Lecture Series
Winter Term 2012/13
Innsbruck University

UNIVERSITY OF INNSBRUCK

Many-Body Physics with Cold Atoms

IQOQI
AUSTRIAN ACADEMY OF SCIENCES

SFB
Coherent Control of Quantum Systems

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Introduction: Cold Atoms vs. Condensed Matter

Q: What can cold atoms add to many body physics?

- New models of own interest
  - Bose-Hubbard model
  - Strongly interacting continuum systems: BCS-BEC Crossover; Efimov effect
  - long range interactions other than Coulomb; SU(N) Heisenberg models with variable N...
- Quantum Simulation: clean/ controllable realization of model Hamiltonians which are
  - less clear to what extent realized in condensed matter
  - extremely hard to analyze theoretically

  } e.g. 2d Fermi-Hubbard model
- Nonequilibrium Physics, time dependence:
  - Condensed matter: thermodynamic equilibrium and ground state physics.
  - Cold atoms: e.g. creation of excited many-body states, study their dynamic behavior
- Scalability:
  - Study crossover from systems with few- to (thermodynamically) many degrees of freedom: Change of concepts?
- Integrate quantum optics concepts and many-body theory, coherent-dissipative manipulation, non-equilibrium stationary states

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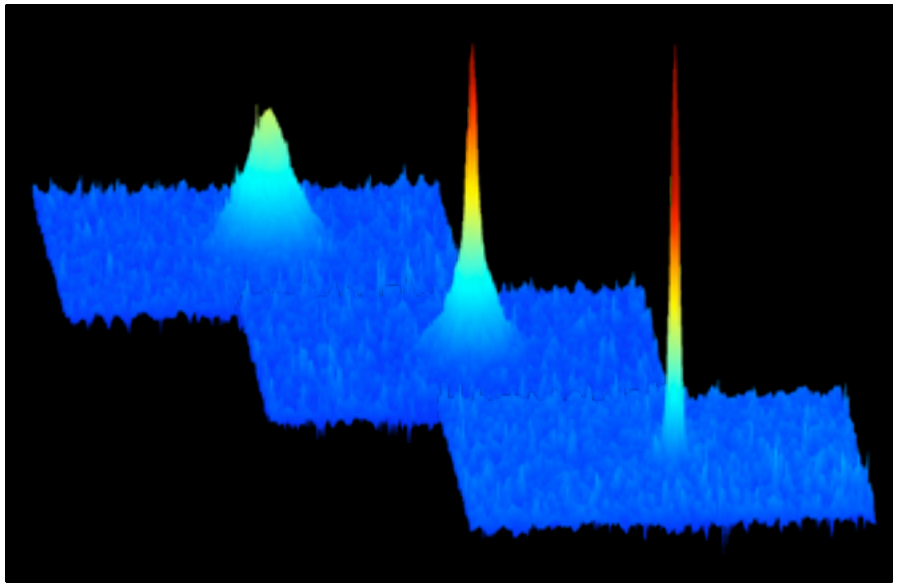
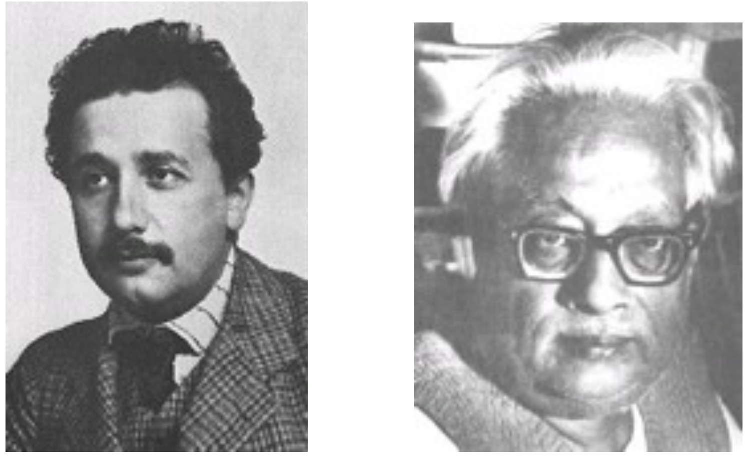
A Brief History of cold atoms and BEC research



A Brief History of cold atoms and BEC research

^{4}He liquified by K. Onnes — 1908

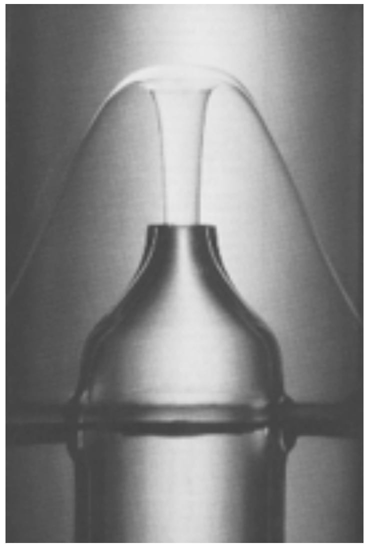
Bose studies statistical Properties of photons — 1924



1925 — Bose/Einstein predict condensation of a noninteracting atomic Bose gas

Kapitza / Allen & Misener discover superfluidity of ^{4}He — 1938

Allen & Jones discover fountain effect



1938 — London makes first connection between ^{4}He superfluidity and BEC

1941 — Landau produces first phenomenological theory of superfluids

1947 — Bogoliubov produces microscopic theory of weakly interacting Bose gas

1949 — Onsager predicts quantized vortices in liquid ^{4}He (+ Feynman 1955)

1951 — Landau & Lifshitz / Penrose link BEC and off-diagonal long range order.

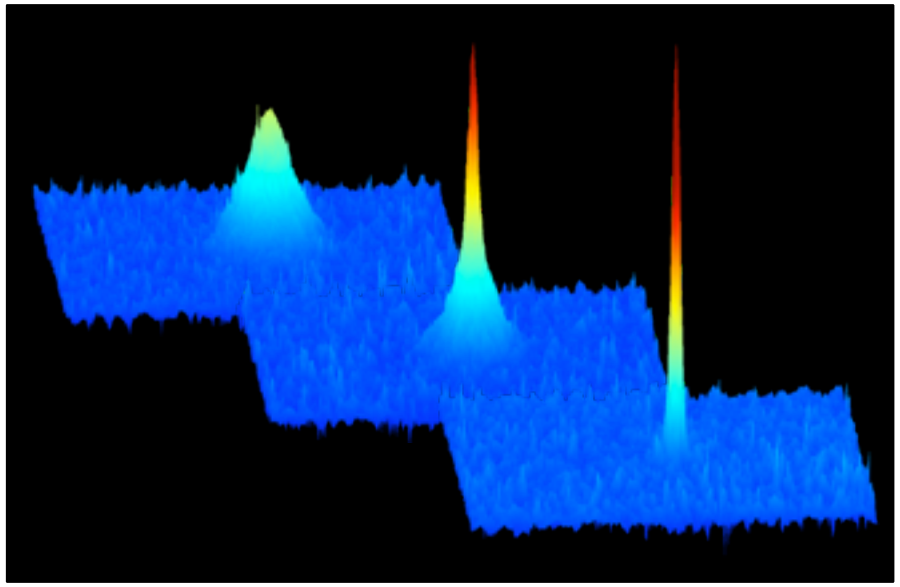
A Brief History of cold atoms and BEC research

1976 Stwalley and Nosanow (following Hecht, 1959) argue spin polarised ^{1}H would be Superfluid BEC (Realised MIT 1998).

Neutral Atom traps:
Gaithersburg (Magnetic)
AT&T Bell Labs
1985

1987 Simultaneous Cooling and Trapping in Magneto-Optical Trap (AT&T Bell labs)

1995 BEC in dilute gases:
JILA (^{87}Rb), MIT (^{23}Na), Rice (^{7}Li)



W. D. Phillips, S. Chu, and C. Cohen-Tannoudji: Nobel Prize for Laser Cooling
1997

E. Cornell, C. Wieman, W. Ketterle: Nobel Prize for BEC in dilute gases
2001

A Brief History of cold atoms and BEC research

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		1995	1997	1998	1998	1998	1998	1999	1999	2001	2001	2002	2002	2002
Rb	1995	9	8	3	1	3	5	2	1	1	1	1		1
Na	1995	3												
Li	1995/97	1		1										
H	1998	1												
He*	2001			2										
K	2001							1						
Cs	2002												1	

Innsbruck
05. Oct. 2002

+ Yb (2004), Cr (2005)

Molecules: Li_2 (2003), K_2 (2003)

Earth alkaline atoms: Ca (2009), Sr (2009)

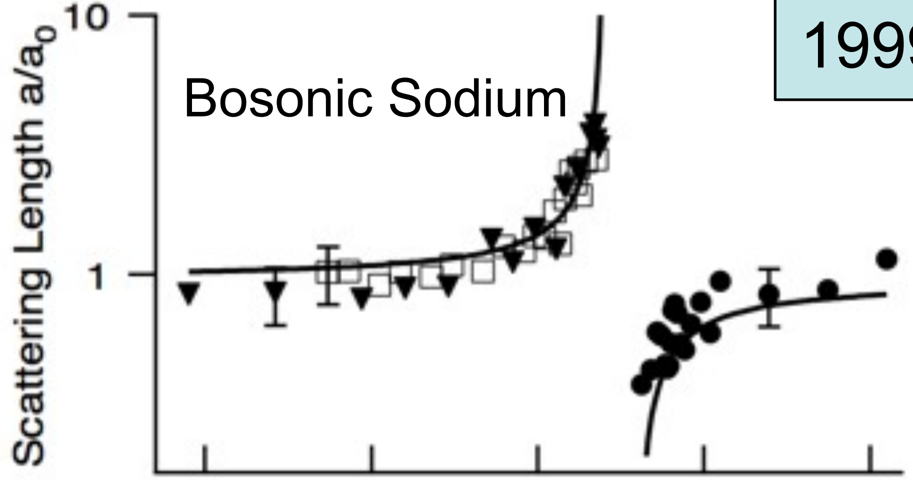
Strongly dipolar atoms: Dy (2011), Er (2012)

A Brief History of cold atoms and BEC research

- Further milestone experiments:

Tunable interations:
Feshbach resonance

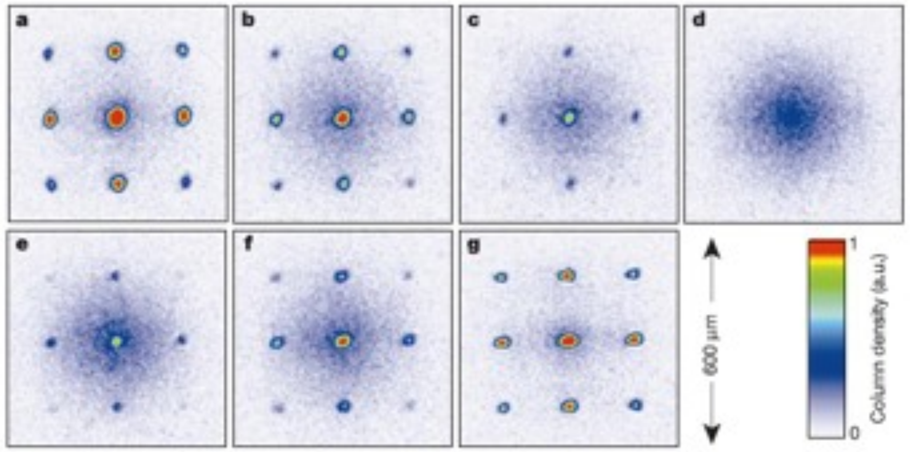
1999



Ketterle Group, MIT

Optical Lattices:
Mott insulator-superfluid
quantum phase transition

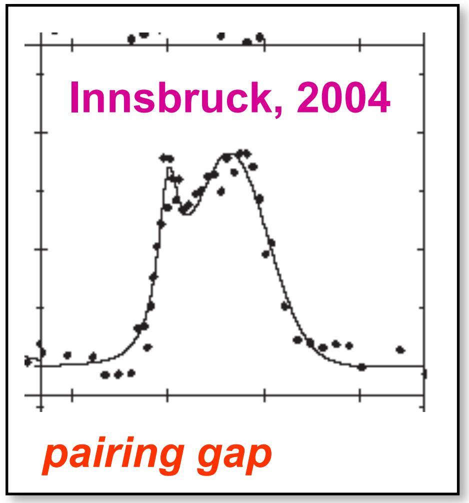
2002



Haensch Group, Munich

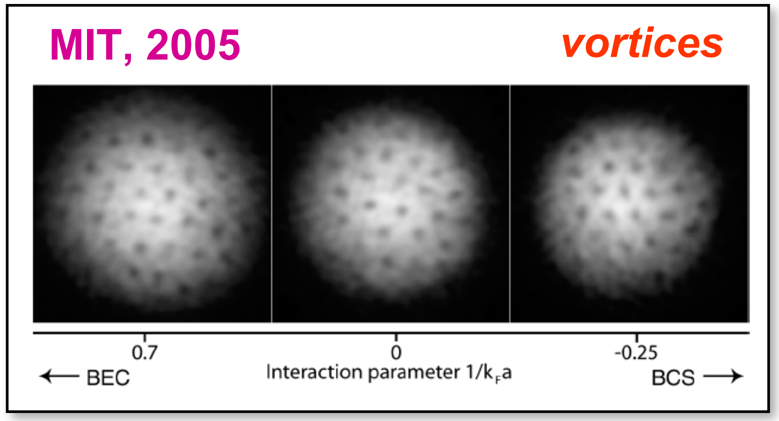
Degenerate and strongly interacting fermions

