(\tau, t)$$

\uparrow
 $\langle \hat{\psi}(\tau, t) \rangle$

\uparrow
 quantum (+ thermal)
 fluctuations

Bogoliubov: Condensate Operator \rightarrow C-number

$$\hat{\psi}(\mathbf{r}, t) = \psi(\mathbf{r}, t) + \tilde{\psi}(\mathbf{r}, t)$$

$$\uparrow$$

$$\langle \hat{\psi}(\mathbf{r}, t) \rangle$$

\uparrow
quantum (+ thermal) fluctuations

$T \rightarrow 0$ neglect $\tilde{\psi}$

\rightarrow NLSE, Gross-Pitaevskii equation for $\psi(\mathbf{r}, t)$

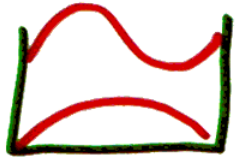
$$i\hbar \frac{\partial \psi}{\partial t} = \left[-\frac{\hbar^2}{2m} \nabla^2 + V_{\text{trap}} + \underbrace{U_0 N |\psi(\mathbf{r}, t)|^2}_{n(\mathbf{r}, t) \text{ density}} \right] \psi(\mathbf{r}, t)$$

$\underbrace{\hspace{10em}}_{\text{mean field potential}}$

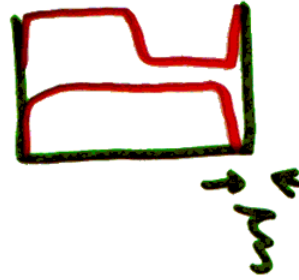
$$U_0 \sum \delta(\mathbf{r}) \rightarrow U_0 n(\mathbf{r}, t)$$

Thomas-Fermi approximation

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→
inter-
actions

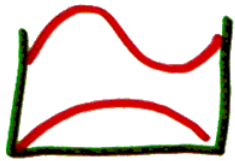


ξ healing length

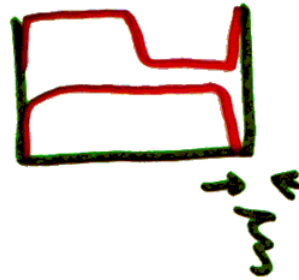
$$\frac{\hbar^2}{2m\xi^2} = U_0$$

$$\xi = (8\pi a n)^{-1/2}$$

Thomas-Fermi approximation



interactions



ξ healing length

$$\frac{\hbar^2}{2m\xi^2} = U_0 n$$

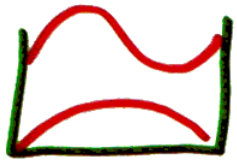
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neglect kinetic energy term

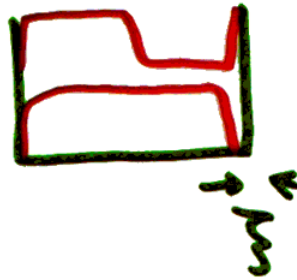
$$\left[\cancel{\frac{\hbar^2}{2m} \nabla^2} + V_{\text{ext}} + U_0 |z(r)|^2 \right] z(r) = \mu z(r)$$

$$\left[V_{\text{ext}} + U_0 |z(r)|^2 - \mu \right] z(r) = 0$$

Thomas-Fermi approximation



interactions



ξ healing length

$$\frac{\hbar^2}{2m\xi^2} = U_0 n$$

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neglect kinetic energy term

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + V_{\text{ext}} + U_0 |\psi(r)|^2 \right] \psi(r) = \mu \psi(r)$$

$$\left[V_{\text{ext}} + U_0 |\psi(r)|^2 - \mu \right] \psi(r) = 0$$

Solution: $|\psi(r)|^2 = \frac{1}{U_0} (\mu - V(r))$



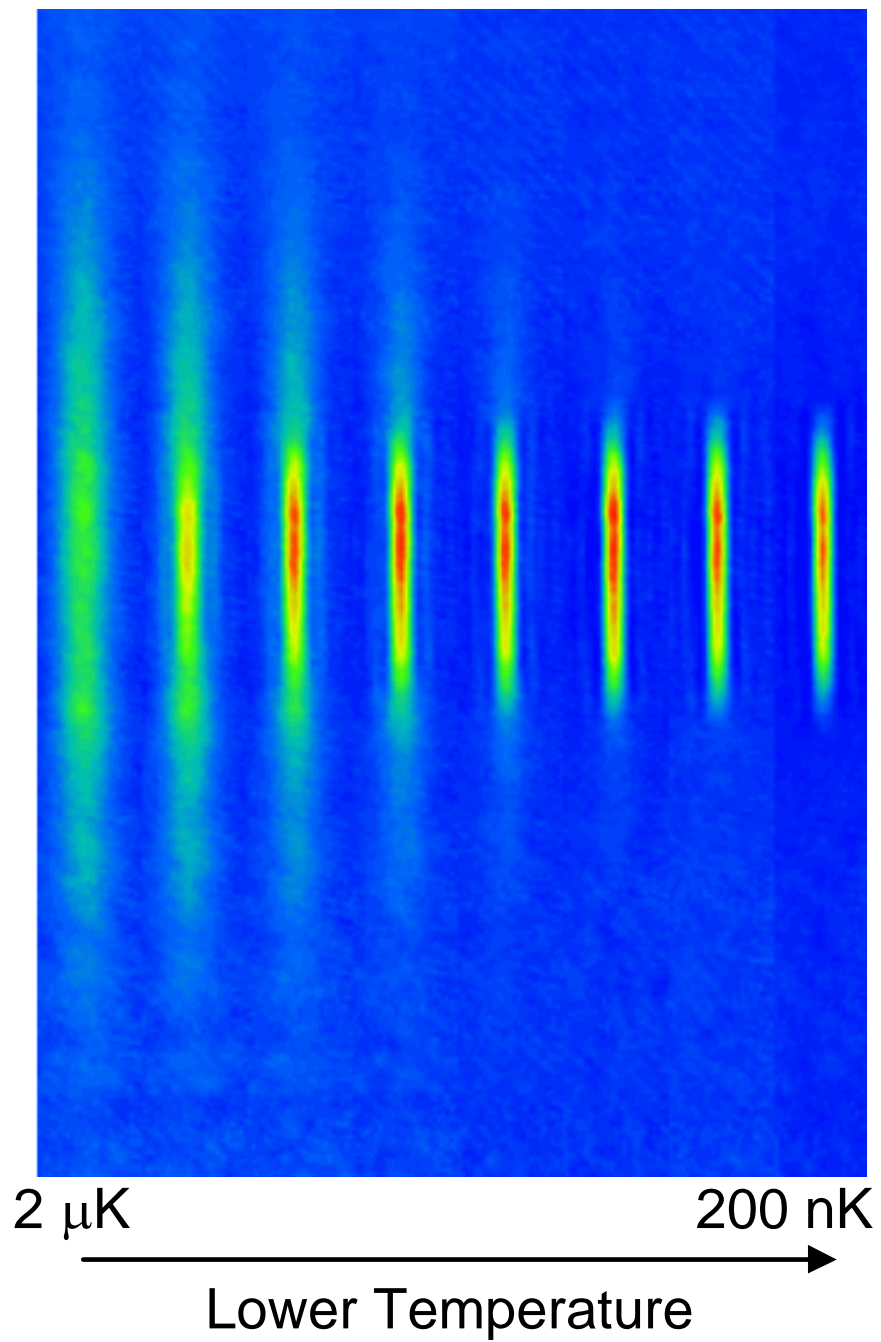
HO: $V(r) = \frac{1}{2} m \omega^2 r^2$

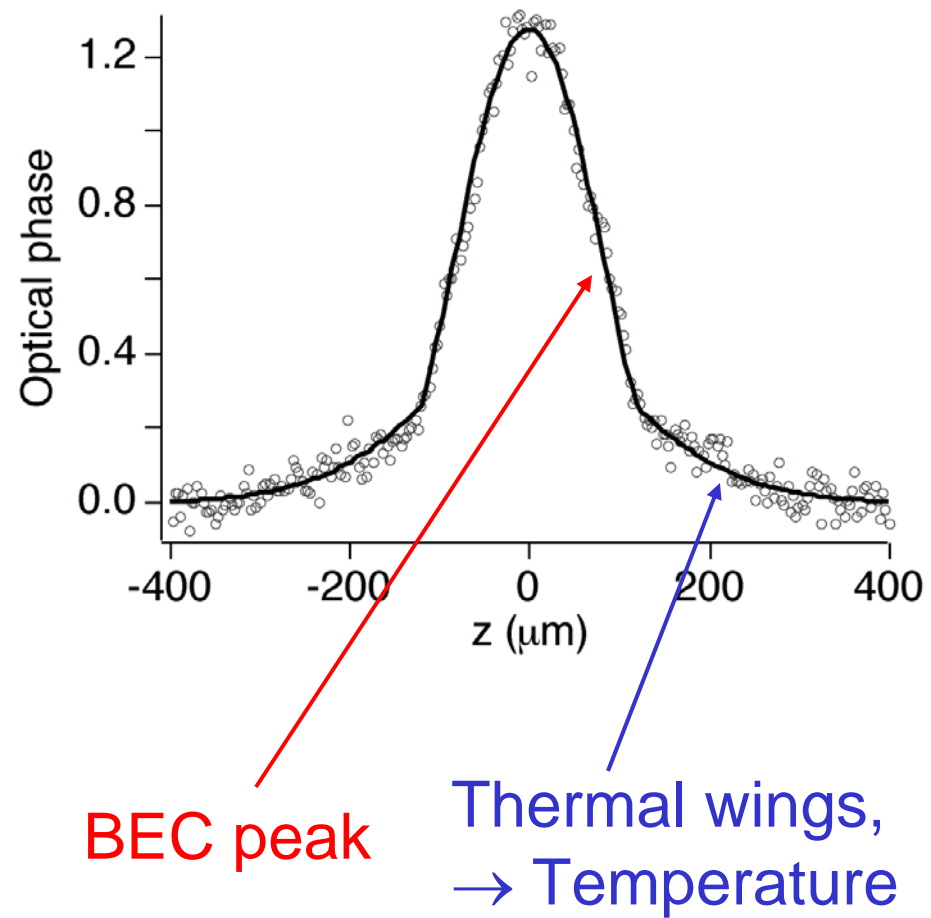
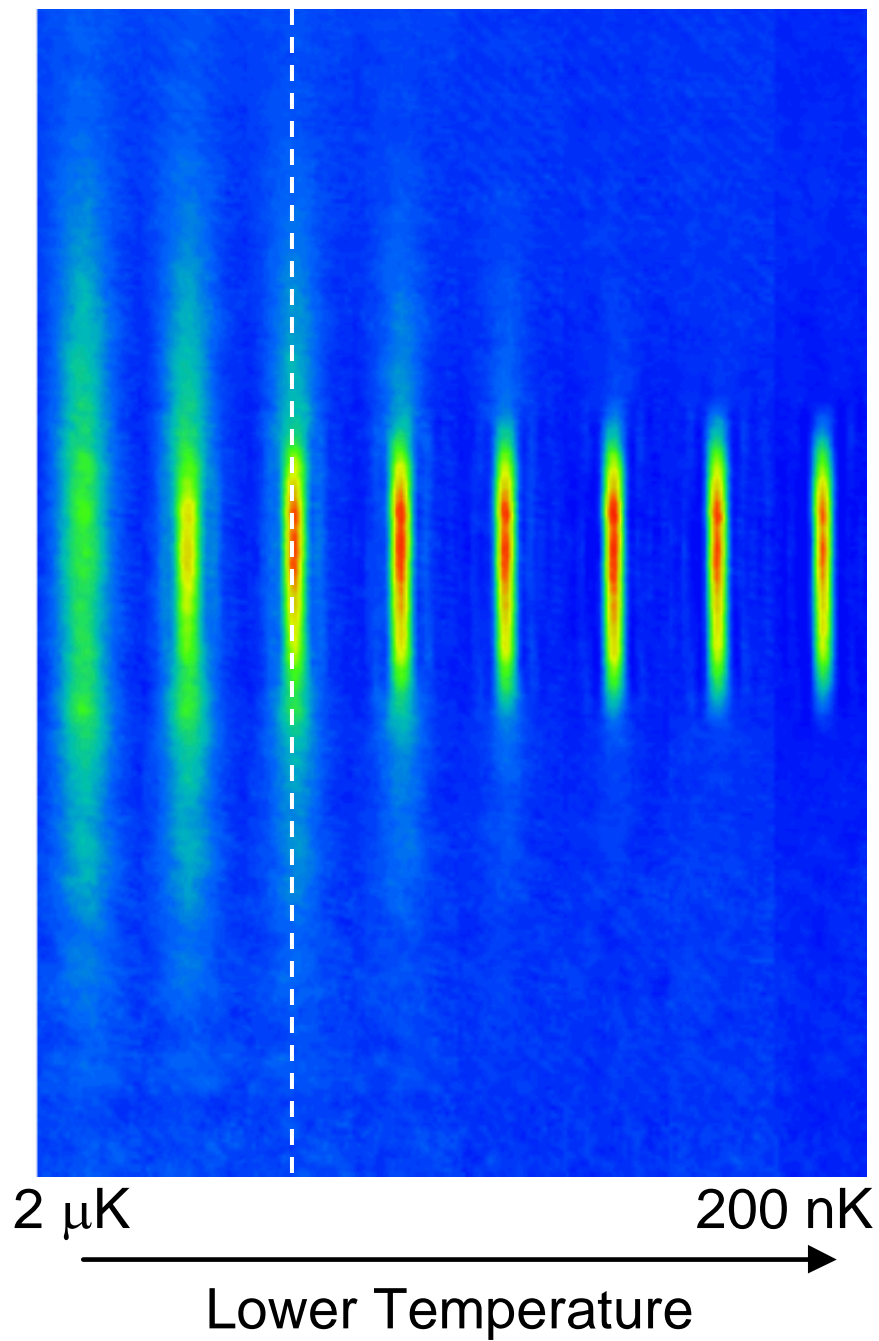
Shape is inverted trapping potential

