Ultra-Cold Gases I – Theory of Cold Atoms

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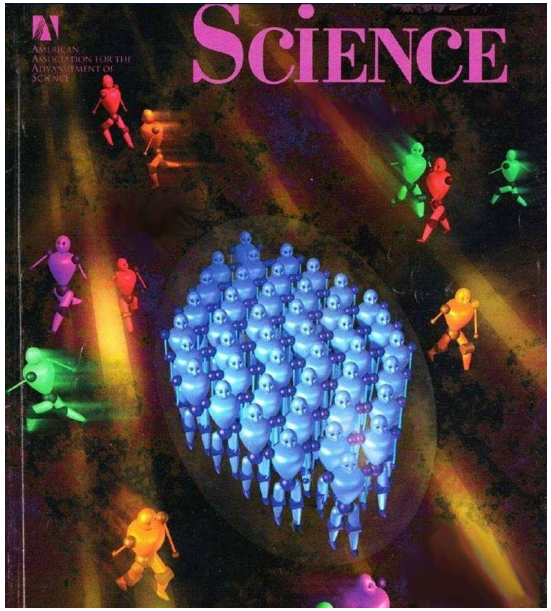
OPTIMAS TU Kaiserslautern

SFB/Transregio 49
Frankfurt – Kaiserslautern - Mainz
Condensed matter systems with variable many-body interactions

SFB/TR 185

1. Introduction
2. Dipolar Quantum Gases
3. Gross-Pitaevskii Theory
4. Quantum Droplets
5. Bosons in Optical Lattices
6. Conclusions



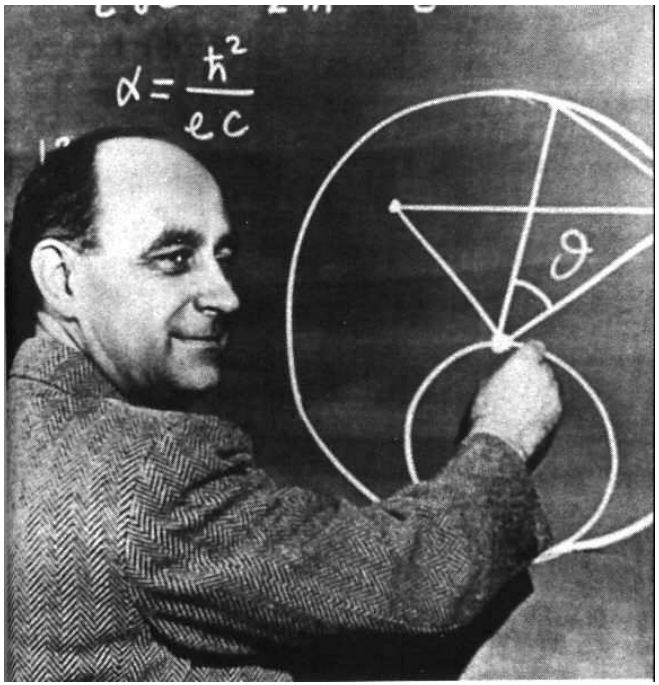
1.1 Identical Quantum Particles

Bosons:

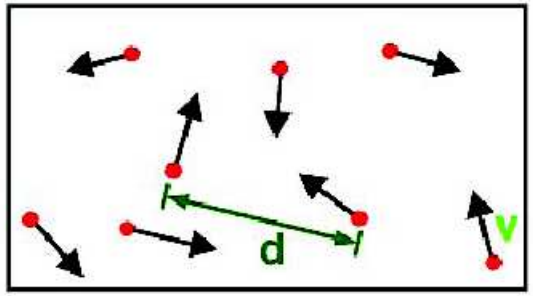
- integer spin
- symmetric wave function

Fermions:

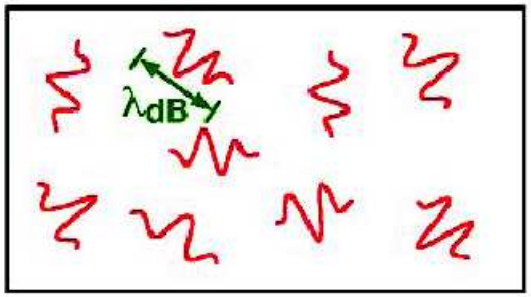
- half-integer spin
- anti-symmetric wave function



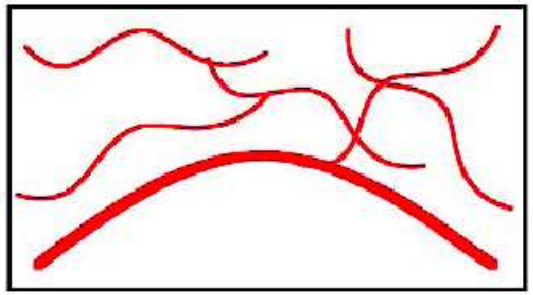
1.2 What is Bose-Einstein Condensation?



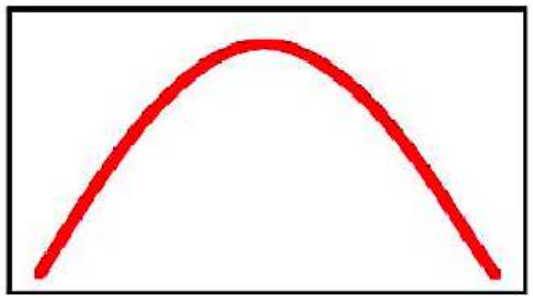
High Temperature T:
thermal velocity v
density d^{-3}
"Billiard balls"



Low Temperature T:
De Broglie wavelength
$\lambda_{dB}=h/mv \propto T^{-1/2}$
"Wave packets"



$T=T_{crit}$: Bose-Einstein Condensation
$\lambda_{dB} \approx d$
"Matter wave overlap"

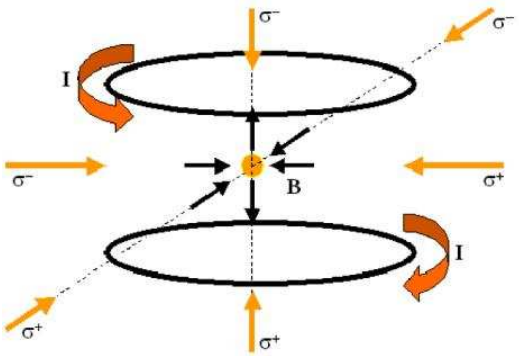


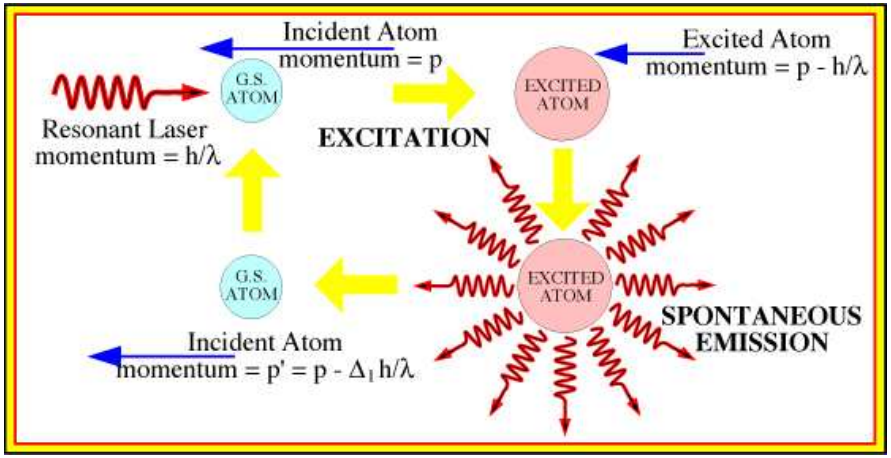
T=0: Pure Bose condensate
"Giant matter wave"

- $\lambda_{\mathrm{dB}} = \dfrac{\hbar}{\sqrt{2Mk_BT}}$
- $n = \dfrac{1}{d^3}$
- $\dfrac{\lambda_{\mathrm{dB}}}{d} \approx 1$
- $T_c \approx \dfrac{\hbar^2 n^{3/2}}{2Mk_B}$