2004



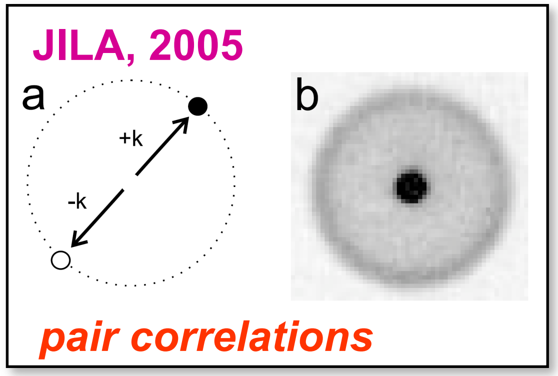
Innsbruck, 2004

pairing gap



MIT, 2005

vortices



JILA, 2005

pair correlations

Absolute Scales in Condensed Matter vs. Cold Atoms

- Compare the absolute scales in of liquid ^{4}He and cold atom BEC

  - Liquid ^{4}He “BEC”
    - Typical density 10^{22} cm^{-3}
    - Condensation temperature ~ 2.17 K
    - Strongly Interacting
    - Small Condensate Fraction

  - BEC in dilute gases
    - Typical density 10^{13} – 10^{15} cm^{-3} (cf. density of air: 3×10^{19} cm^{-3})
    - Condensation temperature < 10^{-5} K (cf. CMB radiation: ~ 2.7K)
    - Weakly interacting
    - Much larger condensate fraction

Modelling in Condensed Matter vs. Cold Atoms

- Compare the way of constructing microscopic models in these systems

  - Condensed Matter
    - given chunk of matter
    - have to guess the microscopic Hamiltonian
    - ex: Fermi-Hubbard model

  - Cold Atoms
    - microscopic parameters from scattering physics (n=T=0)
    - many body physics in separate experiments

➡ Direct experimental access to both micro- and macrophysics

➡ Challenge to theorists to make the connection

➡ Many disciplines and theoretical techniques are involved: Atomic physics, Quantum optics, Condensed matter physics

- Further general properties and features:

Clean system:

- No (uncontrollable) disorder
- Weak dissipation (>1s) (cf. phonons in solid state)

Control:

- tune microscopic parameters,
- modify lattice structure
- choose effective dimensionality

Measurements:

- (quasi-)momentum distribution, noise correlations by releasing atoms.
- Spectroscopy (e.g., lattice modulations / Bragg scattering).

Units

- In these lecture series, we will often work in “natural units”:
  - Quantum mechanical problem:

$$\hbar = 1$$

➡ Measure energy and frequency in the same unit, $E = \hbar\omega$

  - Many-Body problem:

$$k_{\mathrm{B}} = 1$$

➡ Measure energy and temperature in the same unit, $E = \frac{1}{2}k_{\mathrm{B}}T$

  - Nonrelativistic problem: (we often indicate the mass explicitly)

$$2M = 1$$

➡ Measure energy and momentum square in the same unit, $E = \frac{\vec{p}^2}{2M}$

  - Optical problem:

$$c = 1$$

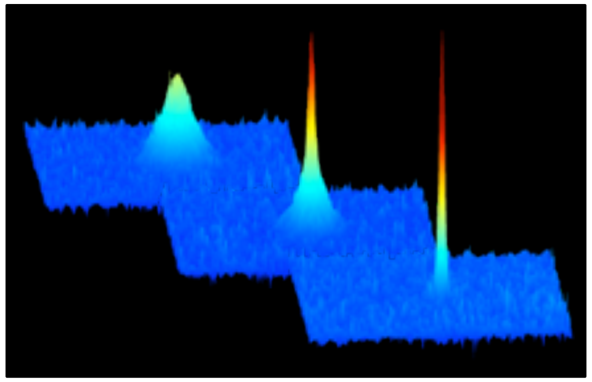
➡ Measure frequency an wave number in the same unit, $\omega = ck$

Lecture Outline

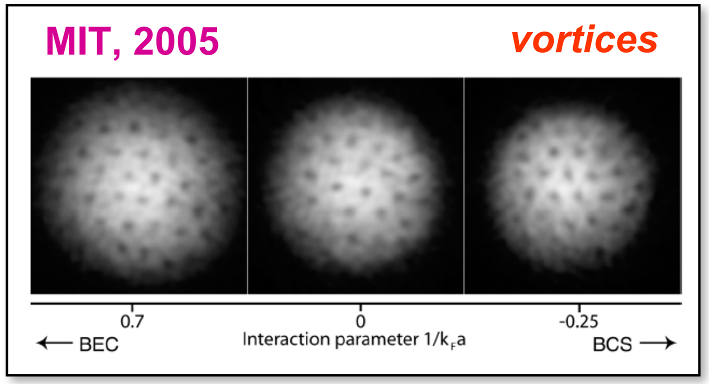
The lecture series consists of two parts:

Part I: Introduction to the theory of ultracold atomic quantum gases

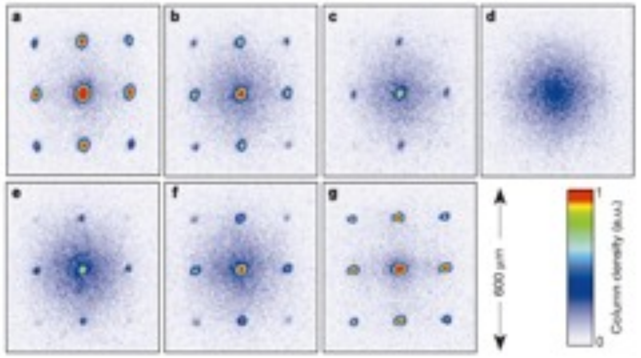
- Physics:
  - Continuum systems:
    - Scales and interactions, Effective theories
    - Weakly interacting Bosons, Bose-Einstein condensation
    - Weakly interacting Fermions, BCS superfluidity
    - Strong interactions, the BCS-BEC crossover
  - Lattice systems:
    - Quantum phase transitions
    - Microscopic derivation of the Bose-Hubbard model
    - Phase Diagram of the Bose-Hubbard model, Mott insulator - superfluid transition
- Methods:
  - Second quantization vs. functional integral techniques



Bose-Einstein Condensation



Fermion Superfluidity



Mott insulator - superfluid transition

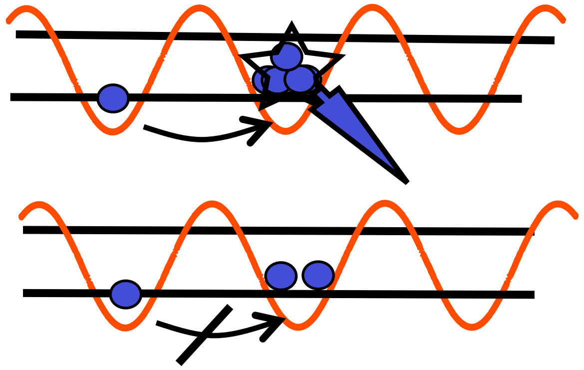
Lecture Outline

The lecture series consists of two parts:

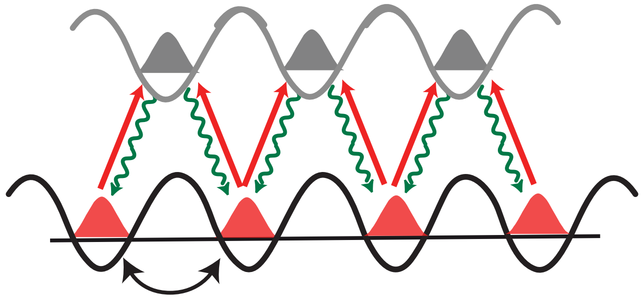
$$\partial_t U_k[\rho] = \frac{1}{2}\mathrm{STr}\,\frac{1}{\Gamma_k^{(2)}[\phi]+R_k}\partial_t R_k$$

Part II: Selected Topics

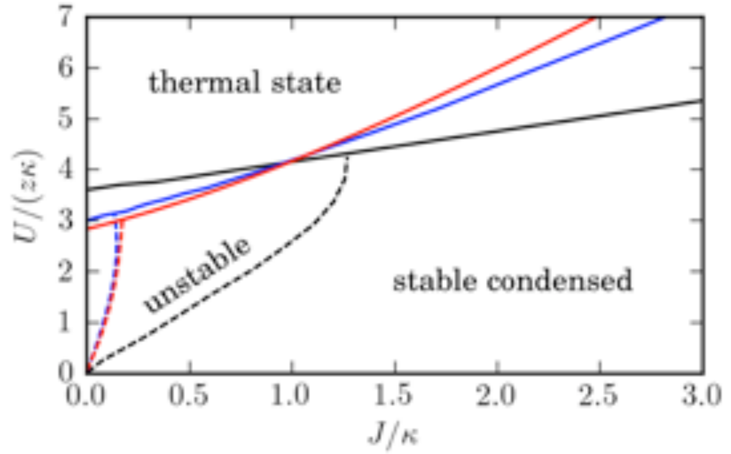
- Advanced field theoretical techniques
  - (Functional) Renormalization Group
  - Application to ultracold atoms: e.g. Efimov effect, quantum criticality in Bose-Hubbard model, Tan effect, ...



- Many-Body Physics with Open Atomic Systems
  - Dissipation engineering, driven-dissipative BEC
  - Nonequilibrium phase transitions: open Dicke model, competing unitary and dissipative dynamics, ...



- Tutorial on Topological Insulators
- Suggestions welcome!

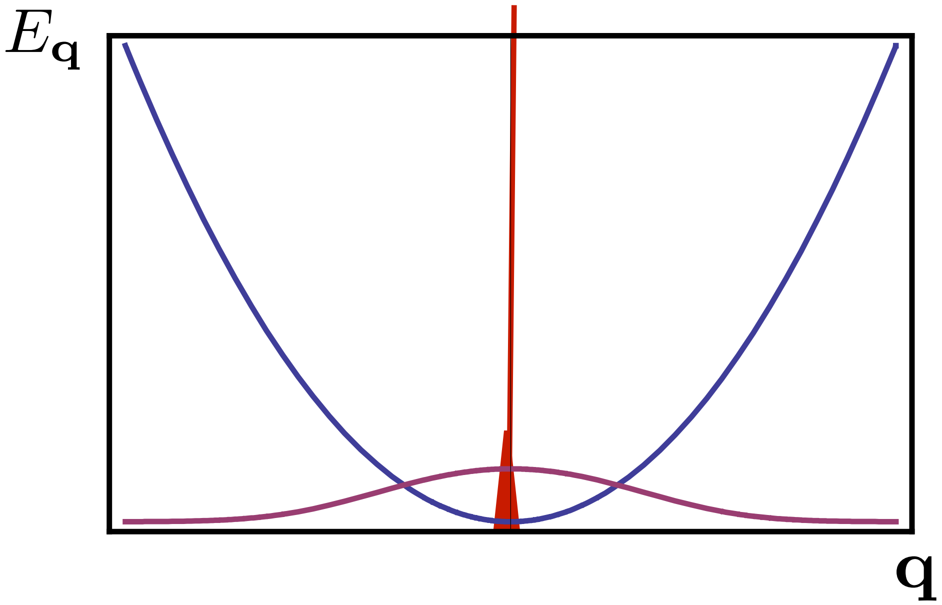


Literature

- General BEC/BCS theory:
  - C. J. Pethick, H. Smith, Bose-Einstein Condensation in Dilute Gases, Cambridge University Press (2002)
  - L. Pitaevski and S. Stringari, Bose-Einstein Condensation, Oxford University Press (2003)
- Recent research review articles:
  - I. Bloch, J. Dalibard and W. Zwerger, Many-Body Physics with Cold Atoms, Rev. Mod. Phys. **80**, 885 (2008)
  - S. Giorgini, L. Pitaevski and S. Stringari, Theory of ultracold atomic Fermi gases, Rev. Mod. Phys. **80**, 1215 (2008)
  - I. Boettcher, J. M. Pawlowski, S. Diehl, Ultracold Atoms and the Functional Renormalization Group, Nucl. Phys. Proc. Suppl. **228,** 63 (2012) arxiv:1204.4394
- Many-Body Physics (with and without cold atoms)
  - J. Negele, H. Orland, Quantum Many-particle Systems, Westview Press (1998)
  - A. Altland and B. Simons, Condensed Matter Field Theory, Cambridge University Press (2006, second edition 2010)
  - S. Sachdev, Quantum Phase Transitions, Cambridge University Press (1999)
  - K. B. Gubbels and H. C. T. Stoof, Ultracold Quantum Fields, Springer Verlag (2009)