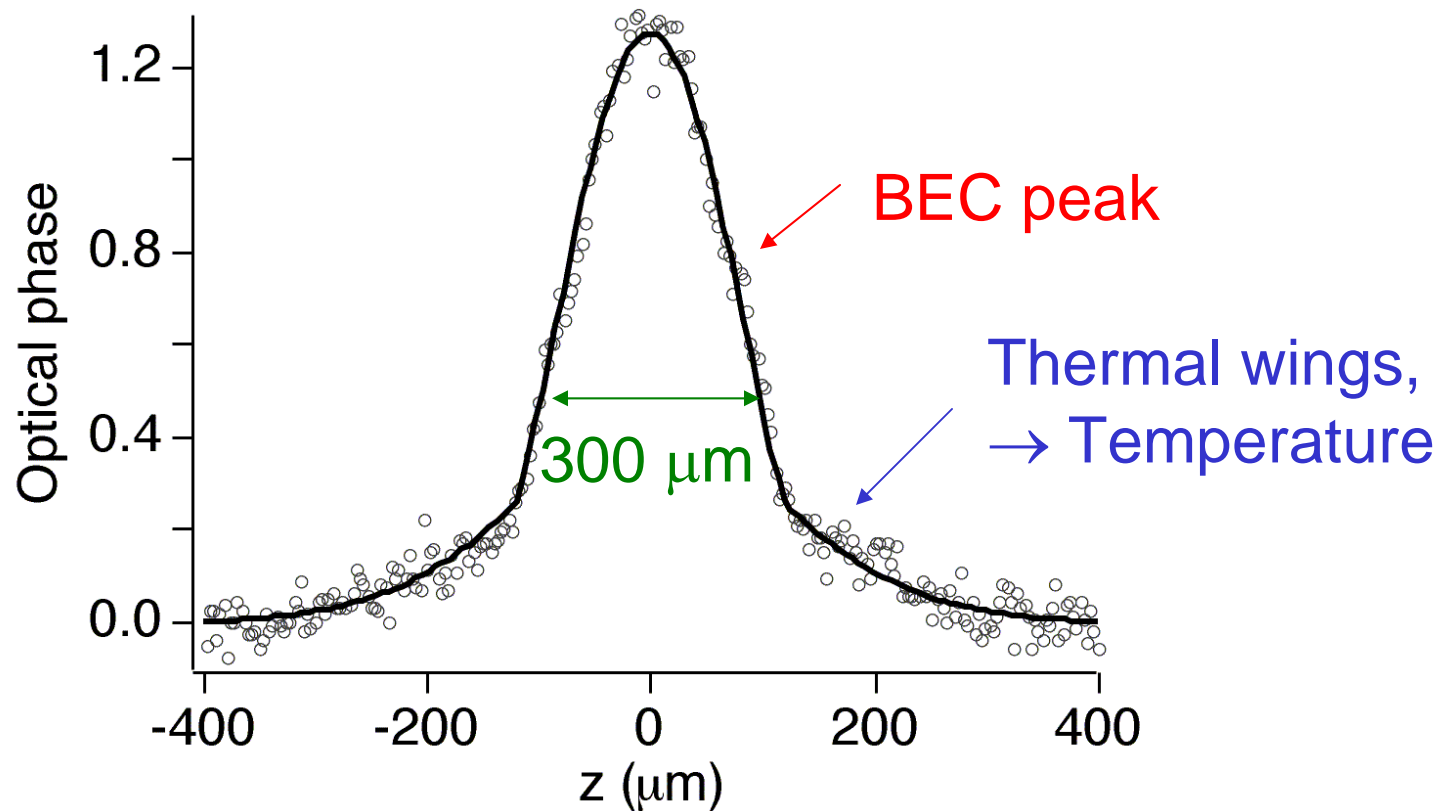
$$\mu = \frac{\hbar \omega}{2} \left(\frac{15 N a}{a_{\text{osc}}} \right)^{2/5} \quad a_{\text{osc}} = \sqrt{\frac{\hbar}{m \omega}}$$