1.3 Cooling Techniques

magneto-optical trap

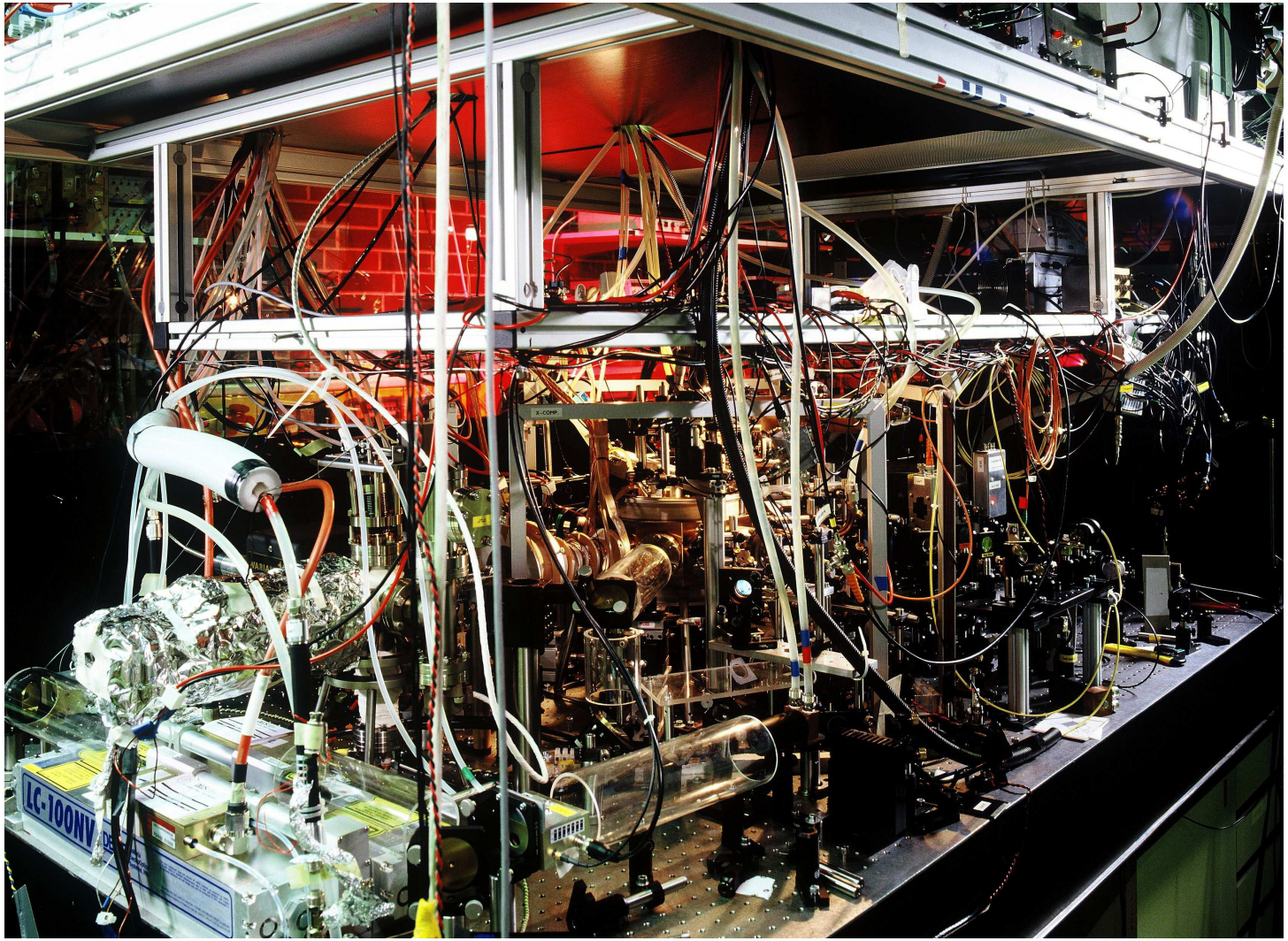




laser cooling

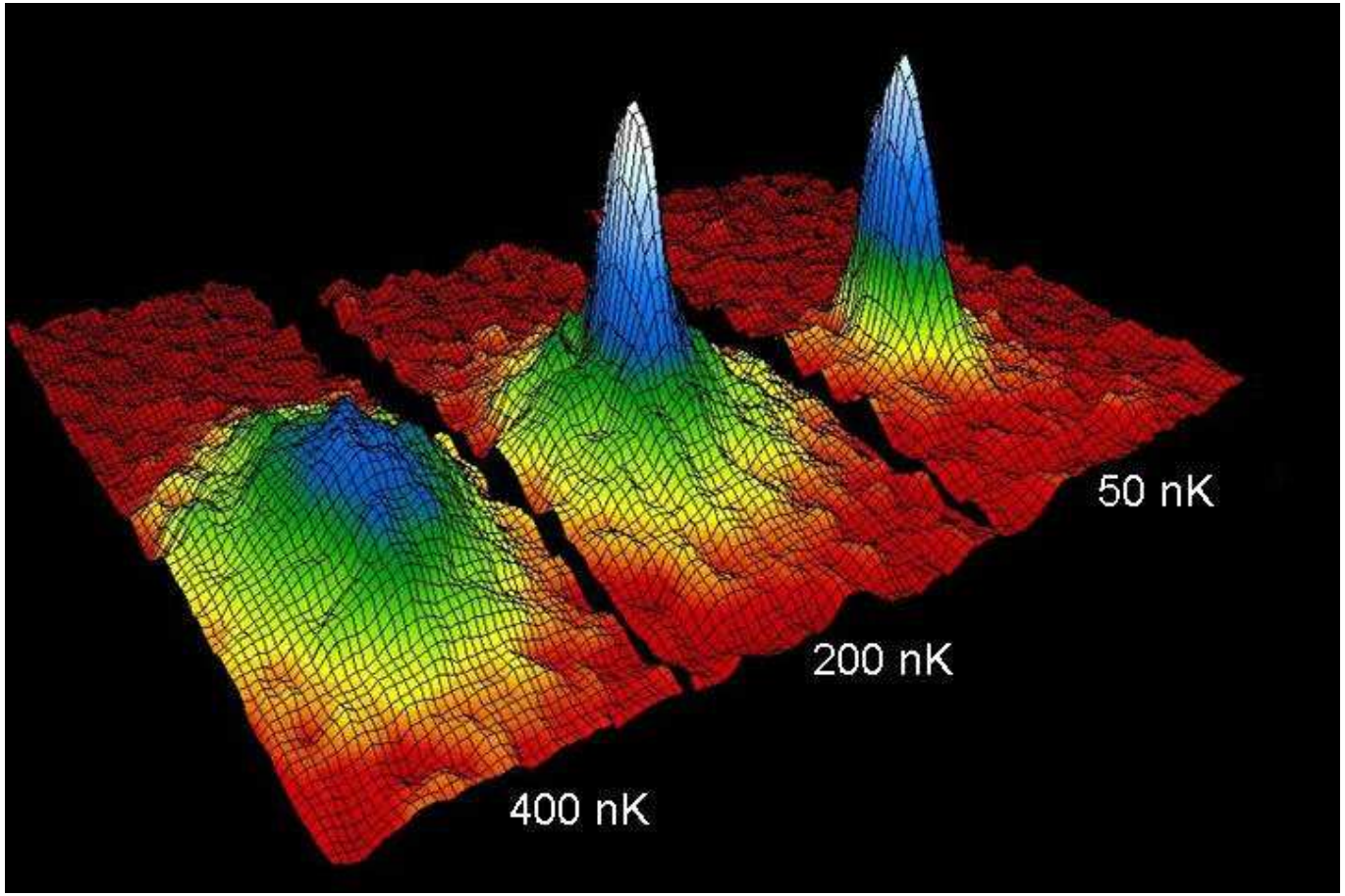
evaporative cooling

1.4 Experimental Apparatus



Costs about 1.000.000 EUR

1.5 Time-of-Flight Absorption Pictures



JILA (1995): $^{87}_{37}$Rb , N=20 000 , $\omega_1 = \omega_2 = \omega_3/\sqrt{8} = 2\pi\times$ 120 Hz