Basic BEC theory

-- scales in ultracold quantum systems



Statistical Mechanics of Noninteracting Bosons

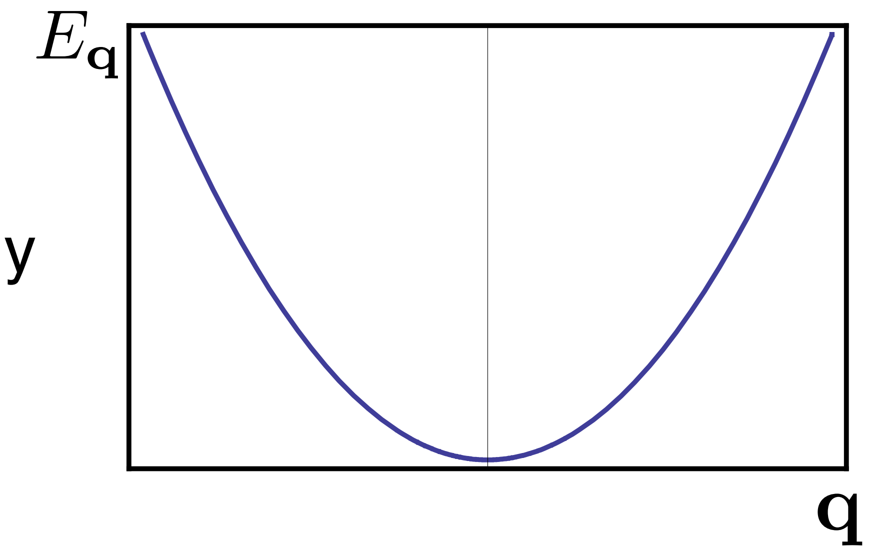
- The Hamiltonian for free particles in occupation number representation ("second quantization")

$$H = \sum_{\mathbf{q}} \frac{\mathbf{q}^2}{2m} a_{\mathbf{q}}^\dagger a_{\mathbf{q}}$$

  - The operator $a_{\mathbf{q}}^\dagger$ creates a particle in the momentum mode **q** : $a_{\mathbf{q}}^{\dagger N}|vac\rangle = \sqrt{(N+1)!}|n_{\mathbf{q}} = N\rangle$. Similarly, $a_{\mathbf{q}}$ annihilates a particle in the mode **q**.
  - The operators satisfy bosonic commutation relations, $[a_{\mathbf{q}}, a_{\mathbf{q}'}^\dagger] = \delta(\mathbf{q}-\mathbf{q}')$ (cf. harmonic oscillator ladder operators, but with an index label **q**).
  - The operator $n_{\mathbf{q}} = a_{\mathbf{q}}^\dagger a_{\mathbf{q}}$ measures the particle number in the momentum mode **q**. The total particle number is $\hat{N} = \sum_{\mathbf{q}} a_{\mathbf{q}}^\dagger a_{\mathbf{q}}$.
  - The dispersion relation is $E_{\mathbf{q}} = \hbar\omega = \frac{\mathbf{q}^2}{2m}$. This is the energy of a single particle in the mode **q**.

- Free particles in occupation number representation = collection of independent harmonic oscillators with energy

$$E_{\mathbf{q}} = \frac{\mathbf{q}^2}{2m}$$



Statistical Mechanics of Noninteracting Bosons

- Statistical properties described by the Free Energy:

$$U = k_B T \log Z, \qquad Z = \mathrm{tr}\exp - \frac{1}{k_B T}(H - \mu \hat{N})$$

temperature

chemical potential

- Trace easily carried out in occupation number basis: H is diagonal:

$$U = k_B T \log \prod_{\mathbf{q}} \sum_{n_{\mathbf{q}}=0}^{\infty} e^{-\frac{1}{k_B T}(\frac{\mathbf{q}^2}{2m} - \mu) n_{\mathbf{q}}} = k_B T \log \prod_{\mathbf{q}} \left(1 - e^{-\frac{1}{k_B T}(\frac{\mathbf{q}^2}{2m} - \mu)}\right)^{-1} = -k_B T \sum_{\mathbf{q}} \log\left(1 - e^{-\frac{1}{k_B T}(\frac{\mathbf{q}^2}{2m} - \mu)}\right)$$

- Consider low temperature behavior of equation of state:

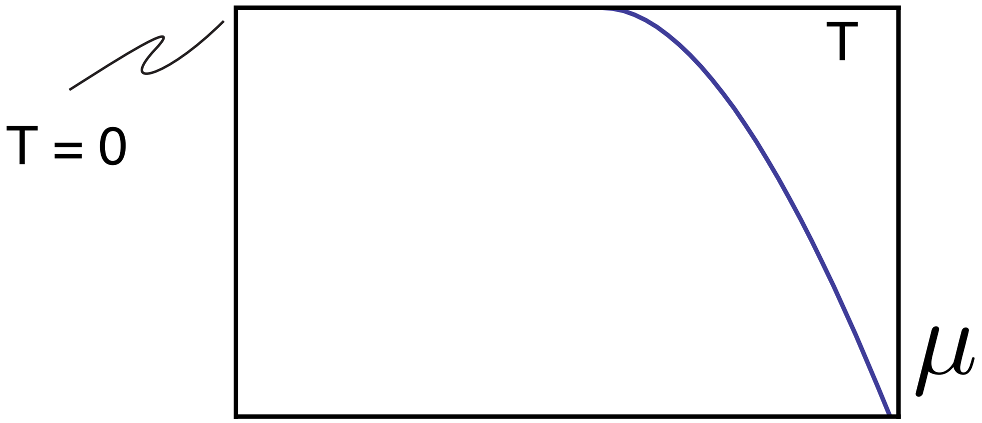
$$N = -\frac{\partial U}{\partial \mu} = \langle \sum_{\mathbf{q}} a^\dagger_{\mathbf{q}} a_{\mathbf{q}} \rangle = \sum_{\mathbf{q}} \langle a^\dagger_{\mathbf{q}} a_{\mathbf{q}} \rangle = \sum_{\mathbf{q}} \frac{1}{e^{\frac{1}{k_B T}(\frac{\mathbf{q}^2}{2m} - \mu)} - 1} \to V \int \frac{d^d q}{(2\pi)^d} \frac{1}{e^{\frac{1}{k_B T}(\frac{\mathbf{q}^2}{2m} - \mu)} - 1}$$

continuum limit

Bose-Einstein distribution

Bose-Einstein Condensation, 3D

- Lower T and study the behavior of μ at fixed n (3D):



$d = 3$

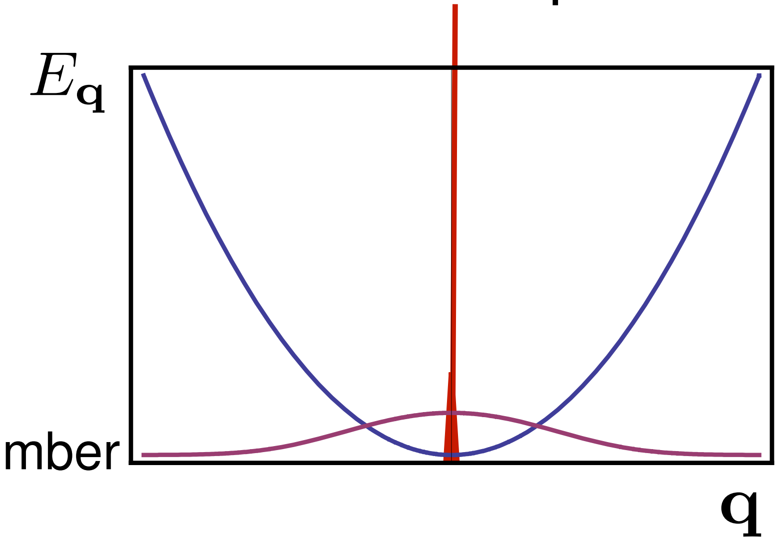
$$n = \frac{N}{V} = \int \frac{d^d q}{(2\pi)^d} \frac{1}{e^{\frac{1}{k_B T}(\frac{\mathbf{q}^2}{2m} - \mu)} - 1}$$

$$= \lambda_{dB}^{-3}(T) g_{3/2}(e^{\mu/k_B T})$$

Polygamma function

$$g_\alpha(z) = \sum_{n=1}^{\infty} \frac{z^n}{n^\alpha}$$

- At a finite T, μ hits zero: below this T_c the equation of state has no solution
- Bose and Einstein (1925): Equation below T_c needs modification due to macroscopic occupation of zero mode:



$$n = \langle a_{\mathbf{0}}^\dagger a_{\mathbf{0}} \rangle + \int \frac{d^d q}{(2\pi)^d} \frac{1}{e^{\frac{\mathbf{q^\wedge 2}}{2mk_B T}} - 1}$$

  - plausible: Bosons can populate single quantum state with arbitrary number
  - macroscopic: $N_0 = \langle a_{\mathbf{0}}^\dagger a_{\mathbf{0}} \rangle = \mathcal{O}(N) \propto V$, i.e. extensive
  - critical temperature: determined by

$$n\lambda_{dB}^3 = g_{3/2}(1) = \zeta(3/2) \approx 2.612$$

=1 above

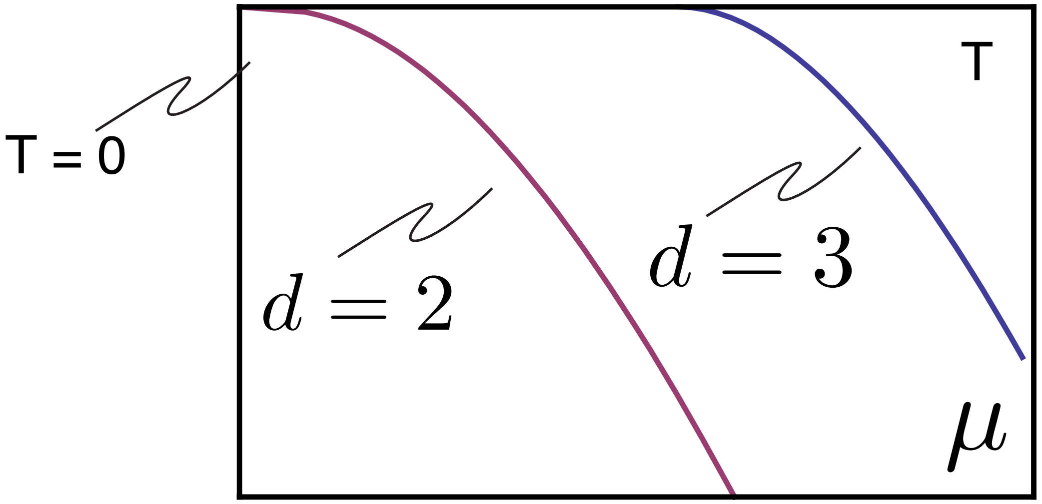
de Broglie wavelength

$$\boxed{\lambda_{dB} = (2\pi\hbar^2/mk_B T)^{1/2} \gtrsim d = n^{-1/3}}$$

interparticle spacing

Role of Dimension: No BEC in 2D

- Lower T and study the behavior of μ at fixed n (2D):



➡ EoS without condensate can be fulfilled for all T:

➡ No BEC in (homogeneous) 2d space

- Reason: Infrared (low momentum) divergence due to smaller phase space

$$\frac{d^2q}{(2\pi)^2}\langle\hat{n}_{\mathbf{q}}\rangle = \frac{d^2q}{(2\pi)^2}\frac{1}{e^{(\frac{q^2}{2m}-\mu)/k_BT}-1} \propto \frac{dqq}{q^2-\mu}$$

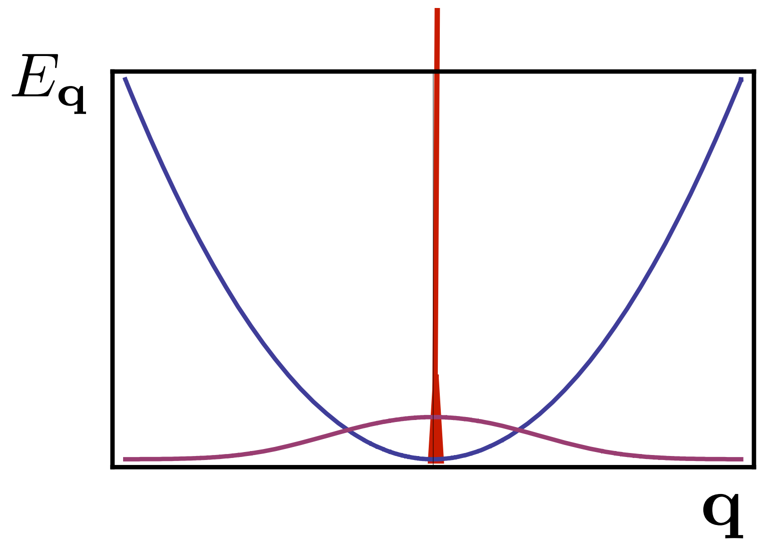
low momenta, small mu

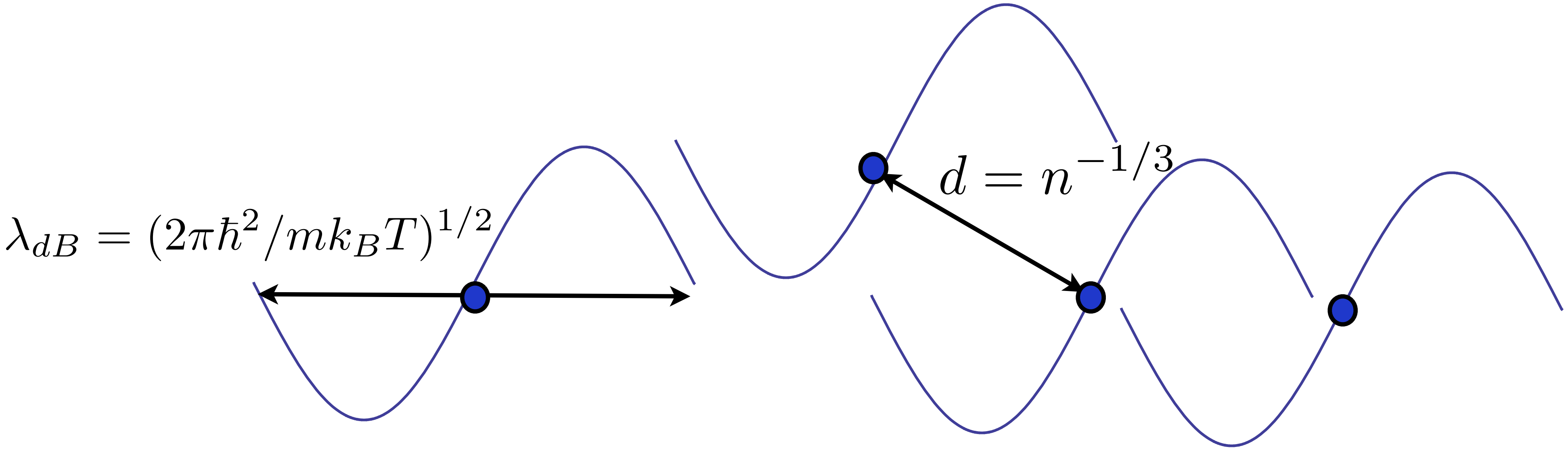
logarithmic divergence

- Remark: More general result
  - No spontaneous breaking of continuous symmetries at finite temperature (Mermin-Wagner Theorem)
  - quasi long range order possible: Kosterlitz-Thouless transition