$$\mu = x^{2/5} \frac{\hbar \omega}{2} = \frac{1}{2} m \omega^2 R^2$$

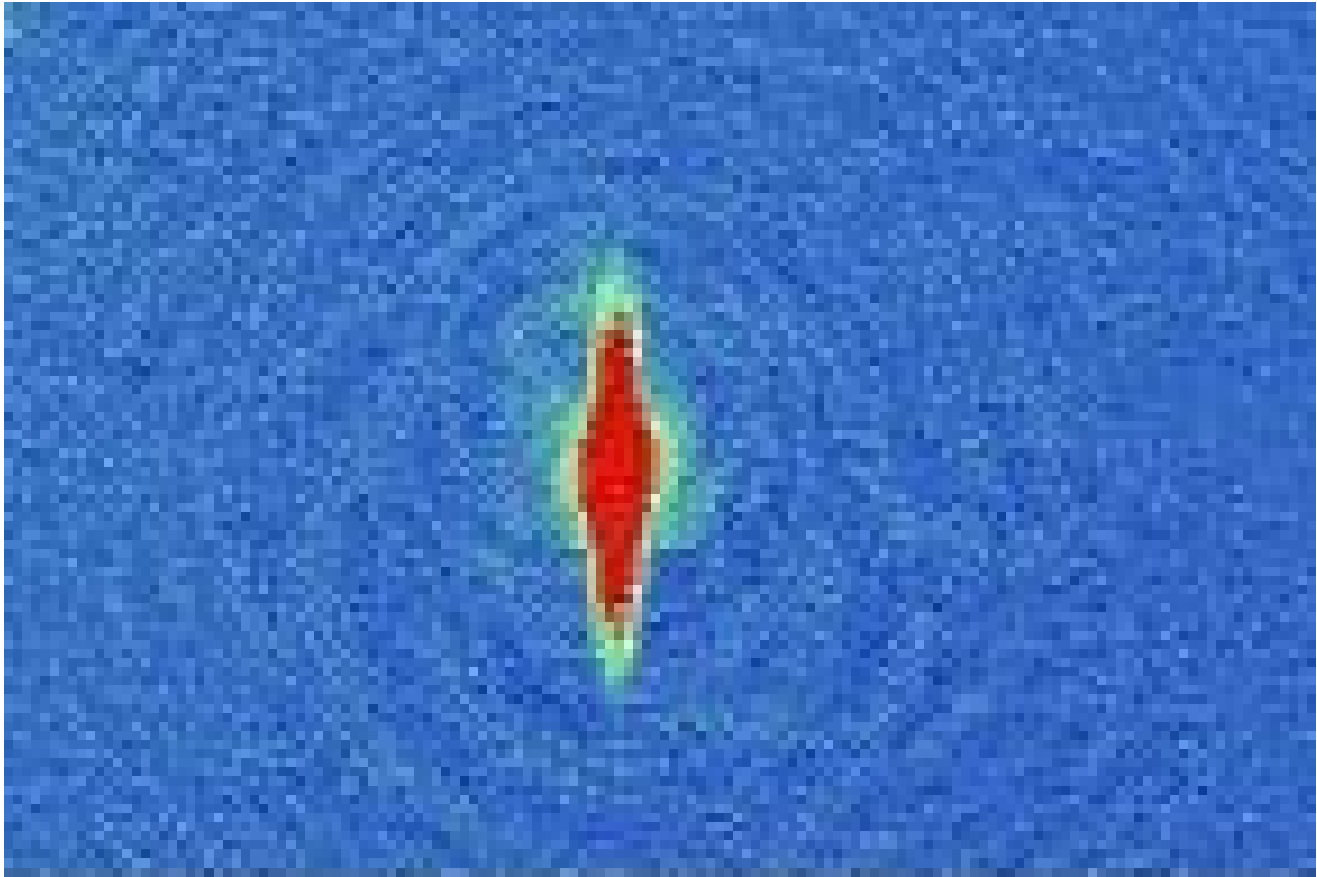
$$R = a_{\text{osc}} x^{1/5}$$





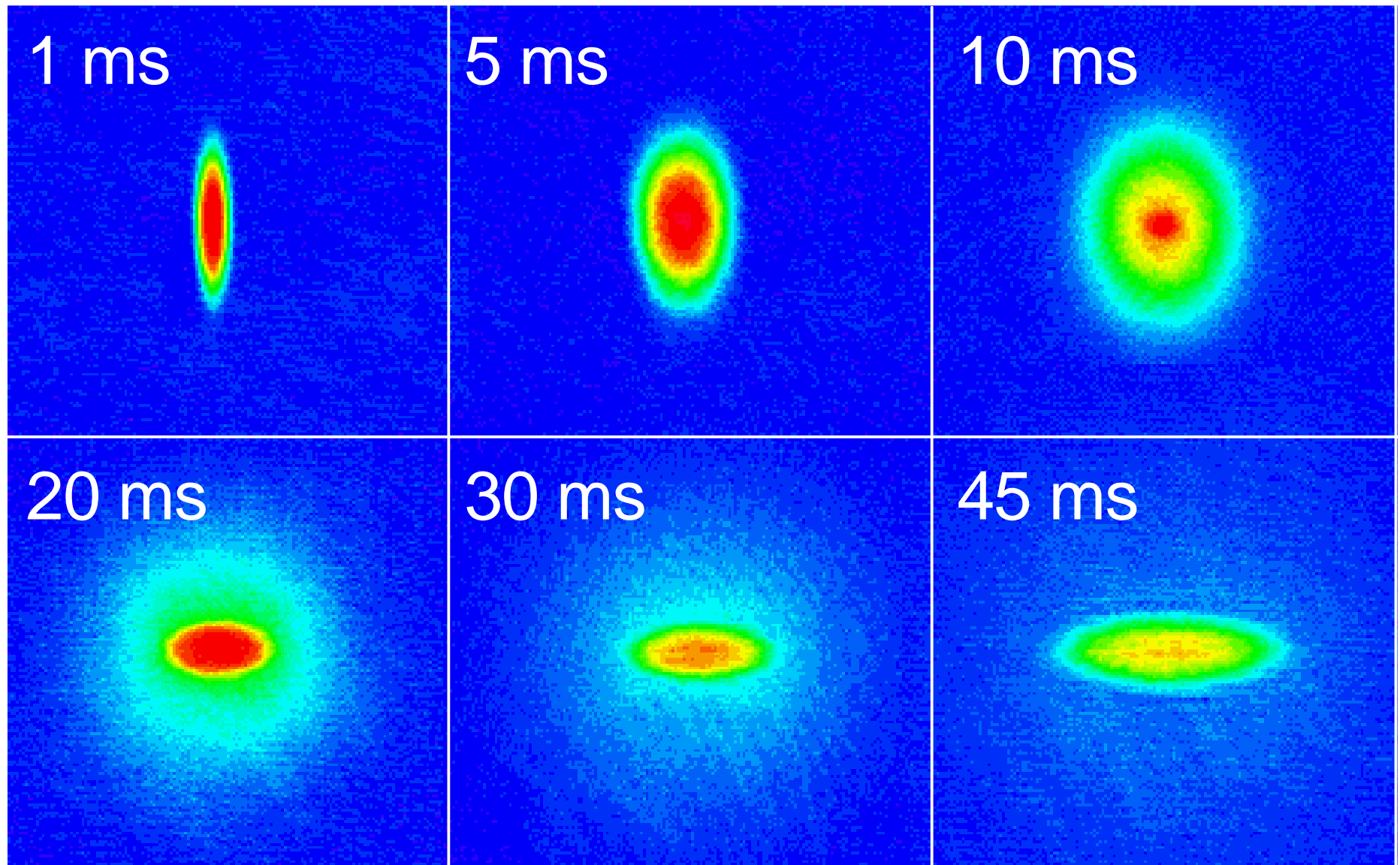


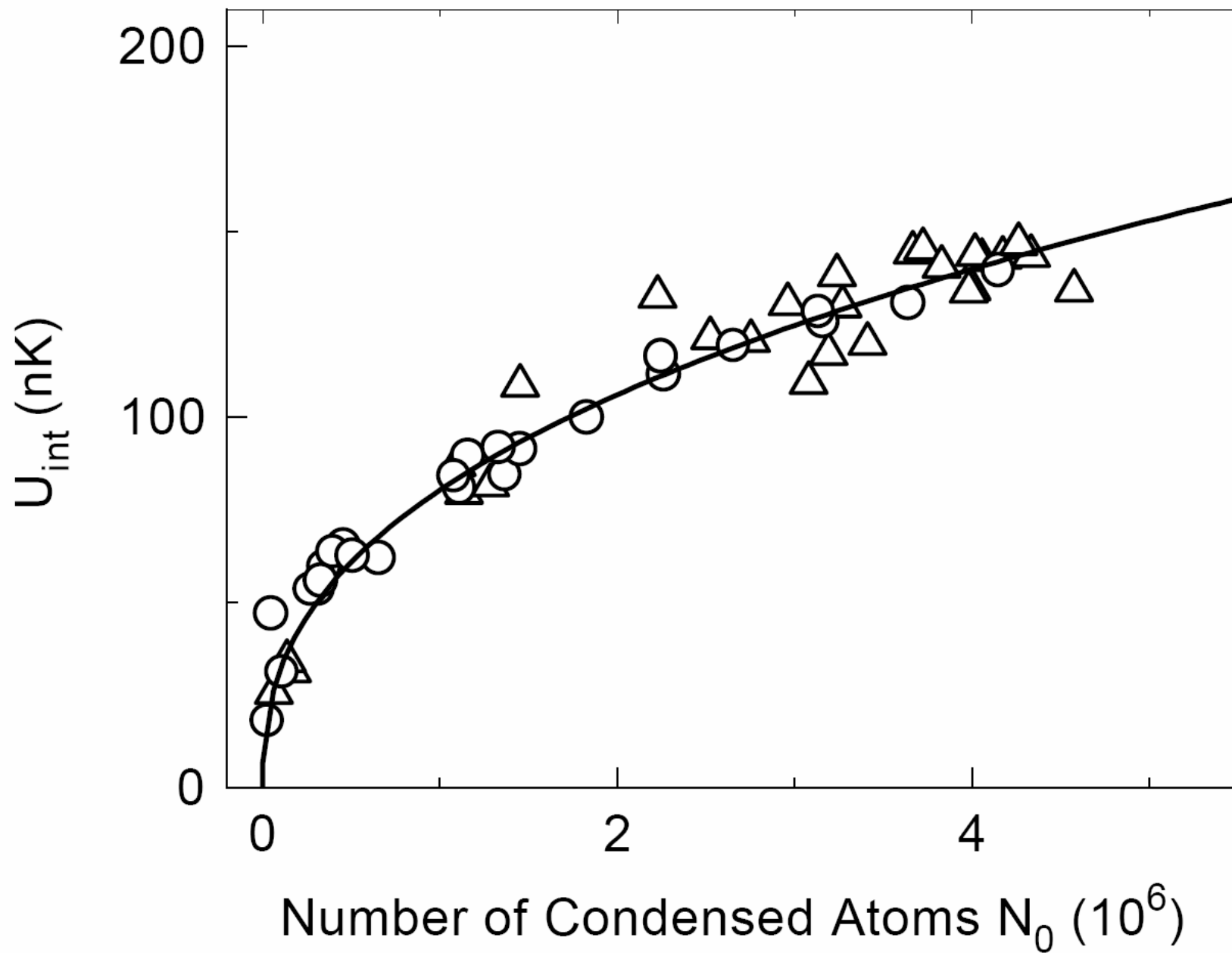
rms width of harmonic oscillator ground state $7 \mu\text{m}$
 \Rightarrow (repulsive) interactions
 \Rightarrow interesting many-body physics



0001 MS

Signatures of BEC: Anisotropic expansion





Vortices

→ NLSE, Gross-Pitaevskii equation for $\psi(\mathbf{r}, t)$

$$i\hbar \frac{\partial \psi}{\partial t} = \left[-\frac{\hbar^2}{2m} \nabla^2 + V_{\text{trap}} + \underbrace{U_0 N |\psi(\mathbf{r}, t)|^2}_{n(\mathbf{r}, t) \text{ density}} \right] \psi(\mathbf{r}, t)$$