1.6 Periodic Table of Chemical Elements

Periode | ☐ = Hauptgruppen | ☐ = Nebengruppen | ☐ = Edelgase | Schale

Periode	I	II	IIIa	IVa	Va	VIa	VIIa	VIIIa			Ia	Ib	III	IV	V	VI	VII	VIII	Schale
1	1,008 H 1 Wasserstoff																	4,003 He 2 Helium	K
2	6,941 Li 3 Litium	9,012 Be 4 Beryllium											10,811 B 5 Bor	12,011 C 6 Kohlenstoff	14,007 N 7 Stickstoff	15,999 O 8 Sauerstoff	18,998 F 9 Fluor	20,180 Ne 10 Neon	L
3	22,990 Na 11 Natrium	24,305 Mg 12 Magnesium											26,982 Al 13 Aluminium	28,086 Si 14 Silicium	30,974 P 15 Phosphor	32,066 S 16 Schwefel	35,453 Cl 17 Chlor	39,948 Ar 18 Argon	M
4	39,098 K 19 Kalium	40,078 Ca 20 Calcium	44,956 Sc 21 Scandium	47,88 Ti 22 Titan	50,942 V 23 Vanadin	51,996 Cr 24 Chrom	54,938 Mn 25 Mangan	55,847 Fe 26 Eisen	58,933 Co 27 Kobalt	58,69 Ni 28 Nickel	63,546 Cu 29 Kupfer	65,39 Zn 30 Zink	69,723 Ga 31 Gallium	72,61 Ge 32 Germanium	74,922 As 33 Arsen	78,96 Se 34 Selen	79,904 Br 35 Brom	83,8 Kr 36 Krypton	N
5	85,468 Rb 37 Rubidium	87,62 Sr 38 Strontium	88,906 Y 39 Yttrium	91,224 Zr 40 Zirconium	92,906 Nb 41 Niob	95,94 Mo 42 Molybdän	98,906 Tc 43 * Technetium	101,07 Ru 44 Ruthenium	102,906 Rh 45 Rhodium	106,42 Pd 46 Palladium	107,868 Ag 47 Silber	112,411 Cd 48 Cadmium	114,82 In 49 Indium	118,71 Sn 50 Zinn	121,75 Sb 51 Antimon	127,6 Te 52 Tellur	126,904 I 53 Iod	131,29 Xe 54 Xenon	O
6	132,905 Cs 55 Cäsium	137,327 Ba 56 Barium	138,906 La 57 Lanthan	178,49 Hf 72 Hafnium	180,948 Ta 73 Tantal	183,85 W 74 Wolfram	186,207 Re 75 Rhenium	190,2 Os 76 Osmium	192,22 Ir 77 Iridium	195,08 Pt 78 Platin	196,967 Au 79 Gold	200,59 Hg 80 Quecksilber	204,383 Tl 81 Thallium	207,2 Pb 82 Blei	208,98 Bi 83 Bismut	208,982 Po 84 * Polonium	209,987 At 85 * Astat	222,018 Rn 86 * Radon	P
7	223,02 Fr 87 * Francium	226,025 Ra 88 * Radium	227,028 Ac 89 * Actinium	261,109 Rf 104 * Rutherfordium	262,114 Ha 105 * Hahnium	263,118 Sg 106 * Seaborgium	262,123 Ns 107 * Nielsbohrium	ca. 265 Hs 108 * Hassium	ca. 268 Mt 109 * Meitnerium	ca. 269 Ds 110 * Darmstadtium	ca. 272 Rg 111 * Roentgenium	ca. 277 ? 112 *		ca. 289 ? 114 *		ca. 289 ? 116 *		ca. 293 ? 118 *	Q

Lanthanide

6	140,12 Ce 58 Cer	140,91 Pr 59 Praseodym	144,24 Nd 60 Neodym	145 Pm 61 * Promethium	150,35 Sm 62 Samarium	151,96 Eu 63 Europium	157,25 Gd 64 Gadolinium	158,92 Tb 65 Terbium	162,50 Dy 66 Dysprosium	164,93 Ho 67 Holmium	167,26 Er 68 Erbium	168,93 Tm 69 Thulium	173,04 Yb 70 Ytterbium	174,97 Lu 71 Lutetium

Actinide

7	232,04 Th 90 * Thorium	231 Pa 91 * Protactinium	238,03 U 92 * Uran	237 Np 93 * Neptunium	244 Pu 94 * Plutonium	243 Am 95 * Americium	247 Cm 96 * Curium	247 Bk 97 * Berkelium	251 Cf 98 * Californium	254 Es 99 * Einsteinium	257 Fm 100 * Fermium	258 Md 101 * Mendelevium	259 No 102 * Nobelium	260 Lr 103 * Lawrencium

Aggregatzustand unter Normalbedingungen:

- Fe fest
- Hg flüssig
- He gasförmig

* = radioaktives Element

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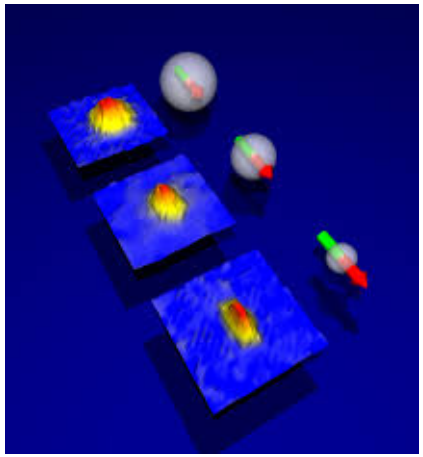


2.1 Magnetic versus Electric Dipolar Systems

- **Magnetic systems:** $C_{\rm dd}^{\mathcal{B}} = \mu_0 m^2$, with $m \sim 1$ to $10\ \mu_B$
  - Realized samples
    Boson: ^{52}Cr Griesmaier *et al.*, PRL **94**, 160401 (2005)
    Boson: ^{87}Rb Vengalattore *et al.*, PRL **100**, 170403 (2008)
    Fermion: ^{53}Cr Chicireanu *et al.*, PRA **73**, 053406 (2006)
    Both: Dy Lu *et al.*, PRL **104**, 063001 (2010); PRL **107**, 190401 (2011)
    Boson: ^{168}Er Aikawa *et al.*, PRL **108**, 210401 (2012)
    Fermion: ^{167}Er Aikawa *et al.*, Science **345**, 1484 (2014)
  - Effects: Bose-nova explosion (Cr), Fermi surface deformation (Er)

- **Electric systems:** $C_{\rm dd}^{\mathcal{E}} = d^2/\epsilon_0$, with $d \sim 1$ Debye
  - Realized samples **(STIRAP: STImulated Raman Adiabatic Passage)**
    Fermion: ^{40}K^{87}Rb Ospelkaus *et al.*, Science **32**, 231 (2008)
    Boson: ^{41}K^{87}Rb Aikawa *et al.*, NJP **11**, 055035 (2009)
  - Effects: thermalization (^{40}K^{87}Rb)

- **Ratio:** $C_{\rm dd}^{\mathcal{B}}/C_{\rm dd}^{\mathcal{E}} \approx \alpha^2 \approx 10^{-4}$, $\qquad \alpha = e^2/(4\pi\epsilon_0\hbar c) \approx 1/137$

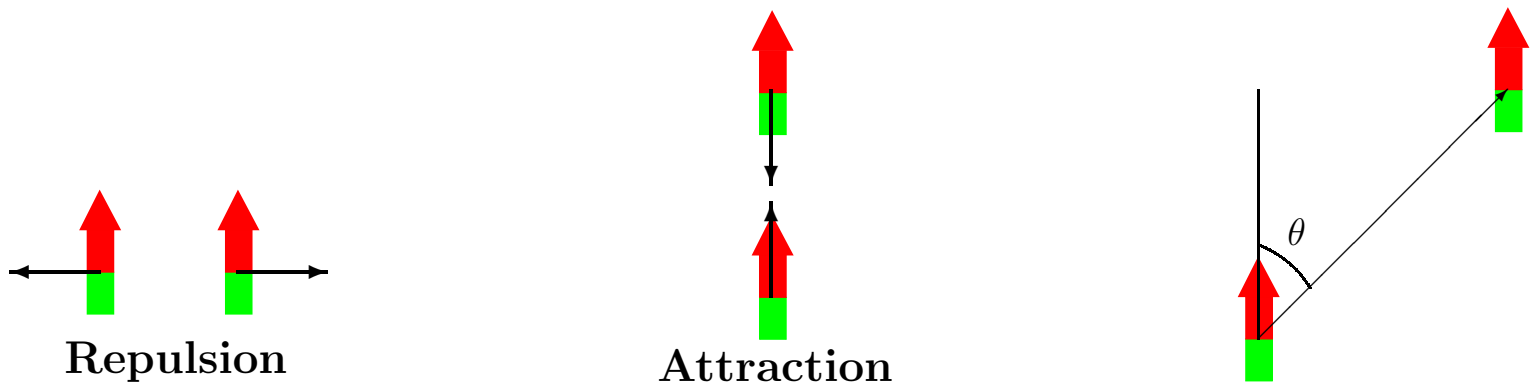
2.2 Trapping and Interaction Potentials

- **Harmonic trap:**

$$U_{\text{trap}}(\mathbf{x}) = \frac{M}{2}\left[\omega_\perp^2\left(x^2+y^2\right)+\omega_z^2 z^2\right]$$