Summary

- BEC is statistical effect, no interaction needed
- BEC is macroscopic population of a single quantum state, the q=0 mode
- quantum degeneracy condition: $\lambda_{dB} \gtrsim d$
- True BEC at finite temperature only in d=3





- Now: more realistic description of ultracold Bose systems
  - Trapping potential
  - Interactions

Trapping Potential and Weak Interactions

- So far: free particles in homogeneous space, continuum limit :

$$H_0 = H - \mu \hat{N} = \int_{\mathbf{q}} a^\dagger_{\mathbf{q}} (\frac{\mathbf{q}^2}{2m} - \mu) a_{\mathbf{q}} = \int_{\mathbf{x}} a^\dagger_{\mathbf{x}} (- \frac{\triangle}{2m} - \mu) a_{\mathbf{x}}$$

after Fourier transform $a_{\mathbf{q}} = \int_{\mathbf{x}} e^{\mathrm{i}\mathbf{q}\mathbf{x}} a_{\mathbf{x}}; \quad [a_{\mathbf{x}}, a^\dagger_{\mathbf{y}}] = \delta(\mathbf{x} - \mathbf{y})$

- Now we aim at a more realistic description of cold atomic gases:
  - Trapping potential: the local density experiences a local potential energy

$$H_{trap} = \int_{\mathbf{x}} V(\mathbf{x}) \hat{n}_{\mathbf{x}}, \quad V(\mathbf{x}) = \tfrac{1}{2} m \omega^2 \mathbf{x}^2$$

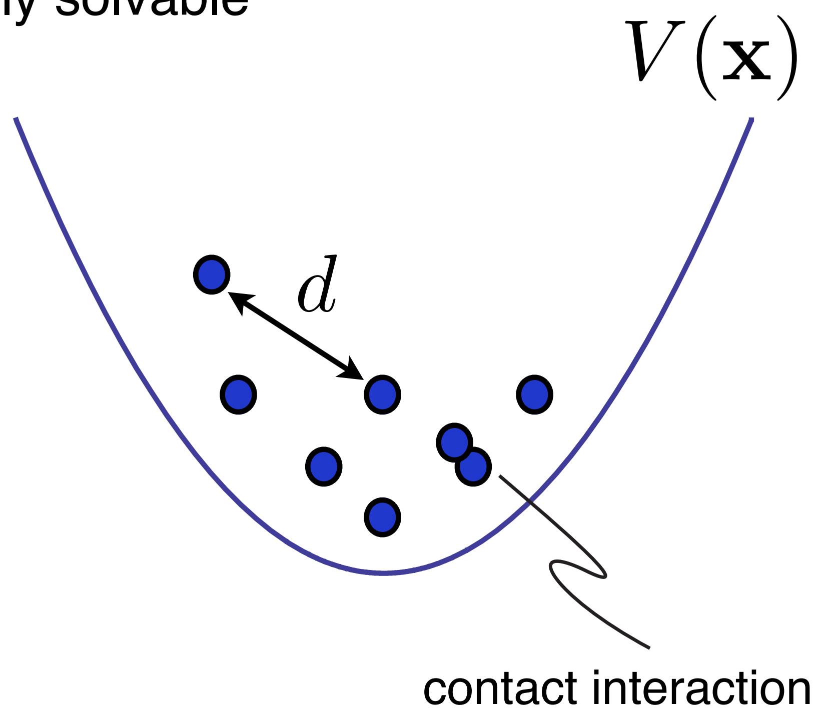
Remark: this is just a collection of local harmonic oscillators: exactly solvable

  - Local two-body interactions:

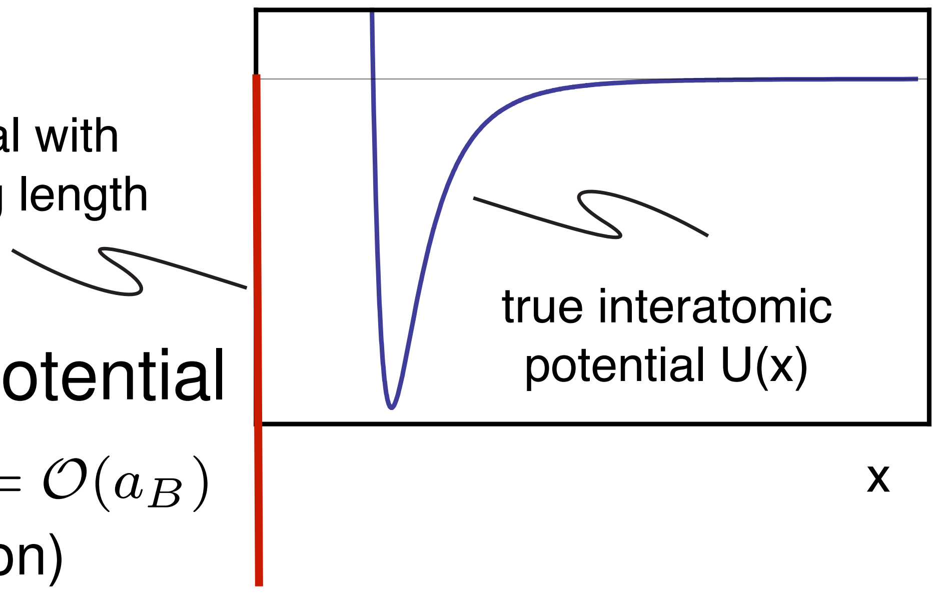
$$H_{int} = \int_{\mathbf{x},\mathbf{y}} g \delta(\mathbf{x} - \mathbf{y}) \hat{n}_{\mathbf{x}} \hat{n}_{\mathbf{y}} = g \int_{\mathbf{x}} \hat{n}^2_{\mathbf{x}}$$

- Our workhorse Hamiltonian is

$$H = H_0 + H_{trap} + H_{int}$$



Microscopic Origin of the Interaction Term



- Microscopic scattering physics: Lennard-Jones (LJ) potential
  - $1/r^{12}$ hard core repulsion: repulsion of electron clouds $r_{rep} = \mathcal{O}(a_B)$
  - $1/r^6$ attraction: van der Waals (induced dipole-dipole interaction)
    $r_{vdW} = (50...200)a_B$ for alkalis: typ. order of magnitude for interaction length scale

- General properties of LJ type potentials at low energies:
  - isotropic s-wave scattering dominates; the scattered wave function behaves asymptotically as $\psi(\mathbf{x}) \sim a/\mathbf{x}$
  - a is the scattering length. Knowledge of this single parameter is sufficient to describe low energy scattering!
  - within Born approximation, it can be calculated as

$$a_{\text{Born}} \sim \int_{\mathbf{x}} U(\mathbf{x})$$

interatomic potential

➡very different interaction potentials may have the same scattering length!

The Model Hamiltonian as an Effective Theory

$$H = \int_{\mathbf{x}} [a^{\dagger}_{\mathbf{x}}\big(-\frac{\triangle}{2m} - \mu + V(x)\big)a_{\mathbf{x}} + g\hat{n}^2_{\mathbf{x}}]$$

- Efficient description by an effective Hamiltonian with few parameters.
- For ultracold bosonic alkali gases, a single parameter, the scattering length a, is sufficient to characterize low energy scattering physics of indistinguishable particles : Effective interaction

$$g = \frac{8\pi\hbar^2}{m}a$$

- A typical order of magnitude for the scattering length is

$$a = \mathcal{O}(r_{vdW}),\ \ r_{vdW}(50...200)a_B$$

- The validity of the model Hamiltonian is restricted to length scales

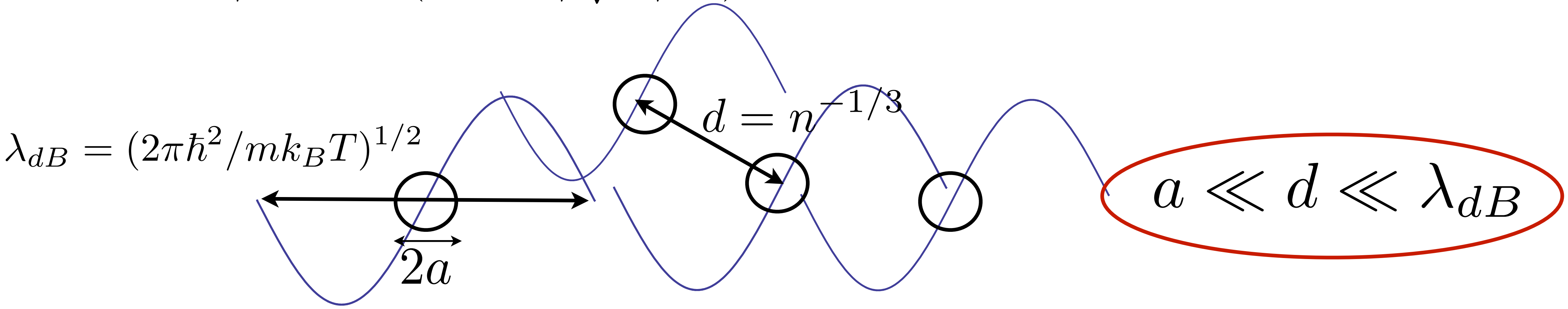
$$l \gtrsim r_{vdW}$$

- For bosons, we must restrict to repulsive interactions a > 0 (else: bosons seek solid ground state, collapse in real space)

- So far: microscopic description; now: many body scales!

Validity of our Hamiltonian: Scales in Cold Dilute Bose Gases

- The effective Hamiltonian is valid because none of many-body length scales can resolve interaction length scale :
- Many-body scales: density and temperature in terms of length scales.
  - diluteness $a/d \ll 1$ $(d = n^{-1/3})$
    - dilute means weakly interacting: interaction energy $gn \sim a/d \cdot d^{-2}$
    - clear: three-body interaction terms irrelevant
  - quantum degeneracy: $d/\lambda_{dB} \ll 1$ $(\lambda_{dB} = (2\pi\hbar^2/mk_BT)^{1/2})$
  - trap frequencies: $\lambda_{dB}/l_{osc} \ll 1$ $(l_{osc} = 1/\sqrt{m/2\omega})$



Summary of length scales

$a_{\rm B} = 5.3 \times 10^{-2}{\rm nm}$ Bohr radius

length	scattering length a/a_B	interparticle sep. d/a_B	de Broglie w.l. λ_{dB}/a_B	trap size l_{osc}/a_B
	(0.05 ... 0.2)10^3	(0.8 ... 3)10^3	(10 ... 40)10^3	(3 ... 300)10^3

phys. meaning of the ratio:

weak interactions/

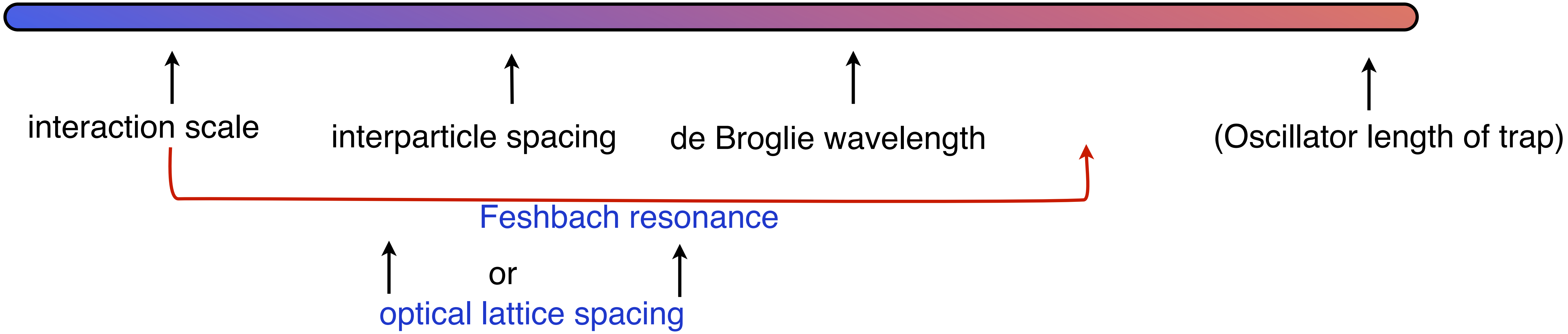
dilute gases

quantum degeneracy

local density approximation valid

Violations of the scale hierarchy

- Generic sequence of scales and possible violations:



interaction scale

interparticle spacing

de Broglie wavelength

(Oscillator length of trap)

Feshbach resonance

or

optical lattice spacing

- With Feshbach resonances, violation of a/d << 1 possible: Dense degenerate system
- With optical lattices, a new length and a new energy scale are introduced:
  - lattice spacing = wavelength of light: high densities (“fillings) become available
  - lattice depth: Kinetic energy is withdrawn more strongly than interaction energy: “strong correlations”

- Both leads to the possibility of “strong interactions/correlations” as we will see

- NB: Despite violation of scale hierarchy for dilute quantum gases, we will be able to give accurate microscopic models

BEC Phenomenology: Gross-Pitaevski Equation

- Heisenberg Equation of motion for the field operator:

$$\partial_t a_{\mathbf{x}}(t) = \mathrm{i}[H, a_{\mathbf{x}}] = -\mathrm{i}\big(-\frac{\triangle}{2m} - \mu + V(\mathbf{x}) + g a^\dagger_{\mathbf{x}} a_{\mathbf{x}} \big) a_{\mathbf{x}}$$

➡ Nonlinear partial differential operator equation...