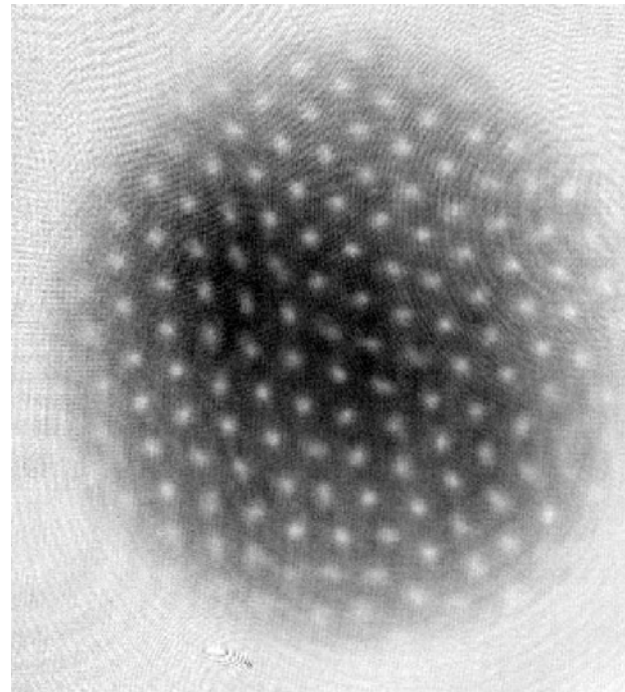
mean field potential

$$U_0 \sum \delta(\mathbf{r}) \rightarrow U_0 n(\mathbf{r}, t)$$

Spinning a Bose-Einstein condensate

The rotating bucket experiment with a superfluid gas
100,000 thinner than air

Rotating
green laser beams



Two-component vortex

Boulder, 1999

Single-component vortices

Paris, 1999

Boulder, 2000

MIT 2001

Oxford 2001

J. Abo-Shaeer, C. Raman, J.M. Vogels,
W.Ketterle, Science, 4/20/2001

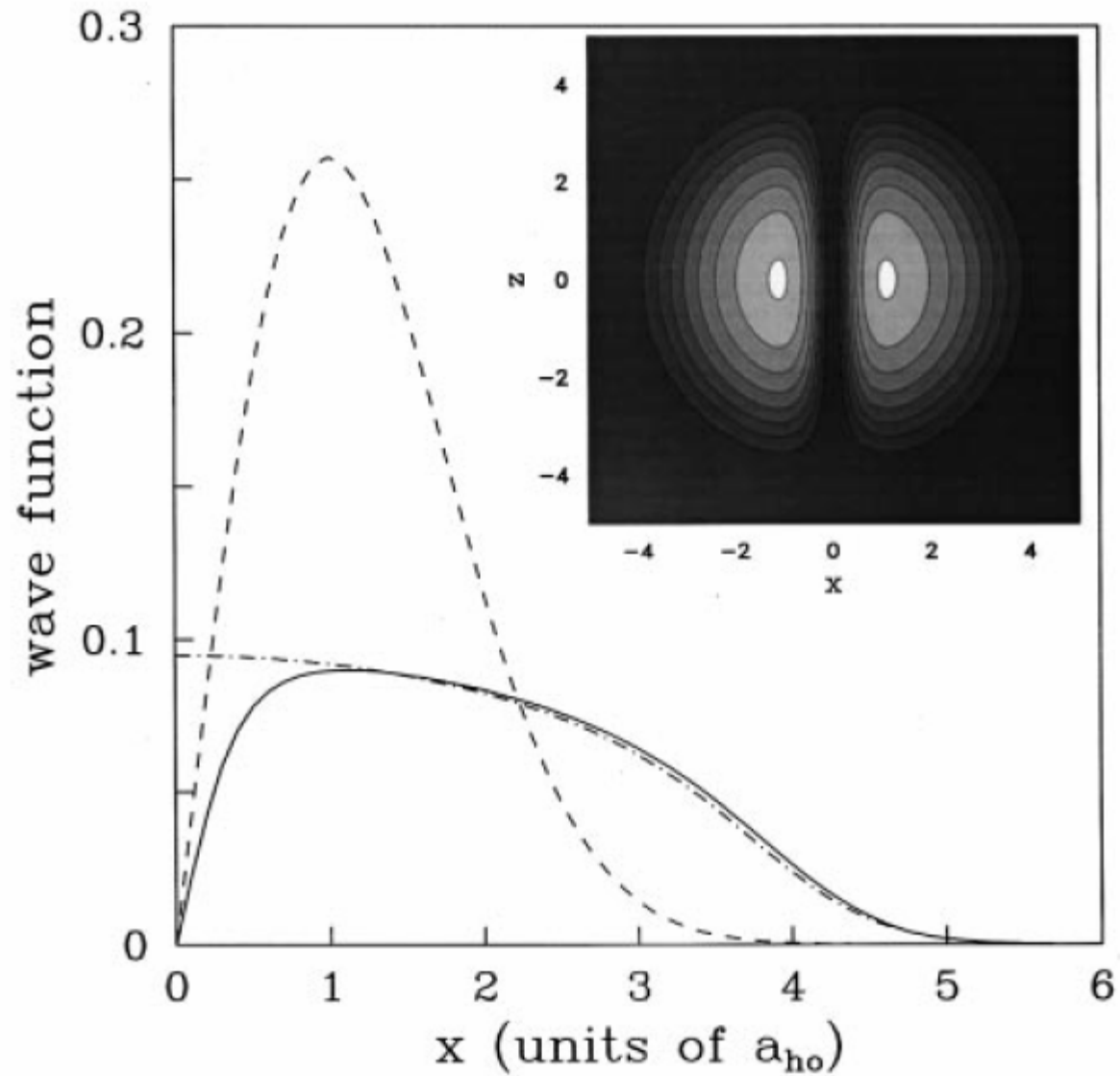
GPE for vortices

Order parameter

$$\phi(\mathbf{r}) = \phi_v(r_\perp, z) \exp[i\kappa\varphi].$$

GPE for modulus

$$\left[-\frac{\hbar^2 \nabla^2}{2m} + \frac{\hbar^2 \kappa^2}{2m r_\perp^2} + \frac{m}{2} (\omega_\perp^2 r_\perp^2 + \omega_z^2 z^2) + g \phi_v^2(r_\perp, z) \right] \phi_v(r_\perp, z) = \mu \phi_v(r_\perp, z)$$



F. Dalfovo, S. Giorgini, L.P. Pitaevskii, and S. Stringari, Rev. Mod. Phys. **71**, 463 (1999)

Hydrodynamics

Hydrodynamic Flow of a Superfluid

15

$$\text{GPE} \quad \left(-\frac{\hbar^2}{2m} \nabla^2 + V(r) + U_0 |\psi|^2 \right) \psi = i\hbar \frac{\partial \psi}{\partial t}$$

* ψ^* , subtract c.c.

$$\frac{\partial |\psi|^2}{\partial t} + \nabla \cdot \frac{\hbar}{2mi} \left(\psi^* \nabla \psi - \psi \nabla \psi^* \right) = 0$$

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$$\frac{\partial n}{\partial t}$$

$$v = \frac{j}{n} = \frac{\psi^* \nabla \psi - \psi \nabla \psi^*}{2mi |\psi|^2}$$

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$$\frac{\partial n}{\partial t} + \nabla \cdot (n v) = 0 \quad \text{Continuity equation}$$

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$\nabla \cdot$ current

$$v = \frac{j}{n} = \frac{\psi^* \nabla \psi - \psi \nabla \psi^*}{2mi |\psi|^2}$$

$$\frac{\partial n}{\partial t} + \nabla \cdot (n v) = 0$$

Continuity equation

$$\psi = f e^{i\phi} \Rightarrow v = \frac{\hbar}{m} \nabla \phi$$

↳ Quant. of circulation $\int \vec{v} \cdot d\vec{s}$
vortices
persistent currents

↑
macroscopic wavefunction "→" SF flow

insert $\psi = f e^{i\phi}$ into NLSE, separate real and im. parts

$$-\hbar \frac{\partial \phi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 f + \frac{1}{2} m v^2 + V(r) + U_0 f^2$$

take ∇

$$m \frac{\partial v}{\partial t} = -\nabla \left(\delta\mu + \frac{1}{2} m v^2 \right)$$

$$\delta\mu = V + U_0 n - \frac{\hbar^2}{2m} \frac{\nabla^2 \sqrt{n}}{\sqrt{n}} - \mu_0$$

$\underbrace{\hspace{10em}}_{\text{arb. const}}$

exact! $\delta\mu = 0 \hat{=} \text{time indep. GPE equation}$

insert $\psi = f e^{i\phi}$ into NLSE, separate real and im. parts

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$\underbrace{\mu_0}_{\text{arb. const}}$

exact! $\delta\mu = 0 \hat{=} \text{time indep. GPE equation}$

Now: Thomas Fermi approx.

neglect ∇f (density derivative)

but not $\nabla \phi$

$$n = n_0 + \delta n \quad \text{where } n_0 U_0 + V = \mu_0$$

$$\delta\mu = U_0 \delta n$$

eliminate $\delta\mu$, neglect v^2 (higher order)

$$m \frac{\partial v}{\partial t} = -\nabla (U_0 \cdot \delta n) \quad | \times n_0, \nabla$$

$$m \nabla \left(n_0 \frac{\partial \mathbf{v}}{\partial t} \right) = -\mu_0 \nabla (n_0 (\nabla \delta n))$$

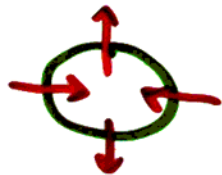
$$\frac{\partial \delta n}{\partial t} + \nabla (n_0 \mathbf{v}) = 0 \quad \text{Linearized}$$

} Combine

$$m \frac{\partial^2 \delta n}{\partial t^2} = \mu_0 \nabla (n_0 \nabla \delta n)$$

- For $n_0 = \text{const}$ Wave equation for δn
velocity $c = \sqrt{\mu_0/m}$ Bogoliubov

- TF solution for n_0
 \Rightarrow discrete modes, $e^{\pm i m \phi}$ in angular mom
e.g. $\omega = \sqrt{2} \omega_{\text{trap}}$



Shape oscillations of the cloud

Collective excitations

(observed in ballistic expansion)