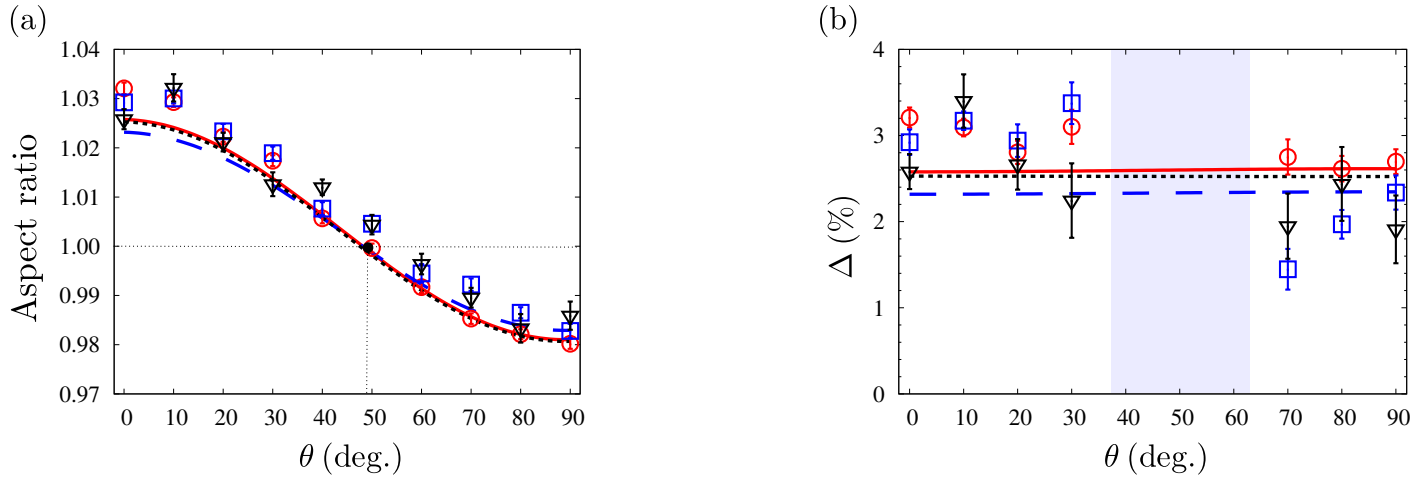
- **Interaction potential:**

$$V_{\text{int}}(\mathbf{x}-\mathbf{x}') = g\left[\delta(\mathbf{x}-\mathbf{x}')+\frac{3\epsilon_{\text{dd}}}{4\pi|\mathbf{x}-\mathbf{x}'|^3}\left(1-3\cos^2\theta\right)\right], \qquad \epsilon_{\text{dd}} = \frac{C_{\text{dd}}}{3g}$$

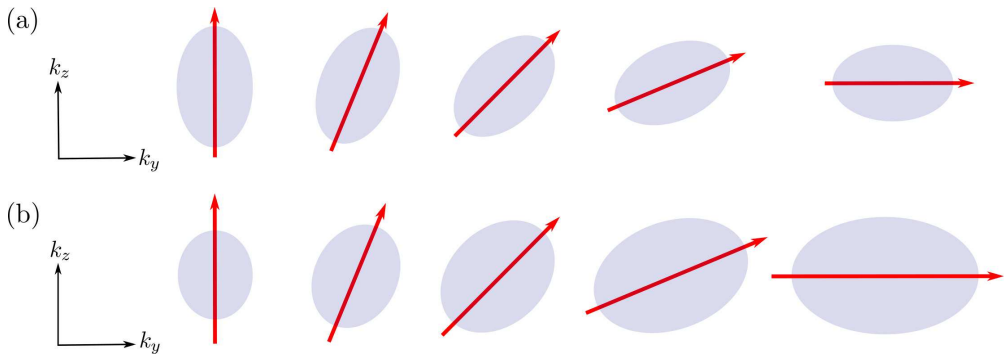


2.3 Fermi Surface Deformation (T=0)

- **Theoretical analysis of Erbium TOF data:**



- **Schematic Fermi surface deformation:**



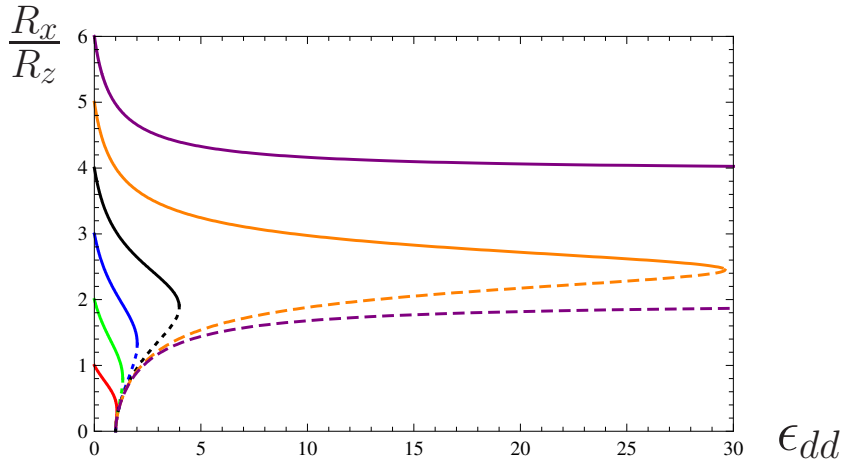
Veljić *et al.*, NJP **20**, 093016 (2018)

2.4 BEC Mean-Field Results (T=0)

- **Aspect ratio:**

  O'Dell *et al.*,

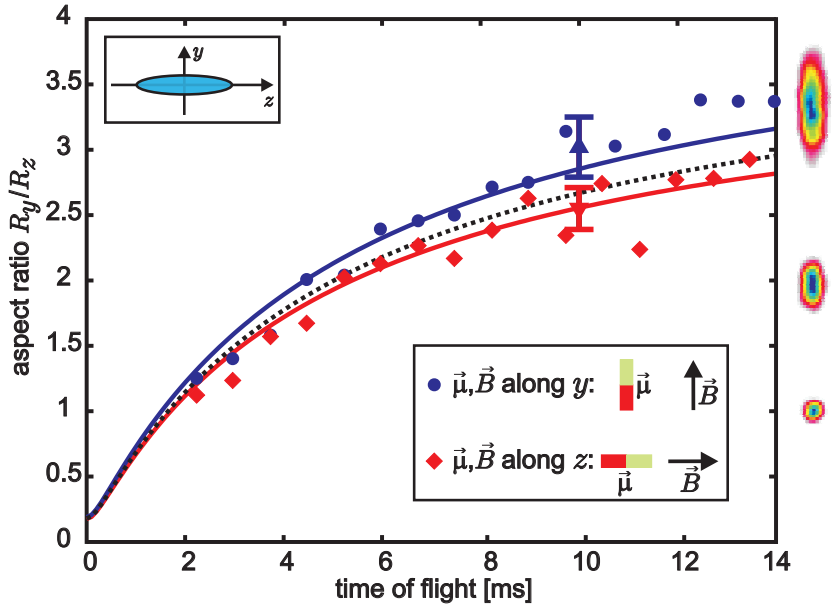
  PRL **92**, 205401 (2004)



- **Time-of-flight:**

  Stuhler *et al.*,

  PRL **95**, 150406 (2005)



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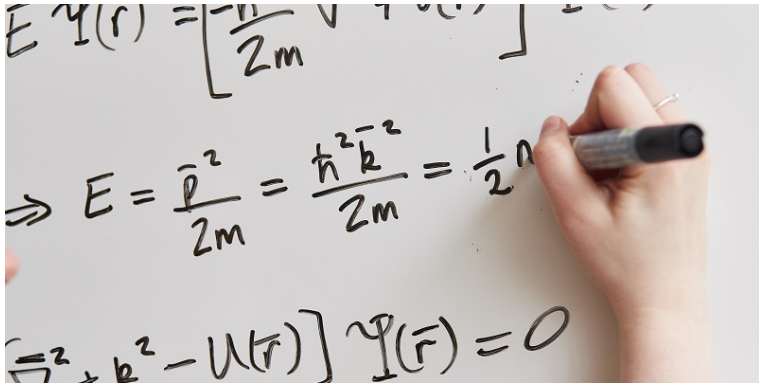


3.1 Many-Body Theory

- **Hamiltonian:** $\hat{H} = \hat{H}_0 + \hat{H}_{\rm int}$

- **Free Hamiltonian:**

$$\hat{H}_0 = \int d^3x\, \hat{\Psi}^\dagger(\mathbf{x},t) \left[-\frac{\hbar^2}{2m}\Delta + U_{\rm trap}(\mathbf{r}) \right] \hat{\Psi}(\mathbf{x},t)$$

- **Interaction Hamiltonian:**

$$\hat{H}_{\rm int} = \frac{1}{2} \int d^3x \int d^3x'\, \hat{\Psi}^\dagger(\mathbf{x},t)\hat{\Psi}^\dagger(\mathbf{x}',t) V_{\rm int}(\mathbf{x}-\mathbf{x}')\hat{\Psi}(\mathbf{x}',t)\hat{\Psi}(\mathbf{x},t)$$

- **Bosonic commutation relations:**

$$\left[\hat{\Psi}(\mathbf{x},t), \hat{\Psi}^\dagger(\mathbf{x}',t)\right] = \delta(\mathbf{x}-\mathbf{x}'), \left[\hat{\Psi}(\mathbf{x},t), \hat{\Psi}(\mathbf{x}',t)\right] = \left[\hat{\Psi}^\dagger(\mathbf{x},t), \hat{\Psi}^\dagger(\mathbf{x}',t)\right] = 0$$

3.2 Mean-Field Theory

- **Nearly all bosons occupy at $T = 0$ the ground state.**

- **Bogoliubov prescription:**

$$\hat{\Psi}(\mathbf{x}, t) = \psi(\mathbf{x}, t) + \delta\hat{\Psi}(\mathbf{x}, t), \qquad \hat{\Psi}^\dagger(\mathbf{x}, t) = \psi^*(\mathbf{x}, t) + \delta\hat{\Psi}^\dagger(\mathbf{x}, t)$$