- Simplifications:
  - $T = 0$, no interactions: whole density sits in the condensate: $\varphi_0 = \sqrt{N}$
  - $T = 0$, weak interactions $(a/d \ll 1)$: expect $\varphi_0 \approx \sqrt{N}$
  - we can formalize this:

complete set of orthogonal functions

$$a_{\mathbf{x}} = \phi_0(\mathbf{x}) a_{\mathbf{0}} + \sum_{\mathbf{q}} \phi_{\mathbf{q}}(\mathbf{x}) a_{\mathbf{q}} = \phi_0(\mathbf{x}) a_{\mathbf{0}} + \delta a_{\mathbf{x}}$$

- macroscopic occupation of zero mode implies: commutator irrelevant, replace with classical c-numbers

$$\langle a^\dagger_{\mathbf{0}} a_{\mathbf{0}} \rangle \approx \langle a_{\mathbf{0}} a^\dagger_{\mathbf{0}} \rangle \approx N \approx \langle a^\dagger_{\mathbf{0}} \rangle \langle a_{\mathbf{0}} \rangle, \text{ thus } a_{\mathbf{0}} \to \sqrt{N}; \;\; \varphi(\mathbf{x}, t) := \phi_0(\mathbf{x}, t)\sqrt{N}$$

- Insert into Heisenberg EoM, keep only terms $\mathcal{O}(\sqrt{N}) \gg 1$

$$\mathrm{i}\partial_t \varphi(\mathbf{x}, t) = \big(-\frac{\hbar^2}{2m} \triangle - \mu + V(\mathbf{x}) + g\varphi^*(\mathbf{x}, t)\varphi(\mathbf{x}, t) \big) \varphi(\mathbf{x}, t)$$

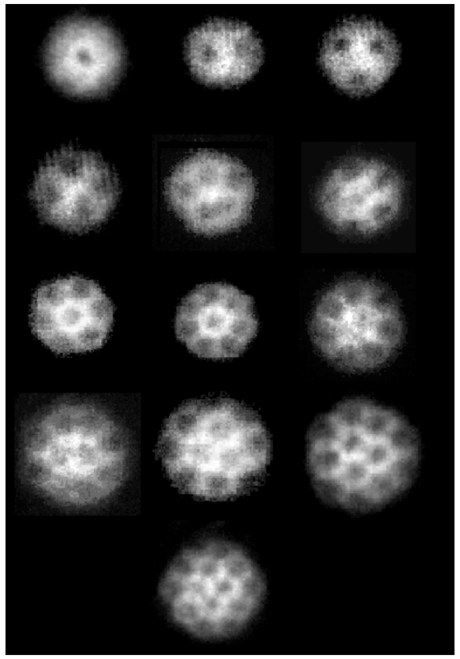
Gross-Pitaevski Equation

Macroscopic wave function

- Gross-Pitaevski Equation :

$$\mathrm{i}\partial_t\varphi(\mathbf{x},t) = \big(-\frac{\hbar^2}{2m}\triangle - \mu + V(\mathbf{x}) + g\varphi^*(\mathbf{x},t)\varphi(\mathbf{x},t)\big)\varphi(\mathbf{x},t)$$

- Properties:
  - Classical field equation (cf. classical electrodynamics vs. QED)
  - for g = 0, or single particle: formally recover linear Schrödinger equation -> expect quantum behavior; interpret φ as "macroscopic wave function"
  - however, in general nonlinear -> richer than Schrödinger equation



- Interplay of quantum mechanics and nonlinearity: quantized vortex solutions
  - uniform case V(x) = 0, search static cylinder symmetric symmetric solutions with no z dependence:

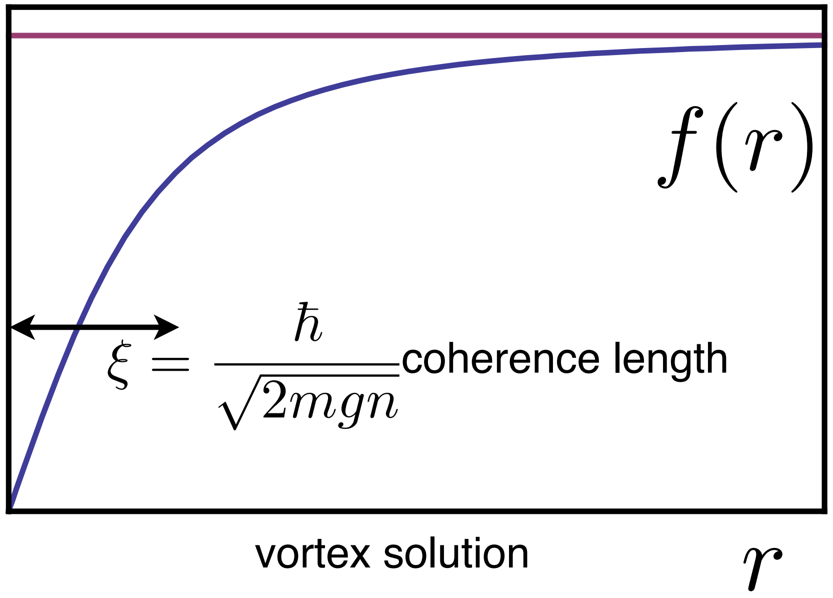
$$\varphi(\mathbf{x},t) = \varphi(r,\phi) = f(r)e^{\mathrm{i}\ell\phi}$$

integer, such that phase returns after 2 pi: unique Wave function

  - GP equation:

$$0 = -\frac{\hbar^2}{2m}\big(f" + \frac{f'}{r} - \frac{\ell^2 f}{r^2}\big) - \mu f + g f^3$$

  - large distances: constant solution, determine chemical pot.
  - short distances: condensate amplitude must vanish due to centrifugal barrier, in turn rooted in the quantization of the phase



Quantum Fluctuations: Bogoliubov Theory

- homogeneous case: plane wave expansion of field operator $(\phi_0(\mathbf{x})a_{\mathbf{0}} = 1/\sqrt{V}\sqrt{N_0} = \sqrt{n_0})$

$$a_{\mathbf{x}} = \sqrt{n_0} + \sum_{\mathbf{q}} e^{\mathrm{i}\mathbf{q}\mathbf{x}} a_{\mathbf{q}}$$

choice of zero phase without loss of generality

- Grand canonical Hamiltonian. Take the fluctuations into account to leading order:

- zero order: homogenous mean field reproduced
- linear terms: vanishes upon proper choice of the chemical potential (equilibrium condition) $\mu = gn_0$
- quadratic part:

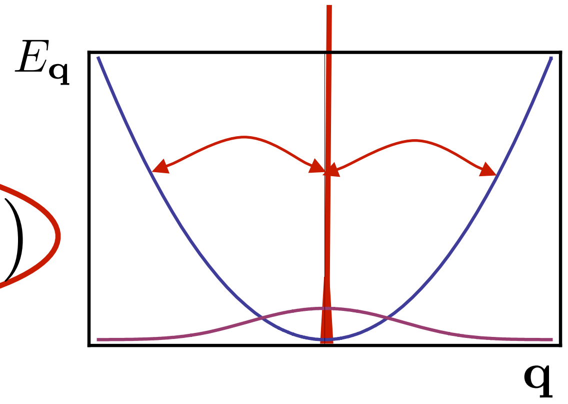
$$H^{(2)}_{Bog} = \sum_{\mathbf{q}} \left(a^\dagger_{\mathbf{q}}\left(\frac{\mathbf{q}^2}{2m} - \mu + 2gn_0\right)a_{\mathbf{q}} + \frac{gn_0}{2}\boxed{(a^\dagger_{\mathbf{q}}a^\dagger_{-\mathbf{q}} + a_{\mathbf{q}}a_{-\mathbf{q}}))}\right.$$

$$= \frac{1}{2}\sum_{\mathbf{q}}(a^\dagger_{\mathbf{q}}, a_{-\mathbf{q}}) \begin{pmatrix} \frac{\mathbf{q}^2}{2m} + gn_0 & gn_0 \\ gn_0 & \frac{\mathbf{q}^2}{2m} + gn_0 \end{pmatrix} \begin{pmatrix} a_{\mathbf{q}} \\ a^\dagger_{-\mathbf{q}} \end{pmatrix} + \text{const.}$$

$\mu = gn_0$

Quantum Fluctuations: Bogoliubov Theory

- quadratic Bogoliubov Hamiltonian:



$$H^{(2)}_{Bog} = \sum_{\mathbf{q}} \left(a^\dagger_{\mathbf{q}}\left(\frac{\mathbf{q}^2}{2m} - \mu + 2gn_0\right)a_{\mathbf{q}} + \boxed{\frac{gn_0}{2}\left(a^\dagger_{\mathbf{q}}a^\dagger_{-\mathbf{q}} + a_{\mathbf{q}}a_{-\mathbf{q}}\right)}\right)$$

$$= \frac{1}{2}\sum_{\mathbf{q}}(a^\dagger_{\mathbf{q}}, a_{-\mathbf{q}}) \begin{pmatrix} \frac{\mathbf{q}^2}{2m} + gn_0 & gn_0 \\ gn_0 & \frac{\mathbf{q}^2}{2m} + gn_0 \end{pmatrix} \begin{pmatrix} a_{\mathbf{q}} \\ a^\dagger_{-\mathbf{q}} \end{pmatrix} + \text{const.}$$

- Discussion:
  - Off-diagonal terms: pairwise creation/annihilation out of the condensate
  - Coupling of modes with opposite momenta
  - Hamiltonian not diagonal in operator space: diagonalize to find spectrum and elementary excitations

- Remarks:
  - An equivalent approach linearizes Heisenberg EoM around homog. GP mean field
  - Validity: The ordering principle is given by the power of the condensate amplitude. Bogoliubov theory is not a systematic perturbation theory in U but becomes good at weak coupling

Bogoliubov Quasiparticles

- Diagonalization in operator space: Bogoliubov transformation

$$\begin{pmatrix} \alpha_{\mathbf{q}} \\ \alpha^\dagger_{-\mathbf{q}} \end{pmatrix} = \begin{pmatrix} u_{\mathbf{q}} & v_{\mathbf{q}} \\ v^*_{\mathbf{q}} & u^*_{\mathbf{q}} \end{pmatrix} \begin{pmatrix} a_{\mathbf{q}} \\ a^\dagger_{-\mathbf{q}} \end{pmatrix}$$

  - The trafo be canonical, $[\alpha_{\mathbf{q}}, \alpha^\dagger_{\mathbf{q}'}] = \delta(\mathbf{q} - \mathbf{q}')$, thus $u^2_{\mathbf{q}} - v^2_{\mathbf{q}} = 1$.