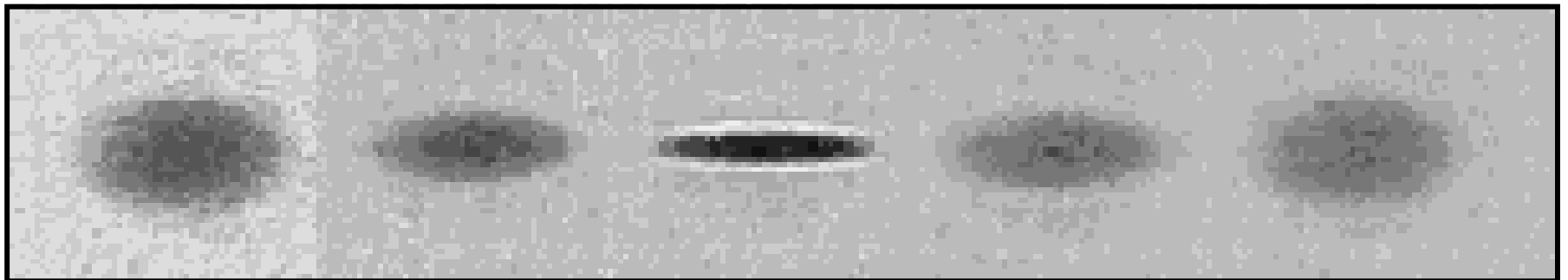
16 ms

23 ms

28 ms

41 ms

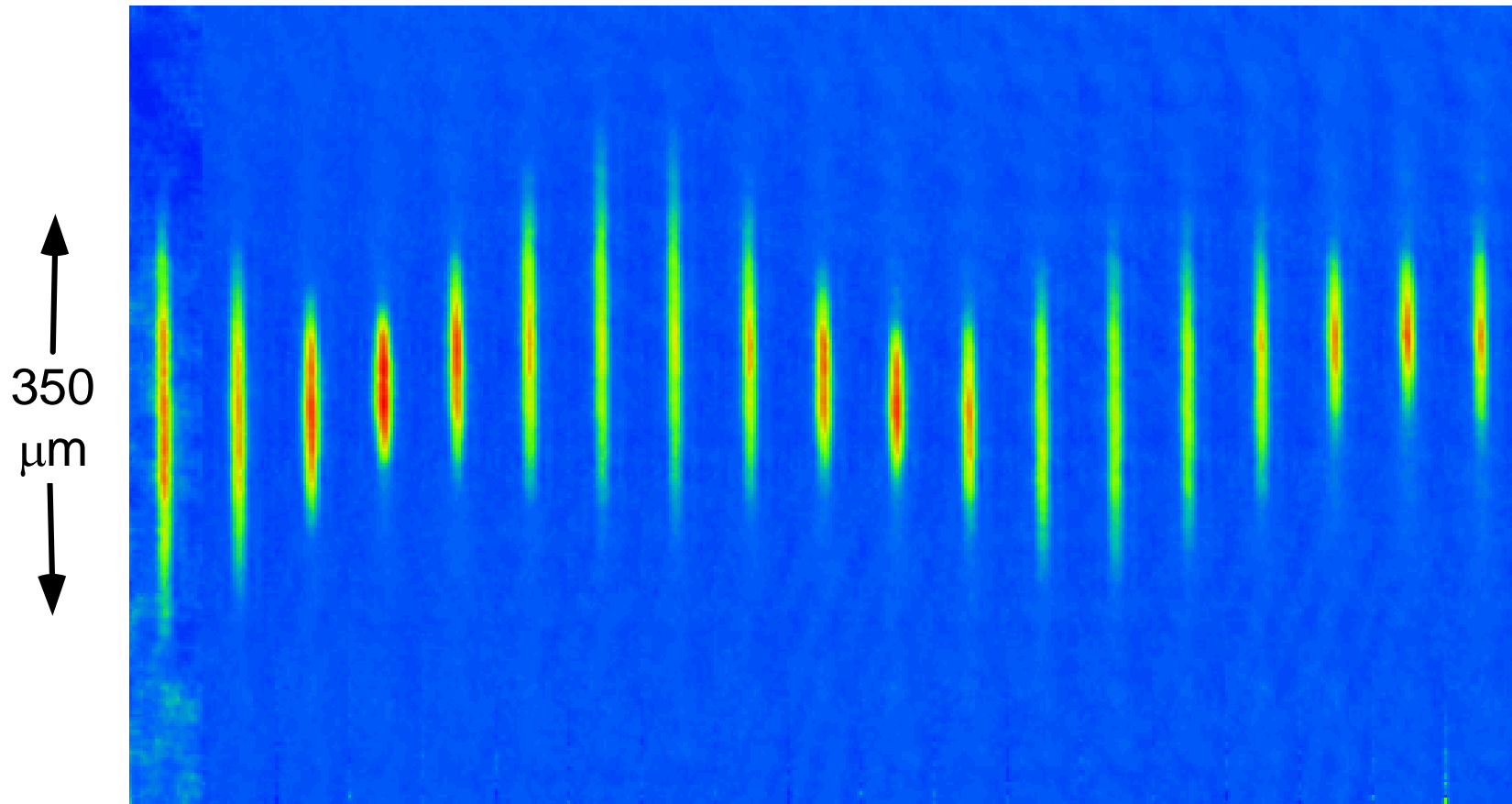
48 ms



Absorption 0%  100%

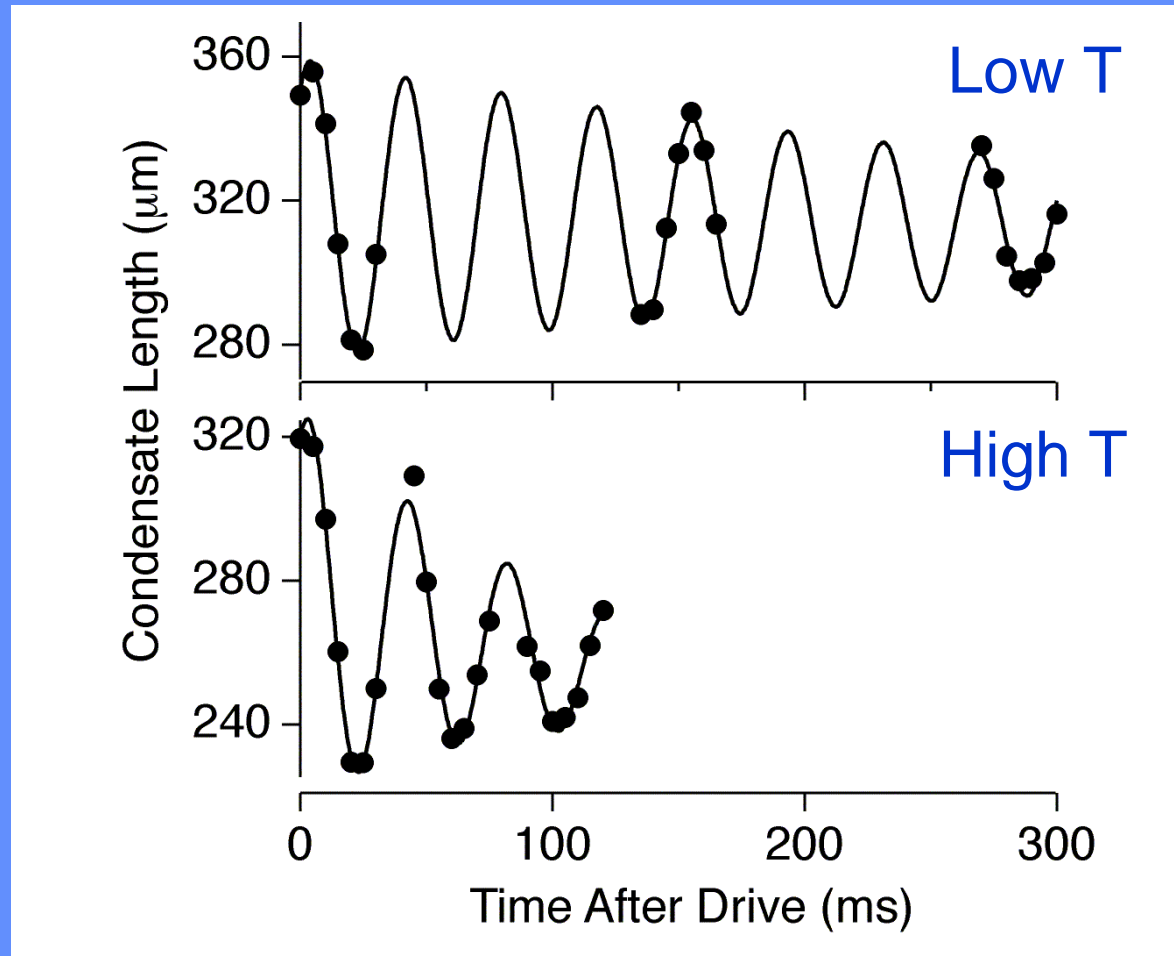
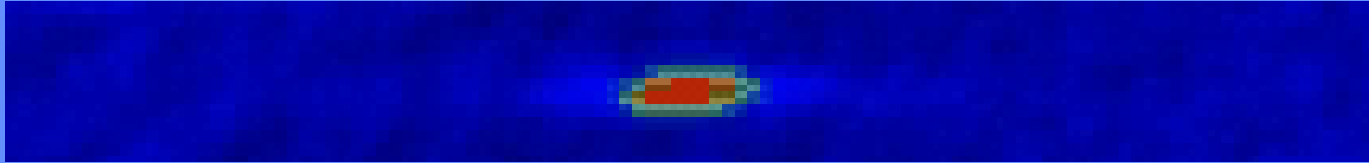
Shape oscillations

“Non-destructive” observation of a time-dependent wave function



5 milliseconds per frame

$m=0$ quadrupole-type oscillation at 29 Hz



Optical Lattices

Superfluid to Mott Insulator Transition

Optical lattice (cubic)

$$V(x, y, z) = V_0 (\sin^2 kx + \sin^2 ky + \sin^2 kz)$$

QM in periodic potentials (1D)

$$H = \frac{\hbar^2}{2m} \nabla^2 - V_0 \sin^2(kx)$$

$$\psi_{q,n} = e^{iqx/\hbar} u_{q,n}(x) \quad \text{Bloch theorem}$$

Quasi momentum
Band index

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Quasi momentum

Band index

periodic

Fourier expansion

$$-V_0 \sin^2(kx) = \sum_r \tilde{V}_r e^{i2rkx}$$

$$\tilde{V}_{-1} = \tilde{V}_1 = V_0/4$$

$$\tilde{V}_0 = -V_0/2$$

$$\sum_l c_l^{q,n} e^{i2lkx}$$

Insert into $H\psi_{q,n} = \epsilon_{q,n}\psi_{q,n}$

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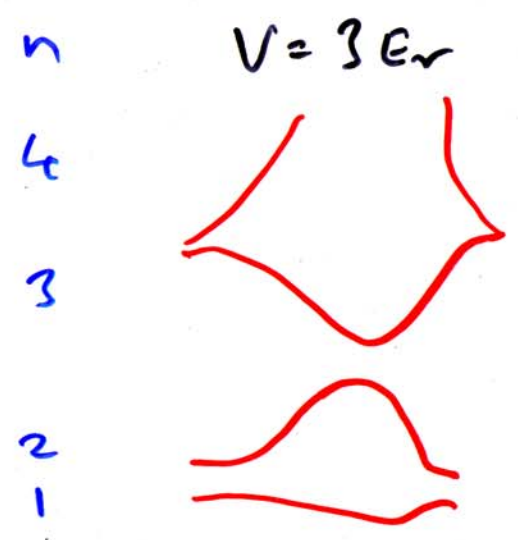
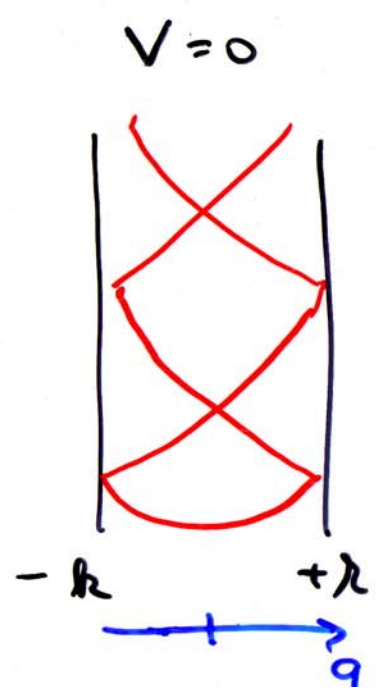
$$\tilde{V}_0 = -V_0/2$$

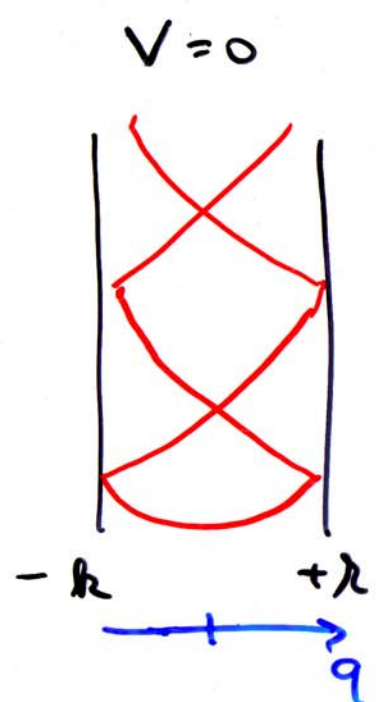
$$\sum_l c_l^{q,n} e^{i2lkx}$$

Insert into $H\psi_{q,n} = \epsilon_{q,n}\psi_{q,n}$

$$\sum_{l'} e^{i(q+2l')x} \left[\left(\frac{q+2l'+k}{2m} \right)^2 - \epsilon_{q,n} \right] c_{l'}^{q,n} + \sum_r \tilde{V}_r c_{l'-r}^{q,n} = 0$$

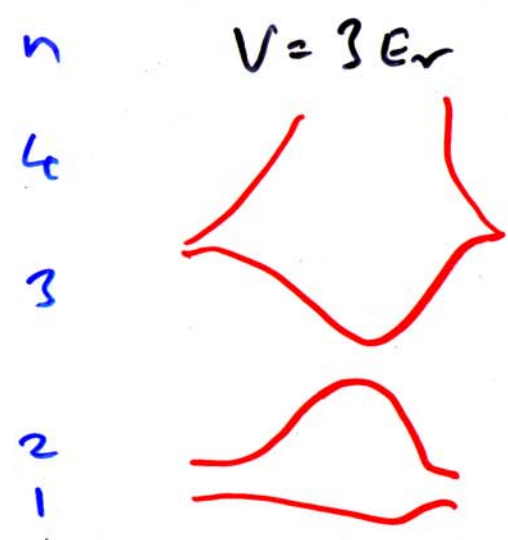
Set of linear equations



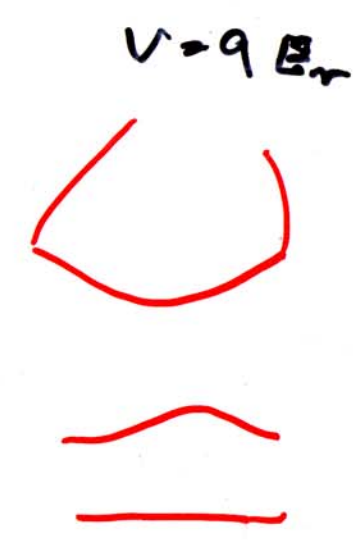


$\frac{V_0}{E_r} \gg 1$

tight binding case
 \Rightarrow harm. confinement
 at each lattice site

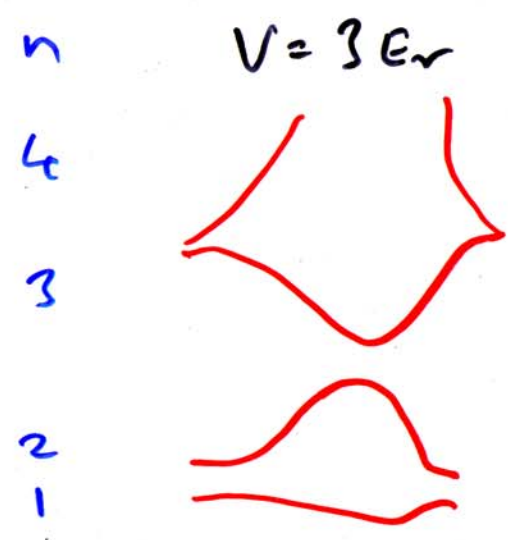
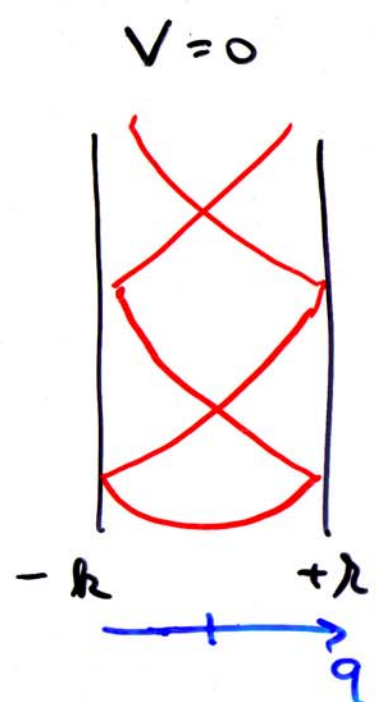