- **Heisenberg equation:** $$i\hbar\frac{\partial}{\partial t}\hat{\Psi}(\mathbf{x}, t) = \left[\hat{\Psi}(\mathbf{x}, t), \hat{H}\right]$$

- **Zeroth order = Gross-Pitaevskii mean-field theory:**

$$\hat{\Psi}(\mathbf{x}, t) \approx \psi(\mathbf{x}, t), \qquad \hat{\Psi}^\dagger(\mathbf{x}, t) \approx \psi^*(\mathbf{x}, t)$$

- **Time-dependent Gross-Pitaevskii equation:**

$$i\hbar\frac{\partial\psi(\mathbf{x}, t)}{\partial t} = \left[-\frac{\hbar^2}{2m}\triangle + U_{\text{trap}}(\mathbf{x}) + \int d^3x'\, V_{\text{int}}(\mathbf{x} - \mathbf{x}')|\psi(\mathbf{x}', t)|^2\right]\psi(\mathbf{x}, t)$$

3.3 Time-Independent Gross-Pitaevskii Equation

- **Separation ansatz:** $\psi(\mathbf{x},t) = \psi(\mathbf{x})e^{-i\mu t/\hbar}$

- **Nonlinear Schrödinger equation:**

$$\left[-\frac{\hbar^2}{2m}\triangle + U_{\text{trap}}(\mathbf{x}) + \int d^3x'\, V_{\text{int}}(\mathbf{x}-\mathbf{x}')|\psi(\mathbf{x}')|^2\right]\psi(\mathbf{x}) = \mu\psi(\mathbf{x})$$

- **Harmonic trap:** $U_{\text{trap}}(\mathbf{x}) = \frac{M}{2}\left[\omega_\perp^2\left(x^2+y^2\right) + \omega_z^2 z^2\right]$

- **Interaction potential:** $V_{\text{int}}(\mathbf{x}-\mathbf{x}') = g\delta(\mathbf{x}-\mathbf{x}') + V_{\text{dd}}(\mathbf{x}-\mathbf{x}')$

- **No interaction:** $\psi(\mathbf{x}) = C\,\exp\left[-\frac{1}{2}\left(\frac{x^2+y^2}{l_\perp^2} + \frac{z^2}{l_z^2}\right)\right]$

- **Oscillator lengths:** $l_\perp = \sqrt{\frac{\hbar}{M\omega_\perp}}, \quad l_z = \sqrt{\frac{\hbar}{M\omega_z}}$

$$\omega_\perp = \omega_z = 2\pi\,100\ \text{Hz}\,, \qquad M\left({}^{87}_{37}\text{Rb}\right) = 87\ u \qquad \Longrightarrow \qquad l_\perp = l_z = 1\mu\text{m}$$

3.4 Thomas-Fermi Approximation: Contact Potential

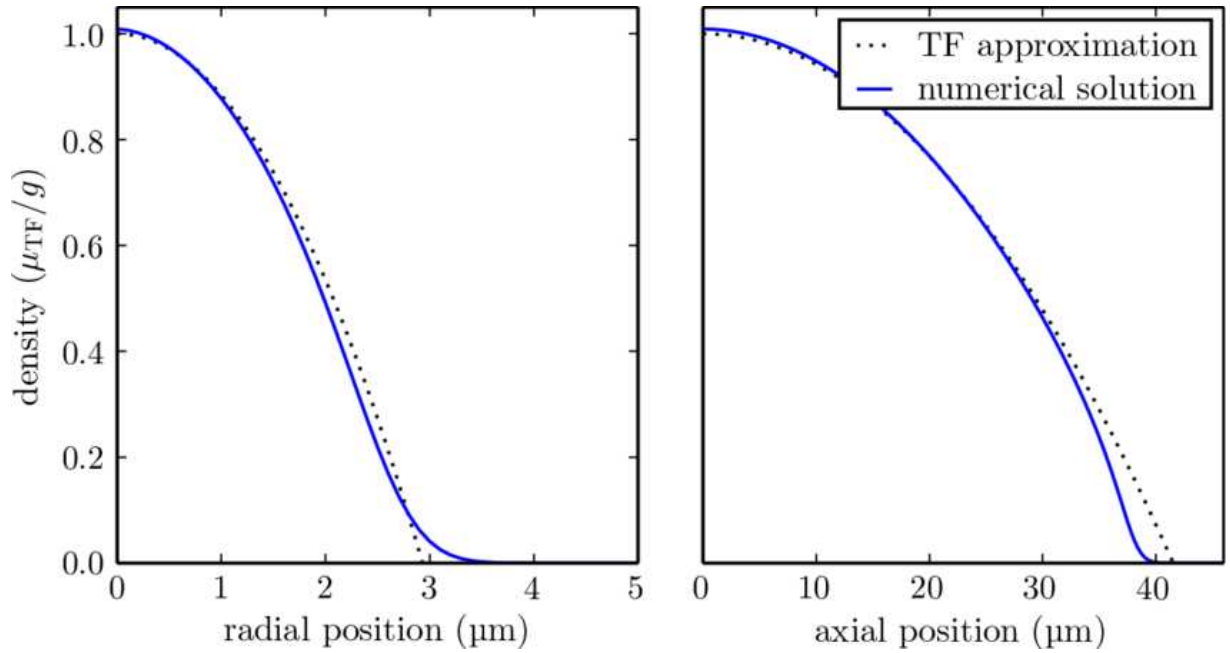
- **Strong contact interaction: neglect kinetic energy**

$$\left[U_{\text{trap}}(\mathbf{x}) + g|\psi(\mathbf{x})|^2\right]\psi(\mathbf{x}) = \mu\psi(\mathbf{x}) \qquad \Longrightarrow \qquad |\psi(\mathbf{x})|^2 = \frac{\mu - U_{\text{trap}}(\mathbf{x})}{g}$$

- **Thomas-Fermi radii:** $R_i = \sqrt{\dfrac{2\mu}{M\omega_i^2}}$

- **Normalization:** $N = \displaystyle\int d^3x\, |\psi(\mathbf{x})|^2 \qquad \Longrightarrow \qquad R_i = \left(15\,\frac{aN}{\tilde{l}}\right)^{1/5}\sqrt{\frac{\tilde{\omega}}{\omega_i}}\, l_i$

$$g = \frac{4\pi\hbar^2}{M}\,a\,, \qquad a\left({}^{87}_{37}\mathrm{Rb}\right) = 100\,a_{\mathrm{B}}\,, \qquad N = 10^6 \qquad \Longrightarrow \qquad R \approx 10\,l$$



3.5 Exercise Sheet

- **Solution of time-independent Gross-Pitaevskii equation with contact and dipolar interaction in Thomas-Fermi approximation**

- **Integral equation:**

$$U_{\text{trap}}(\mathbf{x}) + g \underbrace{|\psi(\mathbf{x})|^2}_{\text{harmonic ansatz}} + \underbrace{\int d^3x' V_{\text{dd}}(\mathbf{x}-\mathbf{x}')|\psi(\mathbf{x}')|^2}_{\text{convolution turns out to be harmonic}} = \mu$$

- **Comparison:**

$$\frac{\kappa^2}{\lambda^2}\left[\frac{3\epsilon_{\text{dd}} f(\kappa)}{1-\kappa^2}\left(\frac{\kappa^2}{\lambda^2}+1\right) - 1 - 2\epsilon_{\text{dd}}\right] = \epsilon_{\text{dd}} - 1$$

trap aspect ratio: $\lambda = \frac{\omega_z}{\omega_\perp}$, **cloud aspect ratio:** $\kappa = \frac{R_\perp}{R_z}$

relative strength: $\epsilon_{\text{dd}} = \frac{\mu_0 m^2}{3g}$, **anisotropy function:** $f(\kappa) = ?$

- **Note:** $\kappa(\epsilon_{\text{dd}} = 0) = \lambda$

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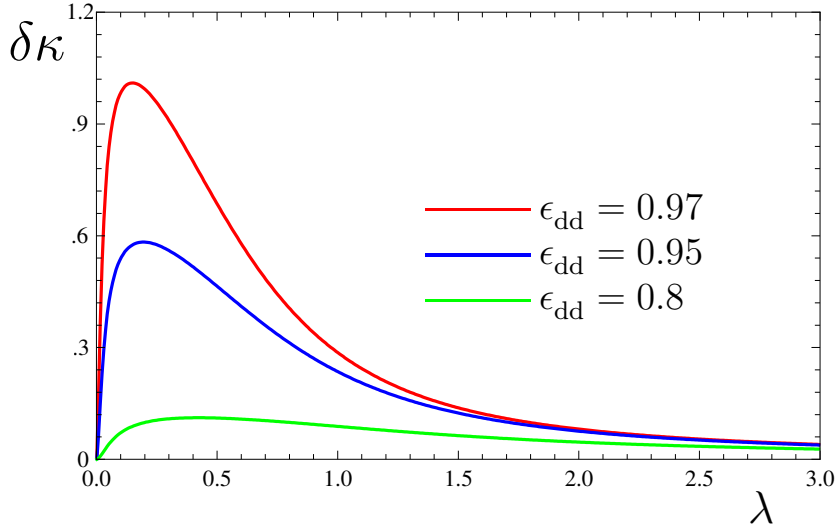
4.1 BEC Beyond Mean-Field Results (T=0)