- The transformation coefficients are chosen to make any off-diagonal contribution in terms of new operators vanish. They can be chosen real and evaluate to

$$u^2_{\mathbf{q}} = \frac{1}{2}(\frac{\xi_{\mathbf{q}}}{E_{\mathbf{q}}} + 1), v^2_{\mathbf{q}} = \frac{1}{2}(\frac{\xi_{\mathbf{q}}}{E_{\mathbf{q}}} - 1) \qquad \xi_{\mathbf{q}} = \epsilon_{\mathbf{q}} + gn_0,\ \epsilon_{\mathbf{q}} = \frac{\mathbf{q}^2}{2M} \qquad E_{\mathbf{q}} = \sqrt{\xi^2_{\mathbf{q}} - \epsilon^2_{\mathbf{q}}}$$

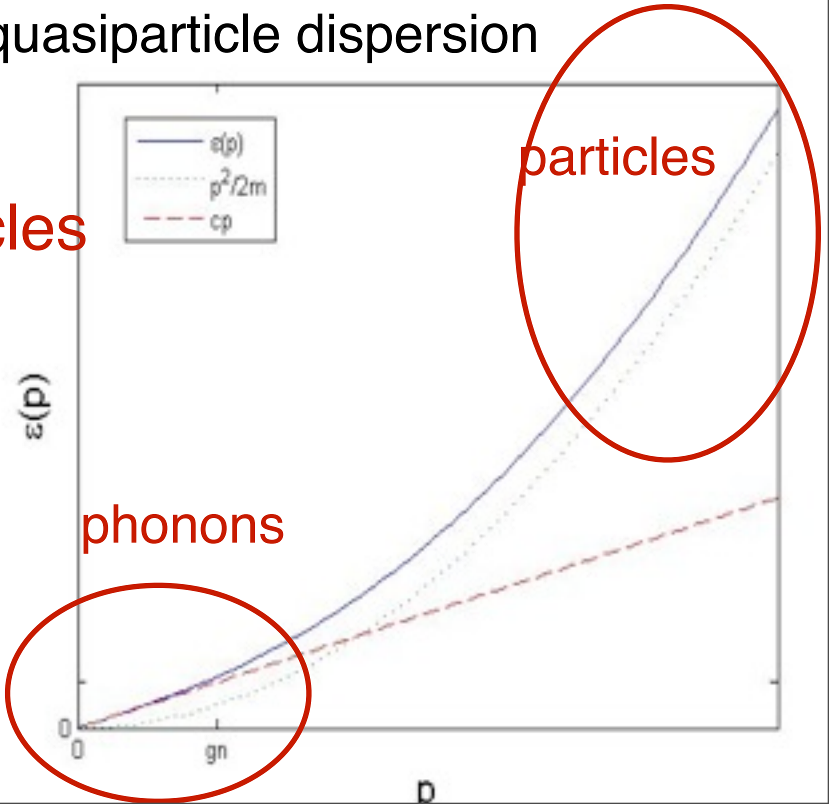
- Rewrite the Hamiltonian with new operators and do normal ordering

$$H = V\frac{gn^2}{2} - \frac{1}{2}\sum_{\mathbf{q}}(\epsilon_{\mathbf{q}} + gn_0 - E_{\mathbf{q}}) + \sum_{\mathbf{q}} E_{\mathbf{q}}\alpha^\dagger_{\mathbf{q}}\alpha_{\mathbf{q}}$$

quasiparticle dispersion

- Result: Collection of harmonic oscillators. New operators: elementary excitations on Bogoliubov ground state: quasiparticles
  - $\alpha^\dagger_{\mathbf{q}}$ creates a quasiparticle excitation and $\alpha_{\mathbf{q}}|0_{Bog}\rangle = 0$
  - Their dispersion is $E_{\mathbf{q}} = \sqrt{2gn_0\epsilon_{\mathbf{q}} + \epsilon^2_{\mathbf{q}}} \overset{\mathbf{q}\to 0}{\to} c|\mathbf{q}|, \quad c = \sqrt{\frac{gn_0}{m}}$
  - At low momenta, this is linear and gapless
  - At high momenta, like free particles: quadratic

speed of sound



Energy Correction and Density Depletion

- Physical effects due to quantum fluctuations:
  - Correction to the total energy:

$$E/V = \langle 0_{Bog}|H|0_{Bog}\rangle/V = \frac{\enclose{circle}{g}n^2}{2} - \frac{1}{2}\int \frac{d^3q}{(2\pi)^3}(\epsilon_{\mathbf{q}} + \enclose{circle}{g}n_0 - E_{\mathbf{q}})$$

interpretation: interaction energy kinetic energy from modes outside the condensate

- Problem: linear high momentum UV divergence
- Reason: too naive treatment of interactions: formally assumed to be constant up to arbitrarily large momenta
- Cure: UV renormalization of interaction (will perform such program explicitly for fermions later)
- Result: $E/V = \frac{gn^2}{2}(1 + \frac{128}{15\pi^{1/2}}(na^3)^{1/2}) \quad g = \frac{8\pi a}{M}$

- Depletion of the condensate (via normal ordering of the particle number operator):

$$n = n_0 + \int_{\mathbf{q}} \langle a^{\dagger}_{\mathbf{q}} a_{\mathbf{q}} \rangle = n_0 + \int_{\mathbf{q}} v^2_{\mathbf{q}} \to \frac{n - n_0}{n} \approx \frac{8}{3\sqrt{\pi}}(na^3)^{1/2}$$

expand in quasiparticle operators

$$na^3 = (a/d)^3$$

interpretation: particles kicked out of condensate

smallness parameter recovered

Phonon Mode and Superfluidity

- Landau criterion of superfluidity: frictionless flow
  - Gedankenexperiment: move an object through a liquid with velocity v.
  - Landau: the creation of an excitation with momentum p and energy $\epsilon_{\mathbf{p}}$ is energetically unfavorable if

$$\boxed{v < v_{\mathbf{c}} = \frac{\epsilon_{\mathbf{p}}}{p}}$$

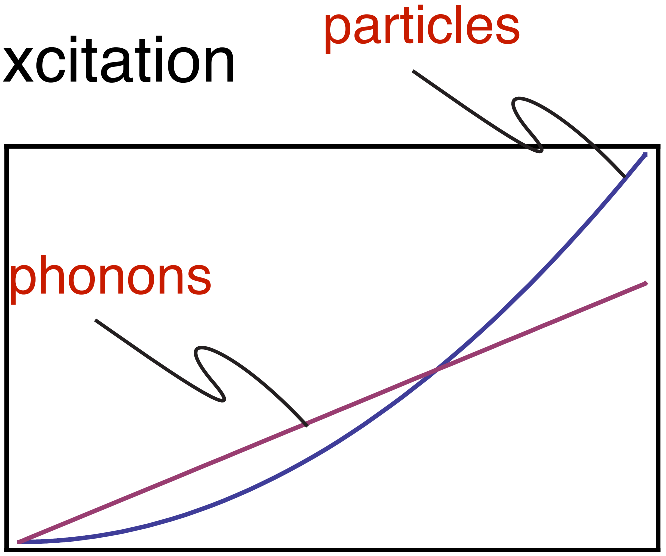
➡in this case, the flow is frictionless, i.e. superfluidity is present

- Weakly interacting Bose gas: Superfluidity through linear phonon excitation

$$\epsilon_{\mathbf{p}} = c|\mathbf{p}|, c = \sqrt{\frac{gn_0}{m}} \to v_c = c$$

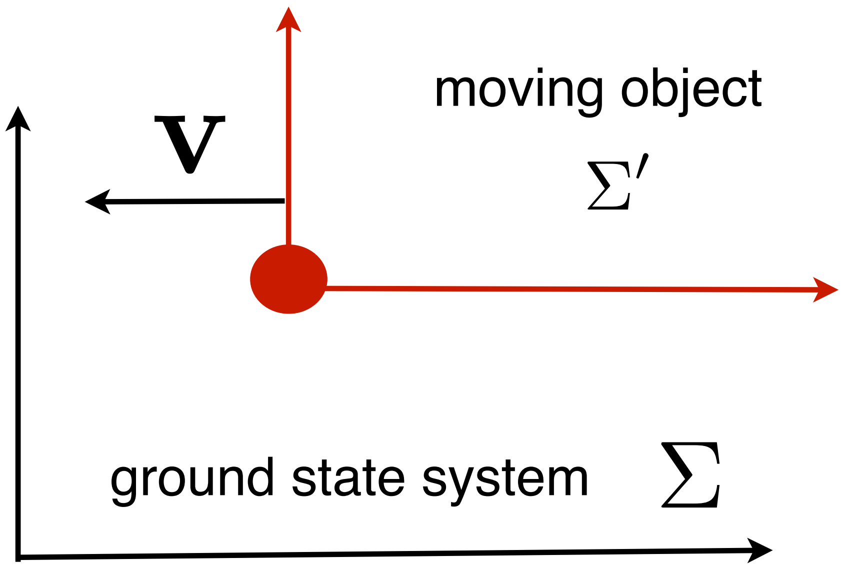
- Free Bose gas: No superfluidity due to soft particle excitations

$$\epsilon_{\mathbf{p}} = \frac{\mathbf{p}^2}{2m} \to v_c = 0$$



➡ Superfluidity is due to linear spectrum of quasiparticle excitations

Idea of Landau Criterion



- Consider moving object in the liquid ground state of a system
- Question: When is it favorable to create excitations?

  - General transformation of energy and momentum under Galilean boost with velocity $\mathbf{v}$

w/o moving object $E, \quad \mathbf{p}$

total system mass

with moving object $E' = E - \mathbf{p}\mathbf{v} + \frac{1}{2}M\mathbf{v}^2, \quad \mathbf{p}' = \mathbf{p} - M\mathbf{v}$

  - Energy and momentum of the ground state

w/o moving object $E_0, \quad \mathbf{p}_0 = 0$

with moving object $E_0' = E_0 + \frac{1}{2}M\mathbf{v}^2, \quad \mathbf{p}_0' = -M\mathbf{v}$

  - Energy and momentum of the ground state plus an excitation with momentum, energy $\mathbf{p}, \epsilon_{\mathbf{p}}$

w/o moving object $E_{\text{ex}} = E_0 + \epsilon_{\mathbf{p}}, \quad \mathbf{p}_{\text{ex}} = \mathbf{p}$

with moving object $E_{\text{ex}}' = E_0 + \epsilon_{\mathbf{p}} - \mathbf{p}\mathbf{v} + \frac{1}{2}M\mathbf{v}^2, \quad \mathbf{p}_{\text{ex}}' = \mathbf{p} - M\mathbf{v}$

  - Creation of excitation unfavorable if

$$E_{\text{ex}}' - E_0' = \epsilon_{\mathbf{p}} - \mathbf{p}\mathbf{v} \geq \epsilon_{\mathbf{p}} - |\mathbf{p}||\mathbf{v}| > 0 \qquad \Rightarrow v < v_c = \frac{\epsilon_{\mathbf{p}}}{p}$$

Summary

- The basic phenomenon of Bose-Einstein condensation is a statistical effect, not driven by interactions.

- Ultracold bosonic quantum gases realize a situation close to that: model Hamiltonians with weak, local, repulsive interactions.

- Important scale hierarchy: $a \ll d \ll \lambda_{dB}$

- In consequence, such systems are well described by relatively simple approximations: at T=0, the physics is well understood in terms of GP equation + quadratic fluctuations.

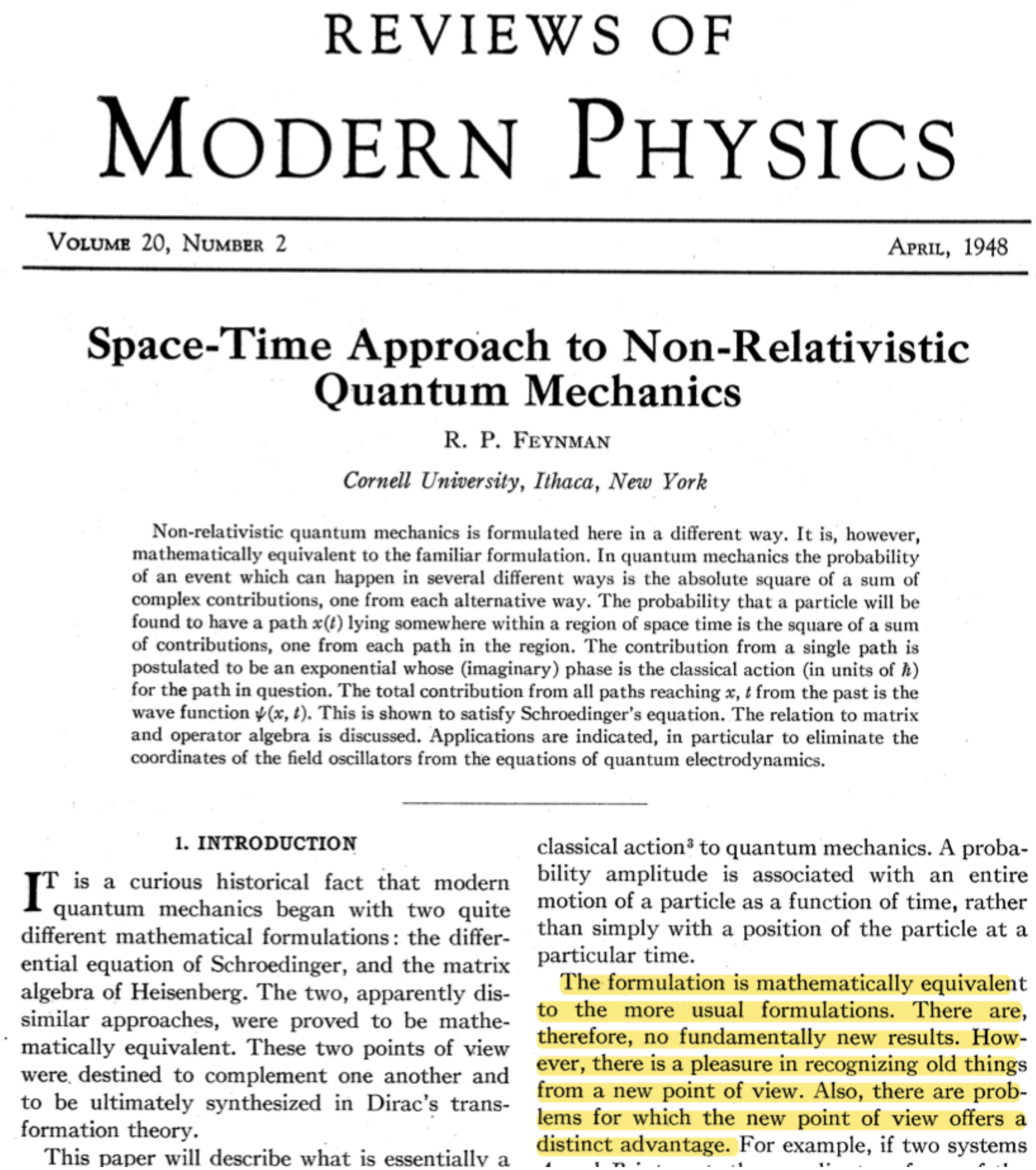
- GP mean field equation = nonlinear Schrödinger equation for macroscopic wave function (hallmark: quantized vortices).