$E_{n,q}$



$E_r = \frac{\hbar^2 k^2}{2m}$

$\hbar \omega_0 = 2 E_r \left(\frac{V_0}{E_r} \right)^{1/2}$



$\frac{V_0}{E_r} \gg 1$

tight binding case
 \Rightarrow harm. confinement
 at each lattice site

$E_r = \frac{\hbar^2 k^2}{2m}$

$\hbar \omega_0 = 2 E_r (V_0/E_r)^{1/2}$

lowest band

$$E_1(q) = \frac{3}{2} \hbar \omega_0 - 2J (\cos q_x a + \cos q_y a + \cos q_z a)$$

$a = \frac{\lambda}{2} = \frac{\pi}{k}$

J : 4 x band width

Wannier Functions

(Orthogonal basis set)

3

$$W_n(x - \underbrace{x_j}_{\text{Site}}) = N^{-1/2} \underbrace{\text{normalization}}_{\text{ization}}$$

Localized

$$\sum e^{iqx_j} \psi_{q,n}(x)$$

Wannier Functions (orthogonal basis set)

$$w_n(x - \underbrace{x_j}_{\text{Site}}) = \underbrace{N^{-1/2}}_{\text{normalization}} \sum e^{iqx_j} \psi_{q,n}(x)$$

localized

$$J = \int w_l(x - x_l) \left[\frac{\hbar^2}{2m} \nabla^2 + V(x) \right] w_l(x - x_j)$$

tunneling from site j to l

J "tunneling energy"
 J/h "tunneling rate"

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localized

$$J = \int w_l(x - x_l) \left[\frac{\hbar^2}{2m} \nabla^2 + V(x) \right] w_l(x - x_j) dx$$

tunneling from site j to l

J "tunneling energy"

J/\hbar "tunneling rate"

deep lattice

$$J = \frac{4}{\sqrt{\pi}} E_r \left(\frac{V_0}{E_r} \right)^{3/4} \exp[-2\sqrt{V_0/E_r}]$$

Tight binding: w_l is Gaussian (solution for HD with Freq. ω_0)

Now: Interactions

Mean field interactions

$$U(x) = \underbrace{\frac{4\pi\hbar^2 a_s}{m}}_g \delta(x)$$

On-site interactions:

$$U = g \int [w_i(x)]^2 d^3x = \sqrt{\frac{8}{\pi}} k a_s E_r \left[\frac{V_0}{E_r} \right]^{3/4}$$

|
tight binding

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|
tight binding

$$H_{\text{Full}} = \int d^3x \psi^\dagger(x) \left(\frac{p^2}{2m} + V(x) \right) \psi(x) \\ + \frac{g}{2} \int d^3x \psi^\dagger(x) \psi^\dagger(x) \psi(x) \psi(x)$$

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On-site interactions:

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|
tight binding

$$H_{Full} = \int d^3x \psi^\dagger(x) \left(\frac{p^2}{2m} + V(x) \right) \psi(x) + \frac{g}{2} \int d^3x \psi^\dagger(x) \psi^\dagger(x) \psi(x) \psi(x)$$

Wannier functions $\hat{\psi}(x) = \sum b_i W_i(x-x_i)$

Assume: only lowest band occupied

$$\Rightarrow H_{Full} = - \sum_{i,j} J_{ij} b_i^\dagger b_j + \frac{1}{2} \sum_{i,j,k,l} U_{ijkl} b_i^\dagger b_j^\dagger b_k b_l$$

$$J_{ij} = - \int dx \psi_i(x-x_i) \left(\frac{p^2}{2m} + V(x) \right) \psi_i(x-x_j)$$

$$U_{ijkl} = g \int dx \psi(x-x_i) \psi(x-x_j) \psi(x-x_k) \psi(x-x_l)$$

$$J_{ij} = - \int dx w_i(x-x_i) \left(\frac{p^2}{2m} + V(x) \right) w_i(x-x_j)$$

$$U_{ijkl} = g \int dx w(x-x_i) w(x-x_j) w(x-x_k) w(x-x_l)$$

Hubbard model

$$J = J_{ij} \neq 0 \quad \text{nearest neighbors}$$

$$U = U_{ijkl} \neq 0 \quad \text{for } i=j=k=l \quad \text{on site}$$

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$$\hat{H} = -J \sum_{ll'} b_l^\dagger b_{l'} + \frac{U}{2} \sum_l n_l(n_l-1) - \mu \sum_l n_l$$

nearest neighbor
 $b_l^\dagger b_l$

n_l : # of bosons/site

Refs: Zwerger, J. Opt. B: Quantum Semi-class. Opt. 5, S9 (2003)
 Jaksch, Zoller, Annals of Phys. 315, 52 (2005)

Two limiting cases:

integer filling \bar{n}

$$U \gg J$$

ground state

$$|Z_{MI}\rangle (J=0, \bar{n}) = \prod_{\ell} (|\bar{n}\rangle_{\ell})$$

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$$U \gg J$$

ground state $|Z_{MI}\rangle (J=0, \bar{n}) = \prod_{\ell} (|\bar{n}\rangle_{\ell})$

$J \gg U$ ideal BEC, all N atoms in $\vec{q}=0$ Bloch state

$$|Z_{SF,N}\rangle (U=0) = \left(\frac{1}{\sqrt{M}} \sum_{\ell=1}^M b_{\ell}^{\dagger} \right)^N |0\rangle \quad M \text{ sites}$$

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Note: Bogoliubov approximation $a_0 = a_0^{\dagger} = \sqrt{N_0}$

does not capture the transition to insulating state

Interactions are treated only approximately

Valid only for small depletion $N - N_0$

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Goal: Find effective onsite Hamiltonian by mean-field

decoupling

van Oosten, van der Straten, Stoof, PRA 63, 053601 (2001).

$$\begin{aligned} \hat{A} \hat{B} &= (\langle A \rangle + \Delta \hat{A}) (\langle B \rangle + \Delta \hat{B}) \approx \langle A \rangle \Delta \hat{B} + \Delta \hat{A} \langle B \rangle + \langle A \rangle \langle B \rangle \\ &= \langle A \rangle \hat{B} + \hat{A} \langle B \rangle - \langle A \rangle \langle B \rangle \end{aligned}$$

Coupling between sites: tunneling $J b_e^\dagger b_{e'}$ 7

$$b_e^\dagger b_{e'} \approx \langle b_e^\dagger \rangle b_{e'} + b_e^\dagger \langle b_{e'} \rangle - \langle b_e^\dagger \rangle \langle b_{e'} \rangle$$

Coupling between sites: tunneling $J b_e^\dagger b_{e'}$ 7

$$b_e^\dagger b_{e'} \approx \underbrace{\langle b_e^\dagger \rangle}_{\zeta} b_{e'} + b_e^\dagger \underbrace{\langle b_{e'} \rangle}_{\zeta} - \underbrace{\langle b_e^\dagger \rangle \langle b_{e'} \rangle}_{\zeta^2}$$

SF order parameter $\zeta = \sqrt{n_e} = \langle b_e^\dagger \rangle = \langle b_e \rangle$

Coupling between sites: tunneling $J b_e^\dagger b_{e'}$ 7

$$b_e^\dagger b_{e'} \approx \underbrace{\langle b_e^\dagger \rangle}_{z} b_{e'} + b_e^\dagger \underbrace{\langle b_{e'} \rangle}_{z} - \underbrace{\langle b_e^\dagger \rangle \langle b_{e'} \rangle}_{z^2}$$

SF order parameter $z = \sqrt{n_e} = \langle b_e^\dagger \rangle = \langle b_e \rangle$

z # of nearest neighbors

$$H_{\text{eff}} = -z J z \sum_e (b_e^\dagger + b_e) + z \underbrace{J M z^2}_{\text{\# of sites}} + \frac{u}{2} \sum_e n_e (n_e - 1) - \mu \sum_e n_e$$

Coupling between sites: tunneling $J b_e^\dagger b_{e'}$ 7

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$$H_{\text{eff}} = z J \sum H_{\text{eff},e} \quad \bar{u} = u/zJ \quad \bar{\mu} = \mu/zJ$$

$$H_{\text{eff},e} = \frac{1}{2} \bar{u} n_e (n_e - 1) - \bar{\mu} n_e - z (b_e^\dagger + b_e) + z^2$$

Coupling between sites: tunneling $J b_e^\dagger b_{e'}$ 7

$$b_e^\dagger b_{e'} \approx \underbrace{\langle b_e^\dagger \rangle}_{z} b_{e'} + b_e^\dagger \underbrace{\langle b_{e'} \rangle}_{z} - \underbrace{\langle b_e^\dagger \rangle \langle b_{e'} \rangle}_{z^2}$$

SF order parameter $z = \sqrt{n_e} = \langle b_e^\dagger \rangle = \langle b_e \rangle$

z # of nearest neighbors

$$H_{\text{ell}} = -z J \sum_e (b_e^\dagger + b_e) + z \underbrace{J M z^2}_{\text{\# of sites}} + \frac{u}{2} \sum n_e (n_e - 1) - \mu \sum n_e$$

$$H_{\text{ell}} = z J \sum H_{\text{ell},e} \quad \bar{u} = u/zJ \quad \bar{\mu} = \mu/zJ$$

$$H_{\text{ell},e} = \frac{1}{2} \bar{u} n_e (n_e - 1) - \bar{\mu} n_e - z (b_e^\dagger + b_e) + z^2$$

$$= H^{(0)} + z V \quad \text{with } V = - (b_e^\dagger + b_e)$$

$$H^{(0)} = \frac{1}{2} \bar{u} \hat{n} (\hat{n} - 1) - \bar{\mu} \hat{n} + z^2 \quad \text{diagonal in } \hat{n}$$

ground state for $H^{(0)}$

$$\text{If } \bar{u}(j-1) < \bar{\mu} < \bar{u} j$$

$$\Rightarrow E_j^{(0)} = \frac{1}{2} \bar{u} j (j-1) - \bar{\mu} j$$

j occupation #

8

ground state for $H^{(0)}$

$$\text{If } \bar{u}(j-1) < \bar{\mu} < \bar{u} j$$

$$\Rightarrow E_j^{(0)} = \frac{1}{2} \bar{u} j (j-1) - \bar{\mu} j$$

j occupation #

V : couples $\Delta n = \pm 1$

second order perturbation theory

$$E_j^{(2)} = 2^2 \sum_{n \neq j} \frac{|\langle j | V | n \rangle|^2}{E_j^{(0)} - E_n^{(0)}}$$
$$= \frac{j}{\bar{u}(j-1) - \bar{\mu}} + \frac{j+1}{\bar{\mu} - \bar{u} j}$$