- **Aspect ratio:**

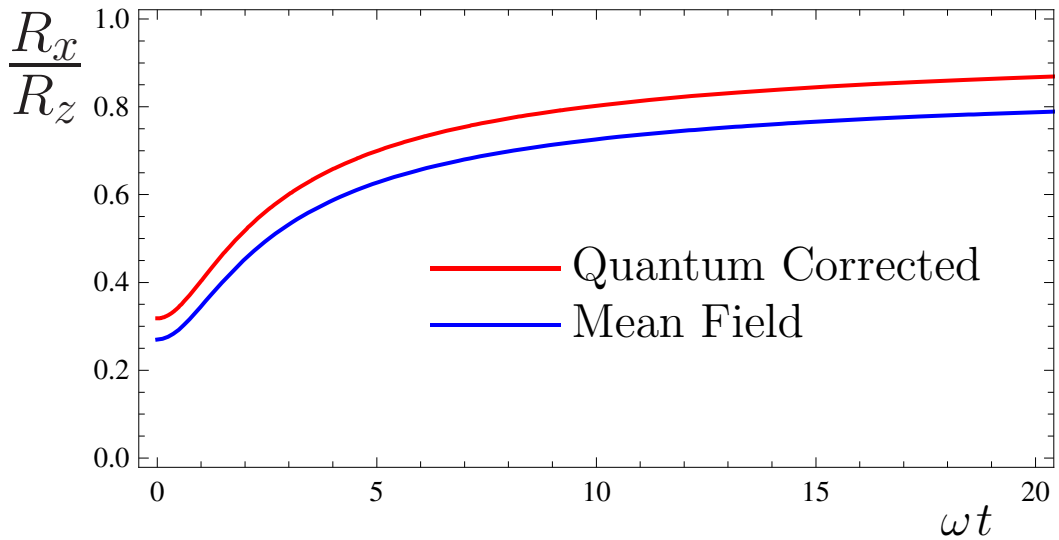
$$\frac{R_x}{R_z} = \kappa_{\mathrm{MF}}\left(1 + \delta\kappa\right)$$



- **Time-of-flight:**

expected for Dy

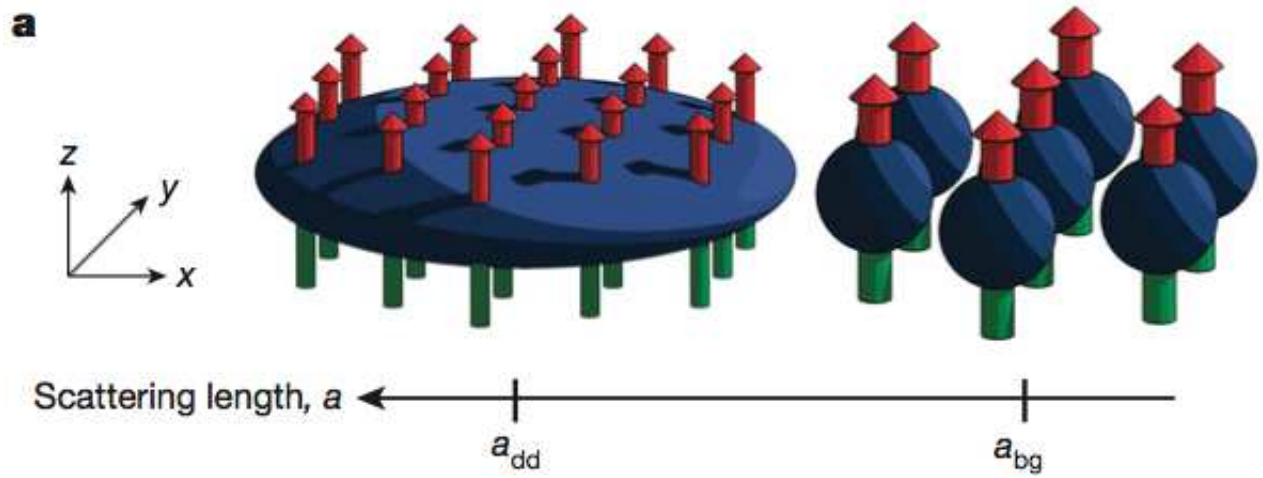
$\epsilon_{\mathrm{dd}} = 0.9$



Lima and Pelster, PRA **84**, 041604(R) (2011); PRA **86**, 063609 (2012)

4.2 Quantum Droplets - A New State of Matter

- **Spontaneous transition from BEC to quantum droplets:**



Kadau *et al.*, Nature **530**, 194 (2016)

- **Three-body interaction?**

Xi and Saito, PRA **93**, 011604(R) (2016)

Bisset and Blakie, PRA **92**, 061603(R) (2015); Blakie, PRA **93**, 033644 (2016)

- **Quantum fluctuations!**

Wächtler and Santos, PRA **93**, 061603(R) (2016)

4.3 Theory for Quantum Droplets

- **Extended Gross-Pitaevskii Equation:**

$$i\hbar\frac{\partial\psi(\mathbf{x},t)}{\partial t} = \left[-\frac{\hbar^2}{2m}\triangle + U_{\text{trap}}(\mathbf{x}) + \int d^3x'\, V_{\text{int}}(\mathbf{x}-\mathbf{x}')|\psi(\mathbf{x}',t)|^2 + V_{\text{QF}}(\mathbf{x},t)\right]\psi(\mathbf{x},t)$$

Wächtler and Santos, PRA **93**, 061603(R) (2016)

- **Quantum fluctuations with Local Density Approximation (LDA):**

$$V_{\text{QF}}(\mathbf{x},t) = \frac{32}{3}g\sqrt{\frac{a^3}{\pi}}\,\mathcal{Q}_5(\epsilon_{\text{dd}})|\psi(\mathbf{x},t)|^3$$

Lima and Pelster, PRA **84**, 041604(R) (2011); PRA **86**, 063609 (2012)

- **Open Questions:**
  - **Imaginary part of quantum fluctuation correction?**
  - **Beyond LDA corrections?**

    Böttcher *et al.*, arXiv:1904.10349 (2019)
  - **Coherence between quantum droplets:**

    Böttcher *et al.*, PRX **9**, 011051 (2019)

    Chomaz *et al.*, PRX **9**, 021012 (2019)

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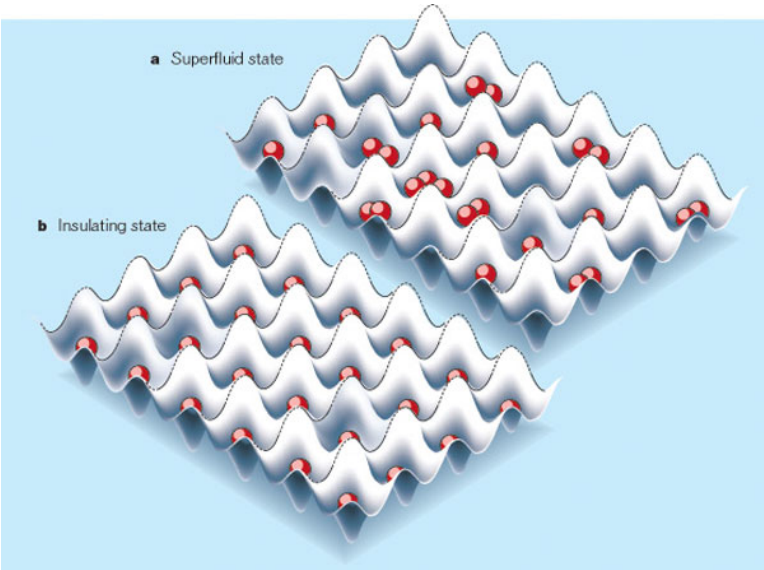
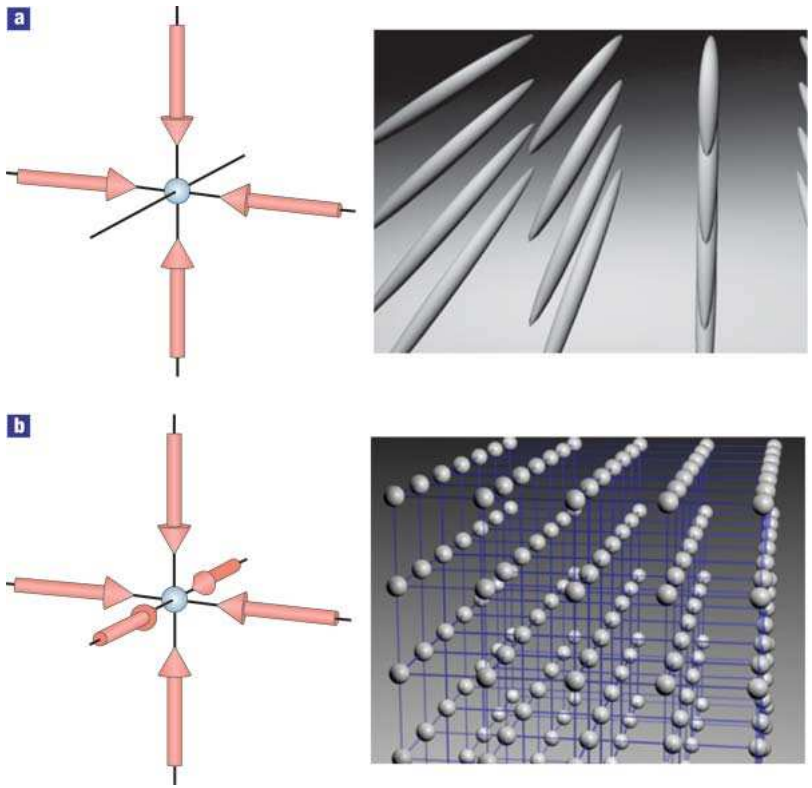