- Bogoliubov theory encompasses quadratic fluctuations around GP mean field and explains superfluidity through existence of phonon mode.

Tutorial:
Functional Integrals
and
Effective Action

$$Z = \mathrm{tr} e^{-\beta \hat{H}} = \int \mathcal{D}(\varphi^*, \varphi) e^{-S[\varphi^*, \varphi]}$$

Feynman’s formulation of quantum mechanics



REVIEWS OF
MODERN PHYSICS

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Space-Time Approach to Non-Relativistic Quantum Mechanics

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Non-relativistic quantum mechanics is formulated here in a different way. It is, however, mathematically equivalent to the familiar formulation. In quantum mechanics the probability of an event which can happen in several different ways is the absolute square of a sum of complex contributions, one from each alternative way. The probability that a particle will be found to have a path $x(t)$ lying somewhere within a region of space time is the square of a sum of contributions, one from each path in the region. The contribution from a single path is postulated to be an exponential whose (imaginary) phase is the classical action (in units of $\hbar$) for the path in question. The total contribution from all paths reaching x, t from the past is the wave function $\psi(x, t)$. This is shown to satisfy Schroedinger's equation. The relation to matrix and operator algebra is discussed. Applications are indicated, in particular to eliminate the coordinates of the field oscillators from the equations of quantum electrodynamics.

1. INTRODUCTION

IT is a curious historical fact that modern quantum mechanics began with two quite different mathematical formulations: the differential equation of Schroedinger, and the matrix algebra of Heisenberg. The two, apparently dissimilar approaches, were proved to be mathematically equivalent. These two points of view were destined to complement one another and to be ultimately synthesized in Dirac's transformation theory.

This paper will describe what is essentially a

classical action[3] to quantum mechanics. A probability amplitude is associated with an entire motion of a particle as a function of time, rather than simply with a position of the particle at a particular time.

The formulation is mathematically equivalent to the more usual formulations. There are, therefore, no fundamentally new results. However, there is a pleasure in recognizing old things from a new point of view. Also, there are problems for which the new point of view offers a distinct advantage. For example, if two systems

Functional Integrals for Statistical Mechanics

- Given a grand canonical Hamiltonian , e.g. with general two-body interactions, normally ordered

$$H - \mu\hat{N} = \sum_{ij}(h_{ij} - \mu\delta_{ij})a_i^\dagger a_j + \sum_{ijkl} V_{ijkl} a_i^\dagger a_j^\dagger a_k a_l$$

- Quantum partition function

$$Z = \mathrm{tr} e^{-\beta(H-\mu\hat{N})} = \sum_{\{\mathrm{n}\}\in \mathrm{Fock\,space}} \langle \mathrm{n}|e^{-\beta(H-\mu\hat{N})}|n\rangle, \quad \beta = 1/k_B T$$

- Here the partition function is represented in Fock space. We now perform a basis change to coherent states leading to the functional integral
- Coherent states (bosons) – eigenstates to the annihilation operators a_i:

$$a_i|\phi\rangle \quad = \phi_i|\phi\rangle,\ \langle\phi|a_i^\dagger = \langle\phi|\phi_i^*$$

- properties:

$$|\phi\rangle \quad = e^{\sum_i \phi_i a_i^\dagger}|\mathrm{vac}\rangle \qquad \text{explicit form}$$

$$\langle\theta|\phi\rangle \quad = e^{\sum_i \theta_i^*\phi_i},\ \langle\phi|\phi\rangle = e^{\sum_i \phi_i^*\phi_i} \qquad \text{overlap and normalization}$$

$$\mathbf{1}_{\mathrm{Fock}} \quad = \int \prod_i \frac{d\phi_i^* d\phi_i}{\pi} e^{-\sum_i \phi_i^*\phi_i}|\phi\rangle\langle\phi| \qquad \text{completeness}$$

- Note: The creation operators do not have eigenstates

Functional Integrals

- Insert identity into quantum partition function

$$\begin{aligned} Z &= \mathrm{tr} e^{-\beta(H-\mu\hat{N})} = \textstyle\sum_{\{\mathrm{n}\}\in \mathrm{Fock\,space}} \langle \mathrm{n}|e^{-\beta(H-\mu\hat{N})}|n\rangle \\ &= \textstyle\int D(\phi^*,\phi) e^{-\sum_i \phi_i^* \phi_i} \langle\phi|e^{-\beta(H-\mu\hat{N})}|\phi\rangle, \quad D(\phi^*,\phi) \equiv \prod_i \frac{d\phi_i^* d\phi_i}{\pi} \end{aligned}$$

- For a normal ordered Hamiltonian $H(a_i^\dagger, a_i) - \mu\hat{N}(a_i^\dagger, a_i)$, we can apply the Feynman strategy of dividing the (imaginary) time interval β into N segments $\Delta\beta = \beta/N$. Note $|\phi_{n=0}\rangle = |\phi_{n=N}\rangle$ – periodic boundary conditions
- Inserting the identity $\mathbf{1}_{\mathrm{Fock}} = \int D(\phi_n^*, \phi_n) e^{-\sum_i \phi_{i,n}^* \phi_{i,n}} |\phi_n\rangle\langle\phi_n|$ after each time step, the respective matrix elements can be calculated explicitly due to the smallness of $\Delta\beta$ with result

$$Z = \int \prod_{n=0}^{N} D(\phi_n^*, \phi_n) e^{-\sum_{n=0}^{N}[\sum_i \phi_{i,n}^*(\phi_{i,n}-\phi_{i,n-1}) + \Delta\beta(H(\phi_{i,n}^*,\phi_{i,n-1}) - \mu N(\phi_{i,n}^*,\phi_{i,n-1}))}$$

  - Here, $H - \mu N$ is a function of classical, but fluctuating variable.
  - The additional index n labels the (imaginary) time evolution. Continuum notation for $N \to \infty$:

$$\Delta\beta \sum_{n=0}^{N} \to \int_0^\beta d\tau, \quad \phi_{i,n} \to \phi_i(\tau), \quad \frac{\phi_{i,n} - \phi_{i,n-1}}{\Delta\beta} \to \partial_\tau \phi_i(\tau), \quad \prod_{n=0}^{N} D(\phi_n^*, \phi_n) \to \mathcal{D}(\phi^*, \phi)$$

Functional Integrals

- Continuum notation for the imaginary time dependence

$$
\begin{aligned}
Z \quad &= \int \mathcal{D}(\phi^*,\phi) e^{-S[\phi^*,\phi]} \\
S[\phi^*,\phi] \quad &= \int_0^\beta d\tau \big[\sum_i \phi_i^*(\tau)(\partial_\tau - \mu)\phi_i(\tau) + H[\phi^*,\phi] \ \big] \\
H[\phi^*,\phi] \quad &= \sum_{ij} h_{ij}\phi_i^*\phi_j + \sum_{ijkl} V_{ijkl}\phi_i^*\phi_j^*\phi_k\phi_l
\end{aligned}
$$

- S is the “classical” or “microscopic” action
- Continuum notation for the discrete indices:
  - interpret indices as spatial indices
  - consider local density-density interactions $V_{ijkl} = v\delta_{ik}\delta_{jl}\delta_{il}$ and h_{ij} such that it describes kinetic energy (1D)

$$
H[\phi^*,\phi] = \sum_{ij} h(\phi_{i+1}^* - \phi_i^*)(\phi_{i+1} - \phi_i) + v\sum_i (\phi_i^*\phi_i)^2
$$

  - the sites $i, i+1$ be separated by a distance a. The continuum limit $a \to 0$ obtains for fixed $\varphi(\tau,x) = a^{-1/2}\phi_i(\tau), 1/2M = ha^2, g/2 = va$, such that

$$
S[\varphi^*,\varphi] \quad = \int_0^\beta d\tau dx [\varphi^*(\tau,x)(\partial_\tau - \tfrac{\triangle}{2M} - \mu)\varphi(\tau,x) + \tfrac{g}{2}(\varphi^*(\tau,x)\varphi(\tau,x))^2]
$$

- S is the “classical” or “microscopic” action of nonrelativistic continuum bosons with local interaction in one spatial dimension

Finite temperatures and Matsubara frequencies

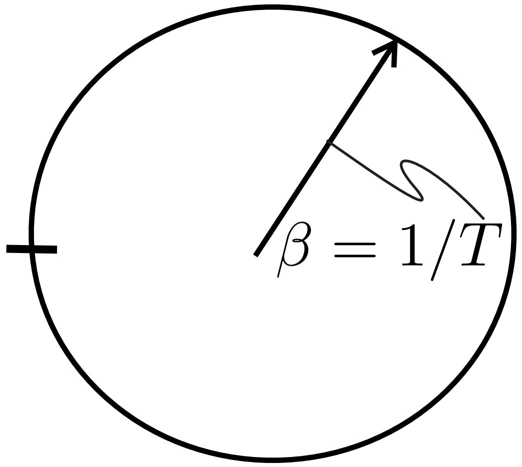
- Unlike the spatial integrations, the imaginary time integrations are restricted to a finite interval
- For bosons, we have used periodic boundary conditions, i.e. $\varphi(\tau = \beta, x) = \varphi(\tau = 0, x)$
- This gives rise to a discreteness in the frequency domain (cf. particle in a box problem) for finite $\beta < \infty \, (T > 0)$: Matsubara modes

$$\begin{aligned} \varphi(\tau, x) &= T \textstyle\sum_n \varphi(\omega_n, x) e^{\mathrm{i}\omega_n \tau}, \; \varphi(\omega_n, x) = \int d\tau \varphi(\tau, x) e^{-\mathrm{i}\omega_n \tau}, \\ \omega_n &= 2\pi n T \end{aligned}$$

- E.g. the free part of the action reads ($\beta^{-1} \int_0^\beta d\tau e^{\mathrm{i}(\omega_n - \omega_m)\tau} = \delta_{\omega_n, \omega_m}$)

$$S[\varphi^*, \varphi] = \sum_n T \int dx [\varphi^*(\omega_n, x)(\mathrm{i\omega_n} - \tfrac{\triangle}{2M} - \mu)\varphi(\omega_n, x)]$$

- In the zero temperature limit, the frequency spacing $\Delta\omega = 2\pi T \to 0$ and the Matsubara summation goes over into a continuum Riemann integral, $\sum_n T \to \int \frac{d\omega}{2\pi}$



$\varphi(\tau = \beta, x) = \varphi(\tau = 0, x)$

Matsubara torus

Formula summary

- Functional integral representation of the quantum partition function for ultracold bosons (3D):

$$
\begin{aligned}
Z &= \int \mathcal{D}(\varphi^*,\varphi) e^{-S[\varphi^*,\varphi]} \\
S[\varphi^*,\varphi] &= \int_0^\beta d\tau \left[\left(\int d^3x \varphi^*(\tau,\mathbf{x})(\partial_\tau - \mu)\varphi(\tau,\mathbf{x}) \right) + H[\varphi^*(\tau,\mathbf{x}),\varphi(\tau,\mathbf{x})] \right] \\
&= \int_0^\beta d\tau \int d^3x \left[\varphi^*(\tau,\mathbf{x})(\partial_\tau - \tfrac{\triangle}{2M} - \mu)\varphi(\tau,\mathbf{x}) + \tfrac{g}{2}(\varphi^*(\tau,x)\varphi(\tau,x))^2 \right]
\end{aligned}
$$

- Discussion:
  - The validity of the microscopic action is based on the validity of the microscopic Hamiltonian
  - The boson fields φ^*, φ are commuting but temporally and spatially fluctuating complex numbers
- Fermions: The same form of the microscopic action is obtained when representing the partition function for continuum fermion fields ψ. Important differences are:
  - Additional spin index, for two-component fermions: $\psi(\tau,\mathbf{x}) = (\psi_\uparrow(\tau,\mathbf{x}), \psi_\downarrow(\tau,\mathbf{x}))^T$
  - Due to the anticommutation relations of the fermion operators, the fermionic fields are anticommuting Grassmann numbers,

$$
\{\psi_\sigma(\tau,\mathbf{x}), \psi^*_{\sigma'}(\tau,\mathbf{x})\} = \{\psi_\sigma(\tau,\mathbf{x}), \psi_{\sigma'}(\tau,\mathbf{x})\} = \{\psi^*_\sigma(\tau,\mathbf{x}), \psi^*_{\sigma'}(\tau,\mathbf{x})\} = 0
$$