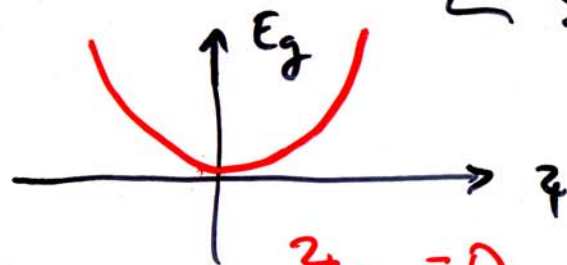
Phase transition

Landau Formalism:

$$E_g(\varphi) = a_0 + a_2 \varphi^2 + o(\varphi^4)$$

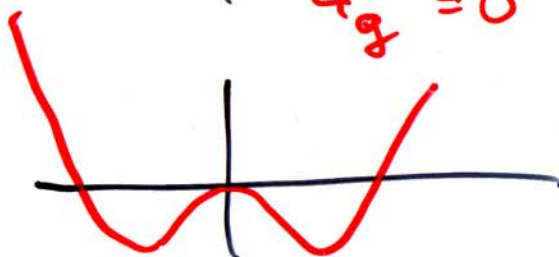
$\hookrightarrow > 0$, see 4th order perturbation theory

$$a_2 > 0$$



$$\varphi_g = 0$$

$$a_2 < 0$$



$$\varphi_g \neq 0$$

Phase transition for

$$a_2 = 0$$

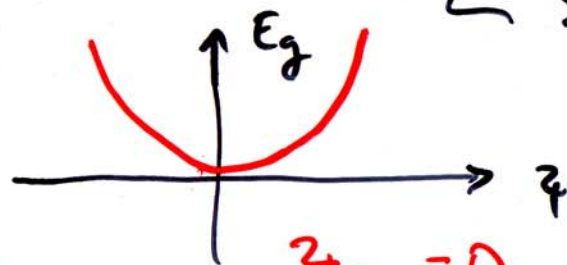
Phase transition

Landau Formalism:

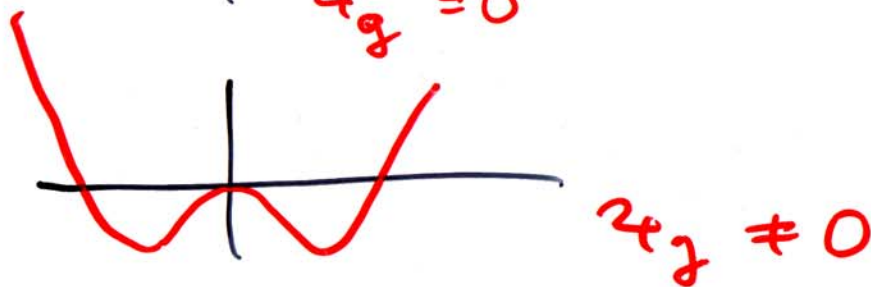
$$E_g(z) = a_0 + a_2 z^2 + o(z^4)$$

$\hookrightarrow > 0$, see 4th order perturbation theory

$$a_2 > 0$$



$$a_2 < 0$$

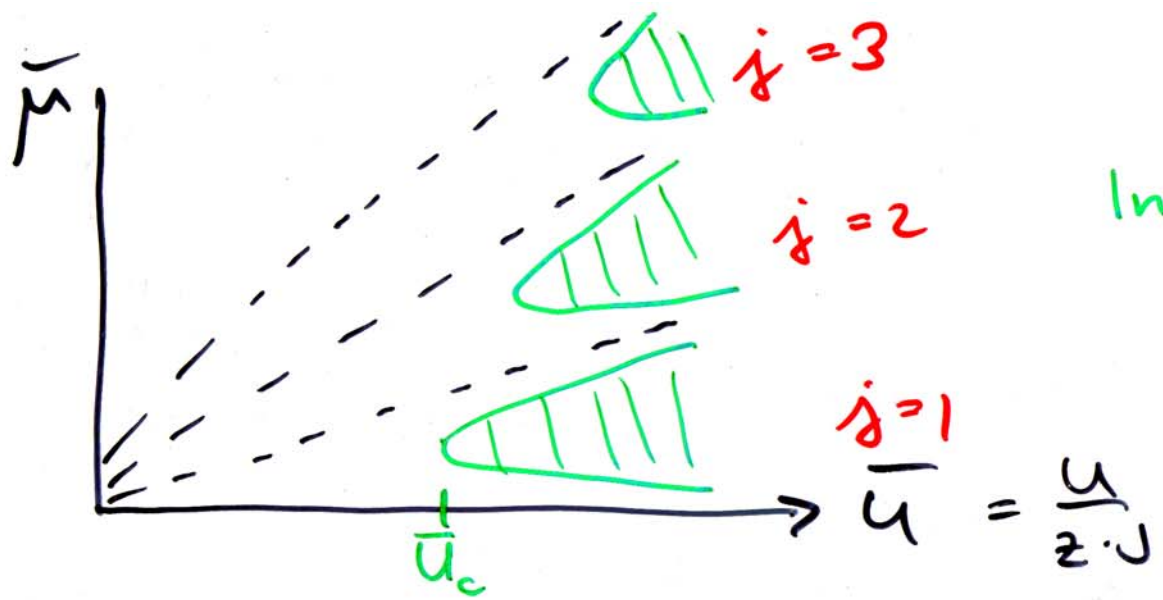


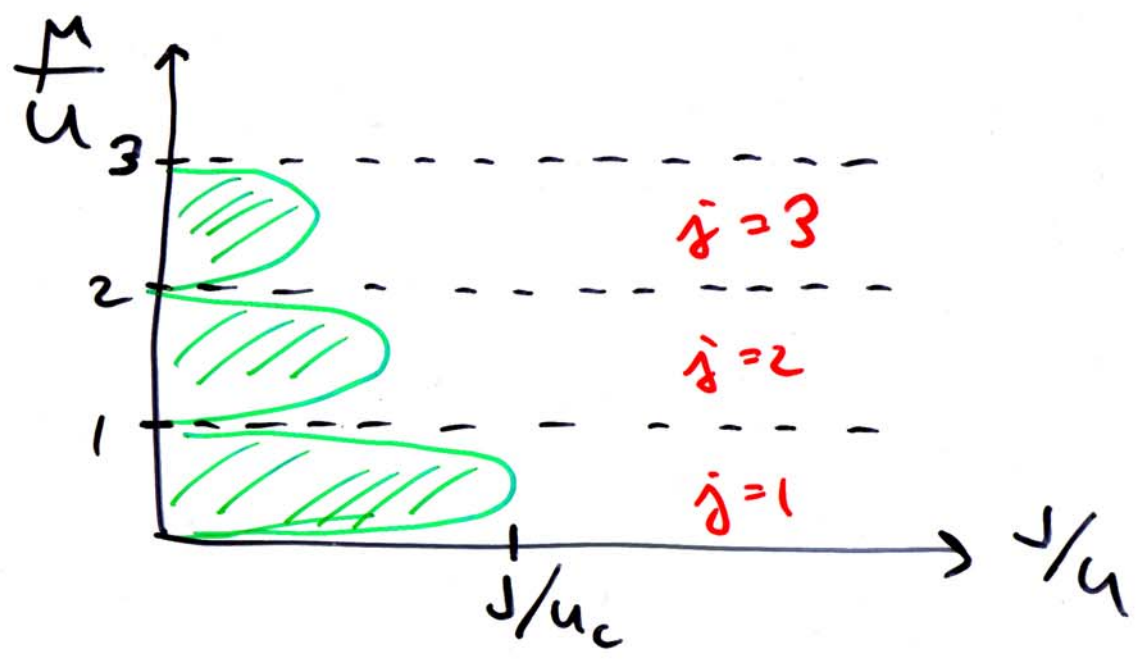
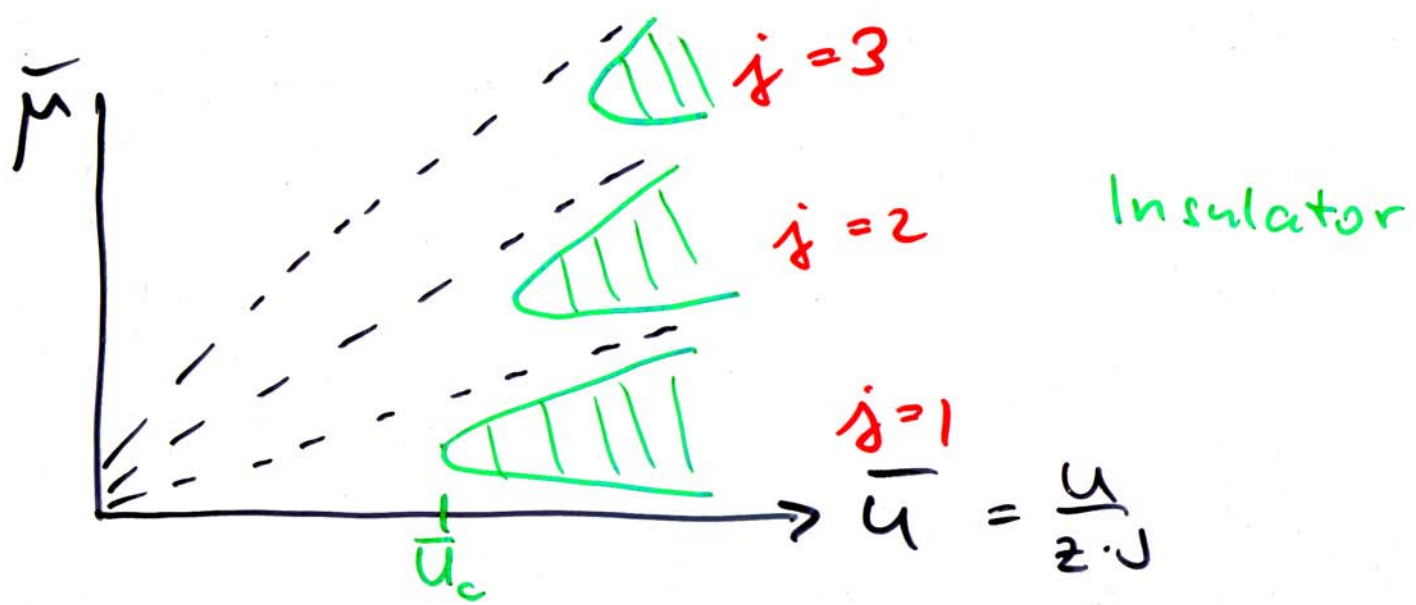
Phase transition for