5.1 Optical Lattice

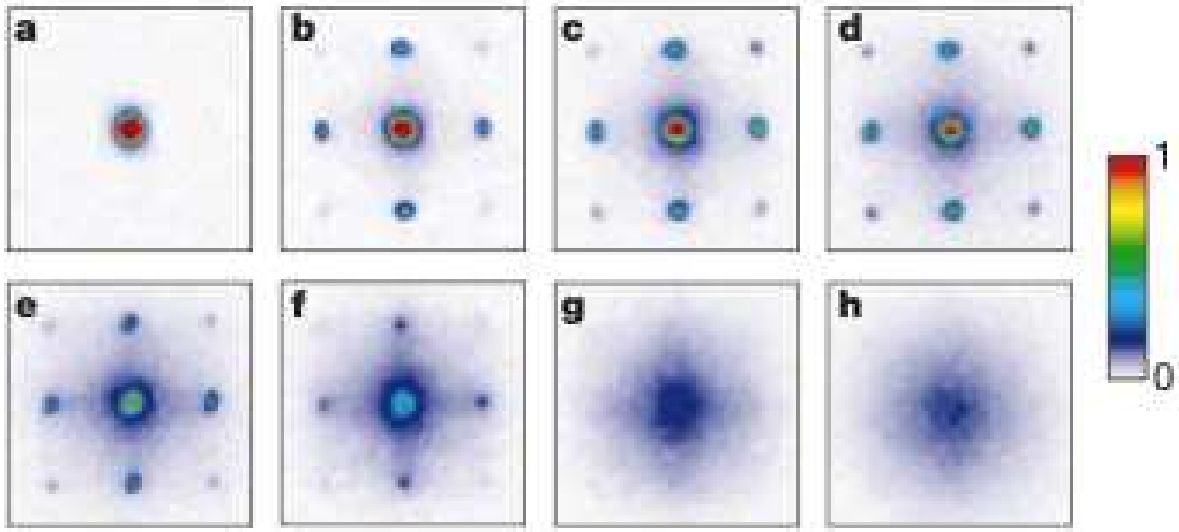
- Counter-propagating laser beams create periodic potential
- Different possible topologies at 1D, 2D, and 3D
- Hopping and interactions are highly controllable



5.2 Time-of-Flight Absorption Pictures

- **Superfluid phase:**
  delocalization in space, localization in Fourier space

- **Mott phase:**
  localization in space, delocalization in Fourier space



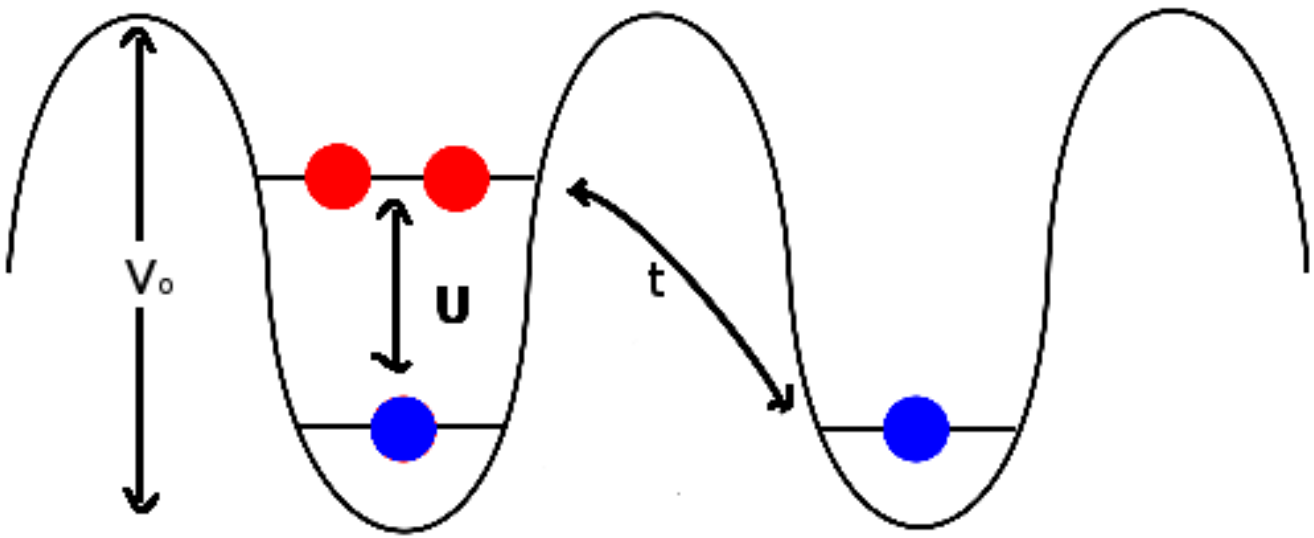
Greiner, Mandel, Esslinger, Hänsch, and Bloch, Nature **415**, 39 (2002)

5.3 Theoretical Description

Bose-Hubbard Hamiltonian:

$$\hat{H}_{\mathrm{BH}} = -t \sum_{\langle i,j \rangle} \hat{a}_i^\dagger \hat{a}_j + \sum_i \left[\frac{U}{2} \hat{n}_i (\hat{n}_i - 1) - \mu \hat{n}_i \right], \qquad \hat{n}_i = \hat{a}_i^\dagger \hat{a}_i$$

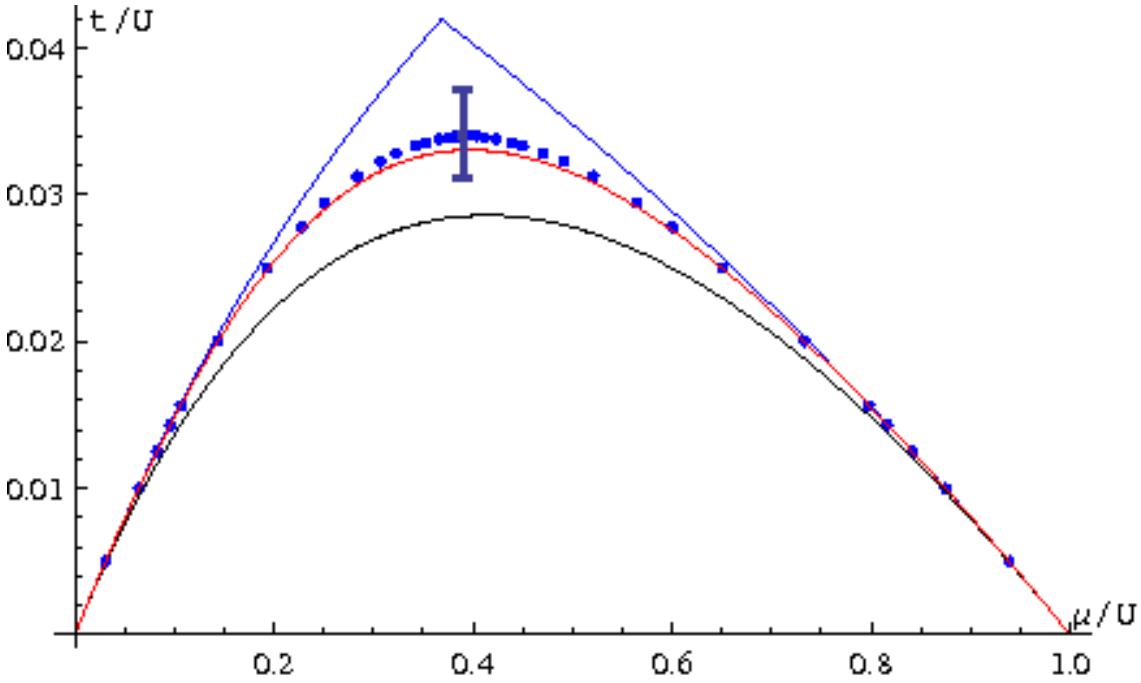
System parameters:



Fisher *et al.*, PRB **40**, 546 (1989)

5.4 Landau Theory

Quantum phase diagram (T=0):



Blue line: 3rd strong-coupling order

Blue dots: Monte-Carlo data

Red line: Landau theory

Black line: Mean-field

Santos and Pelster, PRA **79**, 013614 (2009)

Extension to higher orders:

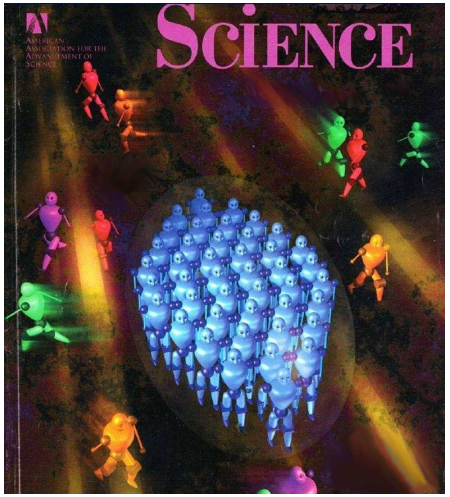
Teichmann, Hinrichs, Holthaus, and Eckardt, PRB **79**, 100503(R) (2009)

Ultra-Cold Gases I – Theory of Cold Atoms

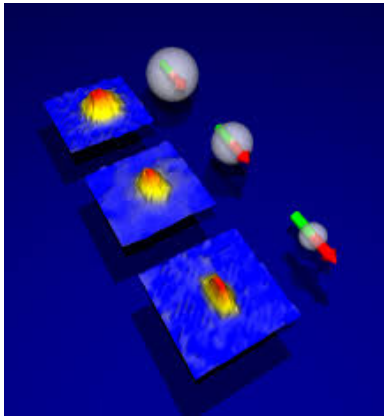
Axel Pelster

1. Introduction
2. Dipolar Quantum Gases
3. Gross-Pitaevskii Theory
4. Quantum Droplets
5. Bosons in Optical Lattices
6. Conclusions

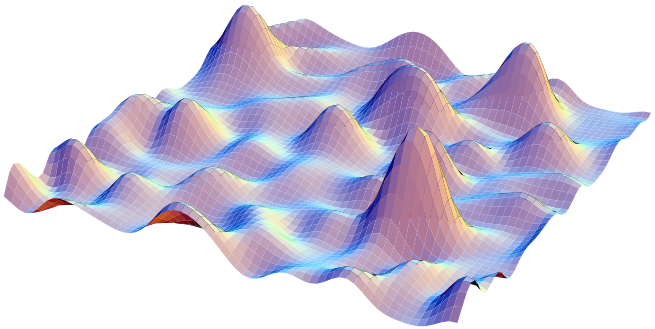
6.1 Summary and Outlook



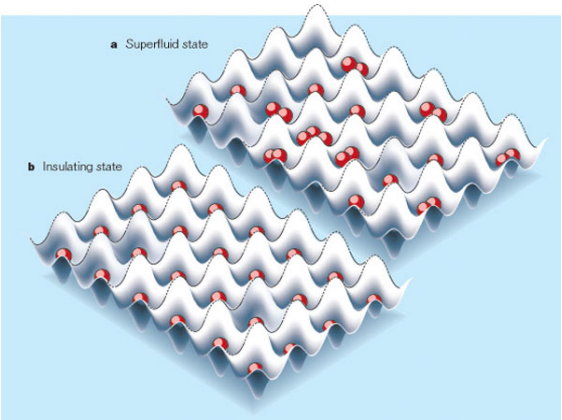
quantum simulation



anisotropic superfluidity



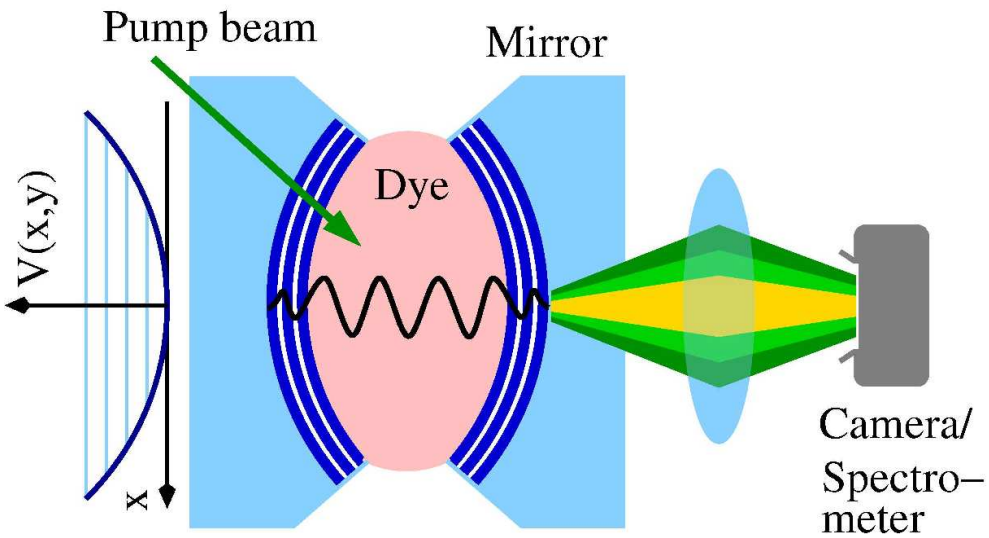
disorder



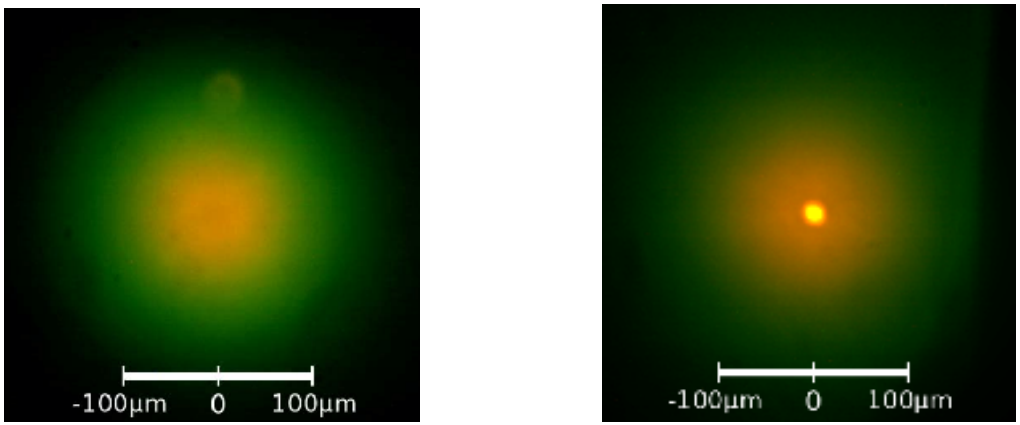
driven optical lattices

6.2 Bose-Einstein Condensation of Light

Set-up



Result



Klaers, Schmitt, Vewinger, and Weitz, Nature **468**, 545 (2010)

Pelster, Physik-Journal **10**, Nr. 1, 20 (2011); Physik-Journal **13**, Nr. 3, 20 (2014)

Radonjić, Kopylov, Balaž, and A. Pelster, NJP **20**, 055014 (2018)

6.3 Bad Honnef Physics School on Methods of Path Integration in Modern Physics

organized by Stefan Kirchner and Axel Pelster

Bad Honnef (Germany); August 25 – 31, 2019

Speakers and Topics:

Lawrence Schulman (Potsdam, USA): *Quantum Mechanics*

Andreas Wipf (Jena, Germany): *Statistical Field Theory*

Carlos Sa de Melo (Atlanta, USA): *Many-body Theory, BEC-BCS Crossover*

Jean Zinn-Justin (Paris, France): *Quantum Field Theory, Large-N Technique*

Victor Dotsenko (Paris, France): *Random Matrix Theory, Replica Trick*

Steve Simon (Oxford, UK): *Wilson Loops Spin, Topology, Holonomy Group*

Wolfhard Janke (Leipzig, Germany): *Quantum Monte Carlo*

Hagen Kleinert (Berlin, Germany): *Vortices and GIMPs*

`https://www.dpg-physik.de/veranstaltungen/2019`

6.4 Master of Science in Advanced Quantum Physics

TECHNISCHE UNIVERSITÄT KAISERSLAUTERN

- **Module topics:**
  - Quantum technologies
  - Many-body quantum systems
  - Laboratory courses
  - Research and master thesis

- **Application deadlines:**

	Winter Term	Summer Term
if visa required	April 30	October 31
if no visa required	July 15	Januar 15

- **Further information:**

`www.physik.uni-kl.de/quantum-master`