$$a_2 = 0$$

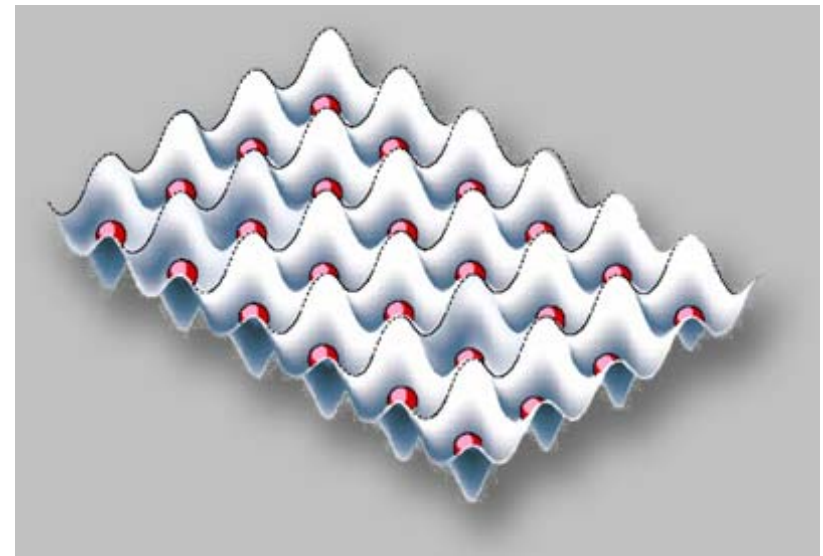
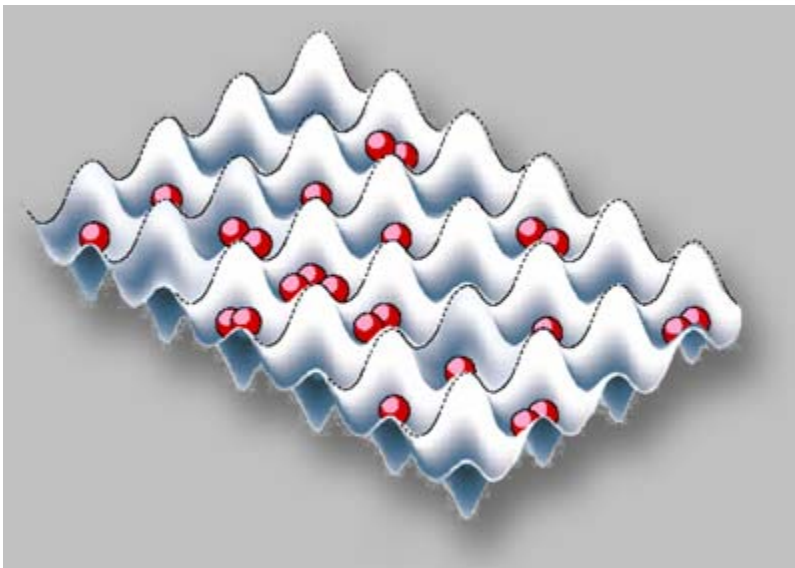
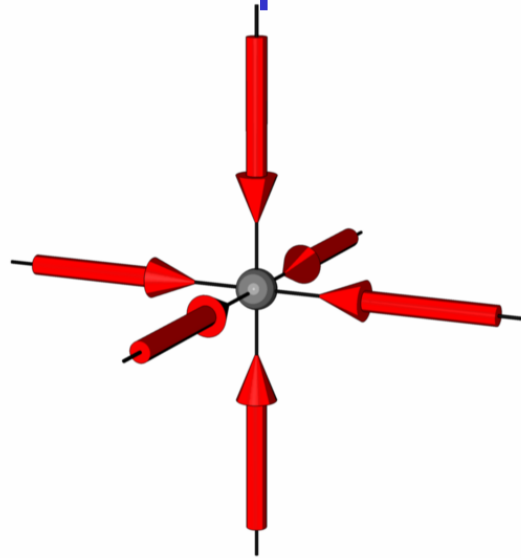
$$a_2 = \frac{j}{\bar{u}(j-1) - \bar{\mu}} + \frac{j+1}{\bar{\mu} - \bar{u}j} + 1 = 0$$

$$\bar{\mu}_{\pm} = \frac{1}{2} [\bar{u}(2j+1) - 1] \pm \frac{1}{2} \sqrt{\bar{u}^2 - 2\bar{u}(2j+1) + 1}$$





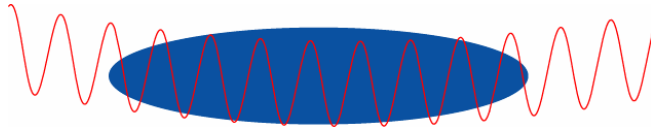
BEC in 3D optical lattice



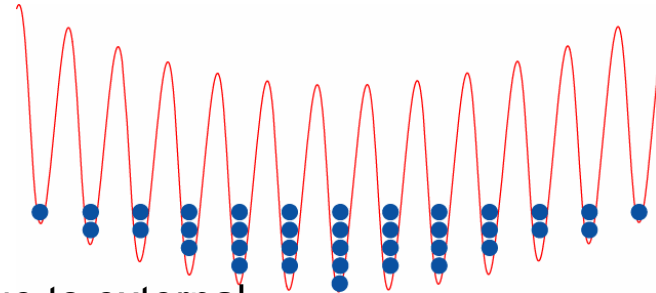
Courtesy Markus Greiner

The Superfluid-Mott Insulator transition

Shallow Lattices - Superfluid



Deep Lattices – Mott Insulator



Energy offset due to external harmonic confinement. Not in condensed matter systems.

$$\hat{H} = -J \sum_{\langle i,j \rangle} \hat{a}_i^\dagger \hat{a}_j + \sum_i \frac{1}{2} U \hat{n}_i (\hat{n}_i - 1) + \sum_i (\epsilon_i - \mu) \hat{n}_i$$

tunneling term between neighboring sites

$$J = \frac{4}{\sqrt{\pi}} E_r \left(\frac{V_0}{E_r} \right)^{3/4} \exp -2 \left(\frac{V_0}{E_r} \right)^{1/2}$$

on-site interaction

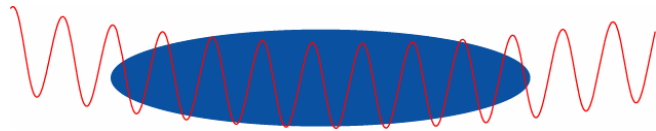
$$U = \left(\frac{4\pi\hbar^2 a}{m} \right) \int |w(x)|^4 d^3x$$

a = s-wave scattering length

Other exp: Mainz, Zurich, NIST Gaithersburg, Innsbruck, MPQ and others

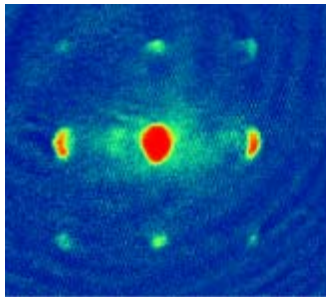
The Superfluid-Mott Insulator transition

Shallow Lattices - Superfluid

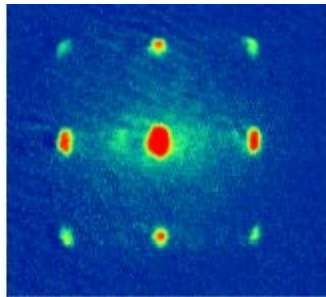


$$|\Psi_{SF}\rangle \propto \left(\sum_{i=1}^M \hat{a}_i^\dagger \right)^N |0\rangle$$

$$\hat{H} = -J \sum_{\langle i,j \rangle} \hat{a}_i^\dagger \hat{a}_j + \sum_i \frac{1}{2} U \hat{n}_i (\hat{n}_i - 1) + \sum_i (\epsilon_i - \mu) \hat{n}_i$$



5 E_{rec}

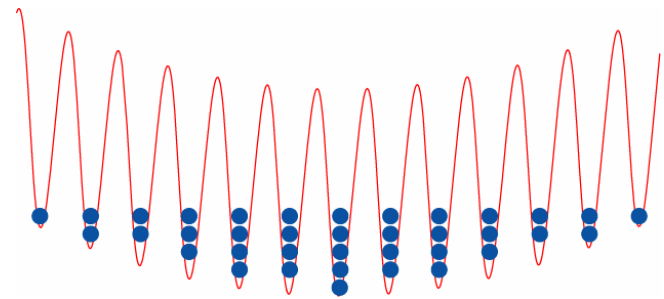


9 E_{rec}

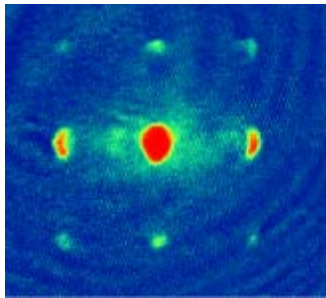
The Superfluid-Mott Insulator transition

Deep Lattices – Mott Insulator

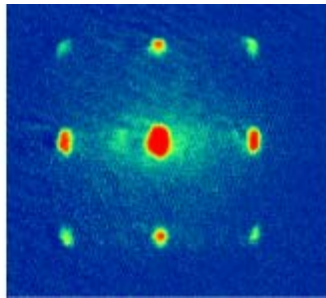
$$|\Psi_{MI}\rangle_{J=0} \propto \prod_{i=1}^M (\hat{a}_i^\dagger)^n |0\rangle$$



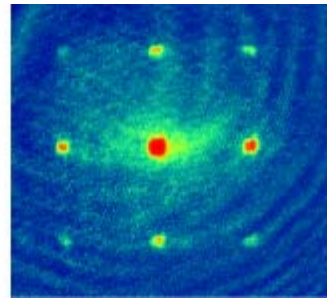
$$\hat{H} = -J \sum_{\langle i,j \rangle} \hat{a}_i^\dagger \hat{a}_j + \sum_i \frac{1}{2} U \hat{n}_i (\hat{n}_i - 1) + \sum_i (\epsilon_i - \mu) \hat{n}_i$$



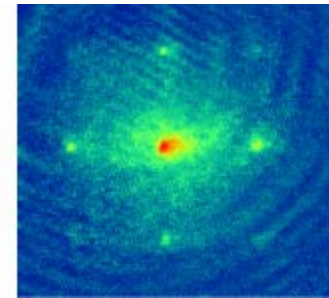
5 E_{rec}



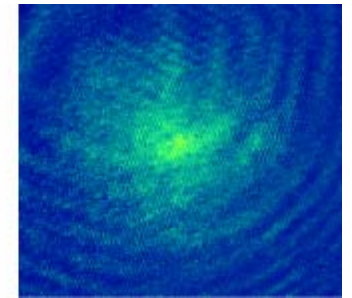
9 E_{rec}



12 E_{rec}



15 E_{rec}



20 E_{rec}

As the lattice depth is increased, J decreases exponentially, and U increases. For $J/U \ll 1$, number fluctuations are suppressed, and the atoms are localized

Nanokelvin atoms are a new toolbox to
address fundamental questions of many-body
physics

**Quantum simulations of strongly correlated,
strongly interacting systems**