  - They obey antiperiodic boundary conditions in imaginary time $\psi_\sigma(\tau=\beta,x) = -\psi_\sigma(\tau=0,x)$, thus $\omega_n = (2n+1)\pi T$
  - Obviously, these properties will strongly affect the concrete evaluation of the functional integrals

From the Partition Function to the Effective Action

Le

- We have stored the information on the many-body system in the partition function

$$Z \quad = \int \mathcal{D}(\varphi^*,\varphi) e^{-S[\varphi^*,\varphi]}$$

- Of interest are the low order correlation functions such as e.g. $\langle \varphi(\tau,\mathbf{x})\varphi^*(0,\mathbf{0})\rangle$
- They can be calculated from introducing (imaginary time and space dependent) artificial sources into the partition function:

$$Z \to Z[j^*(\tau,\mathbf{x}),j(\tau,\mathbf{x})] = \int \mathcal{D}(\varphi^*,\varphi) e^{-S[\varphi^*,\varphi]+\int_{\tau,\mathbf{x}}(j^*(\tau,\mathbf{x})\varphi(\tau,\mathbf{x})+j(\tau,\mathbf{x})\varphi^*(\tau,\mathbf{x}))}$$

- and taking (functional) derivatives evaluated at vanishing sources, e.g.

$$\langle \varphi(\tau,\mathbf{x})\varphi^*(0,\mathbf{0})\rangle = \frac{\delta^2 Z}{\delta j^*(\tau.\mathbf{x})\delta j(0,\mathbf{0})}\Big|_{j=j^*=0}$$

- Remarks:
  - functional derivatives are defined with $\delta f(x)/\delta f(y) = \delta(x-y)$ plus the standard algebraic rules for differentiation
  - successive differentiation generates the “disconnected correlation functions”. The free energy

$$W[j^*,j] = \log Z[j^*,j]$$

generates the “connected correlation functions”

From the Partition Function to the Effective Action

- The information accessible from $Z[j^*, j]$ or $W[j^*, j]$ via derivatives wrt an unphysical source (j^*, j)
- There is a way to store the information in a more intuitive way: Legendre transform of W(cf. classical mechanics, or thermodynamics)

$$\Gamma[\phi^*, \phi] = -W[j^*, j] + \int j^*\phi + j\phi^*, \quad \phi(\tau, \mathbf{x}) = \frac{\delta W[j^*, j]}{\delta j(\tau, \mathbf{x})} = \langle \varphi(\tau, \mathbf{x}) \rangle$$

- Properties and Discussion:
  - The Legendre transform implements a change of the active variable $(j^*, j) \to (\phi^*, \phi)$
  - The expectation value $\phi = \langle \varphi \rangle$ is called the classical field. For ultracold bosons, it has a direct physical interpretation in terms of the condensate mean field
  - The effective action carries the same information as Z and W, only organized differently. It generates the one-particle irreducible correlation functions

From the Partition Function to the Effective Action

- The effective action has a functional integral representation

$$\boxed{\exp -\Gamma[\phi^*,\phi] = \int \mathcal{D}(\delta\varphi^*,\delta\varphi)\exp -S[\phi^*+\delta\varphi^*,\phi+\delta\varphi], \quad \frac{\delta\Gamma[\phi^*,\phi]}{\delta\phi(\tau,\mathbf{x})} = j(\tau,\mathbf{x}) = 0}$$

- Discussion
  - NB: Action principle is leveraged over to full quantum status (see below)
  - The effective action can be understood “classical action plus fluctuations”. It lends itself to semi-classical approximations (small fluctuations around a mean field)
  - Symmetry principles are leveraged over from the classical action to full quantum status

additional material

Effective Action and Propagator

- A useful property: The second derivative of the effective action is the inverse propagator
- Consider a propagation amplitude (in matrix notation)

$$G_{ij} = \langle \delta\varphi_i \delta\varphi_j \rangle = \frac{\delta^2 W}{\delta j_i \delta j_j} = W^{(2)}_{ij}$$

the indices could stand for e.g. $\langle \delta\varphi(\tau, \mathbf{x}) \delta\varphi^*(0, \mathbf{0}) \rangle$

- The above statement is then poperly formulated as the identity

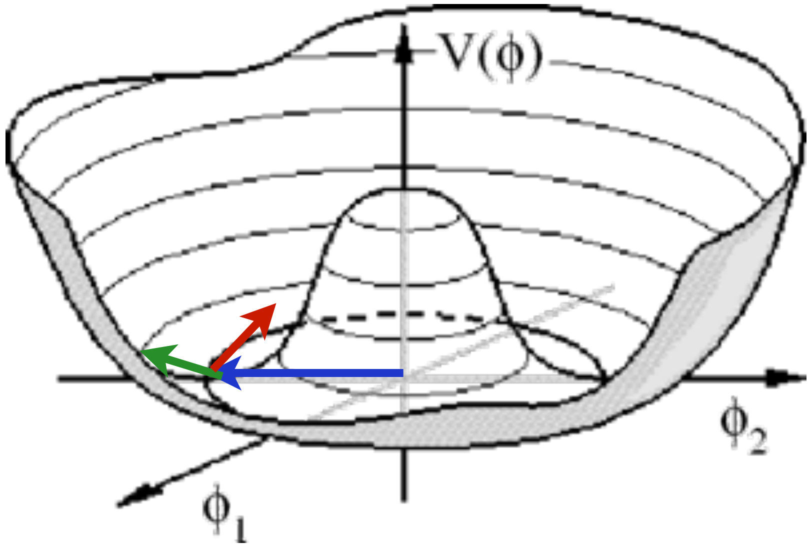
$$\sum_k \Gamma^{(2)}_{ik} G_{kj} = \delta_{ij}$$

- Proof:

$$\sum_k \Gamma^{(2)}_{ik} G_{kj} = \sum_k \frac{\delta^2 \Gamma}{\delta\phi_i \delta\phi_k} \frac{\delta^2 W}{\delta j_k \delta j_j} = \sum_k \frac{\delta^2 \Gamma}{\delta\phi_i \delta\phi_k} \frac{\delta\phi_k}{\delta j_j} = \frac{\delta^2 \Gamma}{\delta\phi_i \delta j_j} = \frac{\delta j_i}{\delta j_j} = \delta_{ij}$$

we have used the chain rule and the field equation for the effective action $\delta\Gamma/\delta\phi_i = j_i$

Functional Integral
for
Weakly Interacting Bosons



Some Introductory Remarks

- This section develops the theory of low temperature weakly interacting boson degrees of freedom from the functional integral point of view. The aim is threefold:

(1) Reproduce the results of Gross-Pitaevski and Bogoliubov theory

(2) Get some familiarity with the functional integral: symmetries, approximations, etc.

(3) The emergence of bosonic quasiparticles at low energies is ubiquitous in a large variety of low temperature quantum systems:

- The concept of quasiparticles/ effective low energy theories is particularly accessible in the functional integral formulation
- Examples of emergent bosonic low energy theories:
    - BCS theory (Cooper pairs)
    - Even more explicitly, BCS-BEC crossover (bound states of fermions: molecules)
    - spin waves in magnetic lattice systems
- A rather universal understanding of such theories is crucial, and accessible within the framework developed here

Recovering the Gross-Pitaevski Equation

- Quantum equation of motion: action principle for the Effective Action

$$0 = \frac{\delta\Gamma}{\delta\phi^*(X)} \propto \int \mathcal{D}(\delta\varphi^*, \delta\varphi)\Big[\frac{\delta S}{\delta\phi^*(X)}\Big]e^{-S[\phi+\delta\varphi]} \qquad X = (\tau, \mathbf{x})$$

- explicitly:

$$\begin{aligned}0 &= (\partial_\tau - \frac{\triangle}{2M} - \mu)\langle\varphi(X)\rangle + g\langle\varphi^*(X)\varphi^2(X)\rangle \\ &= \phi(X)\end{aligned}$$

➡ in general, needs information on 3-point correlation, which needs information on 5-point correlation...: infinite hierarchy

- however, at very low temperature and weak interaction: $\varphi(X) = \phi(X) + \delta\varphi(X)$
  $\mathcal{O}(V^0)$ $\mathcal{O}(V^{-1/2})$

➡ GP Approximation: neglect $\mathcal{O}(V^{-1/2})$

$$0 = (\partial_\tau - \frac{\triangle}{2M} - \mu)\phi(X) + g\phi^*(X)\phi^2(X)$$

➡ “imaginary time” GP equation

Recovering the Gross-Pitaevski Equation

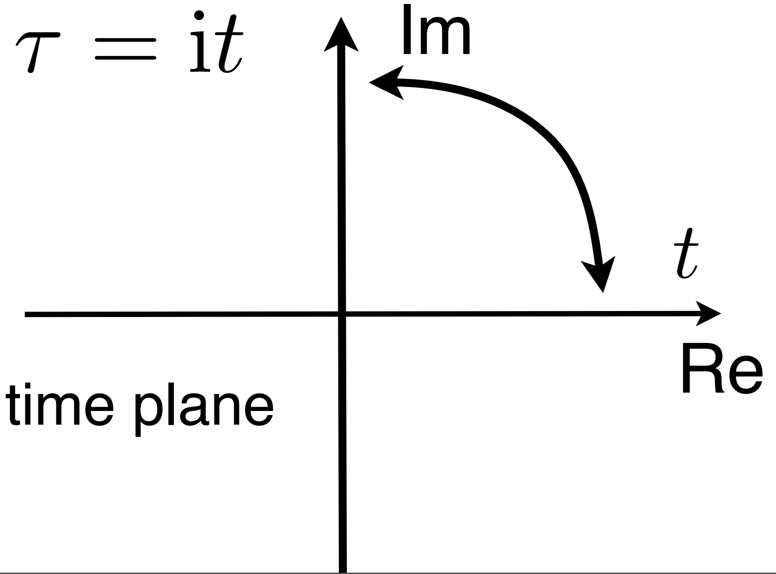
- Indeed, time was introduced rather formally. But the connection to real times is readily made:
- We consider the imaginary time classical action S and and view it as being analytically continued from the real axis (at $T = 0$ or $\beta \to \infty$):

$$\begin{array}{ll} \tau & \to \mathrm{i}t, \quad \phi(\tau, \mathbf{x}) \to \tilde{\phi}(t, \mathbf{x}) \Rightarrow \\ S[\phi^*, \phi] & \to \mathrm{i}S[\tilde{\phi}^*, \tilde{\phi}] = \mathrm{i} \int dt \int d^3x \left[\tilde{\phi}^*(t, \mathbf{x})(-\mathrm{i}\partial_t - \frac{\triangle}{2M} - \mu)\tilde{\phi}(t, \mathbf{x}) + \frac{g}{2}(\tilde{\phi}^*(t, x)\tilde{\phi}(t, x))^2 \right] \end{array}$$

- We derive the field equation of motion for the real time classical action $\delta S / \delta \tilde{\phi}^*(t, \mathbf{x}) = 0$

$$\mathrm{i}\partial_t \tilde{\phi}(t, \mathbf{x}) = \big(- \tfrac{1}{2M} \triangle - \mu + g \tilde{\phi}^*(t, \mathbf{x}) \tilde{\phi}(t, \mathbf{x}) \big) \tilde{\phi}(t, \mathbf{x})$$

- This is precisely the Gross-Pitaevski equation for a weakly interacting Bose-Einstein condensate
- Remark: “classical” refers to the absence of fluctuations. Physically, the global phase coherence implied in this equations is a quantum mechanical effect, with observable consequences: cf. discussion of quantized vortices (see below for more discussion)



Complex time plane

Symmetries of the Microscopic Action

- Gross-Pitaevski action:

$$S[\tilde{\phi}^*, \tilde{\phi}] = \int dt \int d^3x \left[\tilde{\phi}^*(t, \mathbf{x})(-\mathrm{i}\partial_t - \tfrac{\triangle}{2M} - \mu)\tilde{\phi}(t, \mathbf{x}) + \tfrac{g}{2}(\tilde{\phi}^*(t, x)\tilde{\phi}(t, x))^2\right]$$

- Symmetries:
  - Most important is the invariance under global phase rotations $U(1)$. Such transformation is implemented by $\tilde{\phi}(\tau, \mathbf{x}) \to e^{\mathrm{i}\theta}\tilde{\phi}(\tau, \mathbf{x})$, $\tilde{\phi}^*(\tau, \mathbf{x}) \to e^{-\mathrm{i}\theta}\tilde{\phi}^*(\tau, \mathbf{x})$.
  - The associated conserved Noether charge (of the full effective action) is the total particle number $N = \int d^3x \langle \varphi^*(0, \mathbf{x})\varphi(0, \mathbf{x})\rangle$ (NB: needs $U(1)$ symmetry plus linear time derivative)
  - Further continuous "equilibrium" symmetries: time and space translation invariance (energy and momentum conservation) and Galilean invariance (center of mass momentum)

Mean Field Action and Spontaneous Symmetry Breaking

- Homogeneous action: time- and space independent amplitudes ($\int d\tau d^3x = V/T$ -- quantization volume)

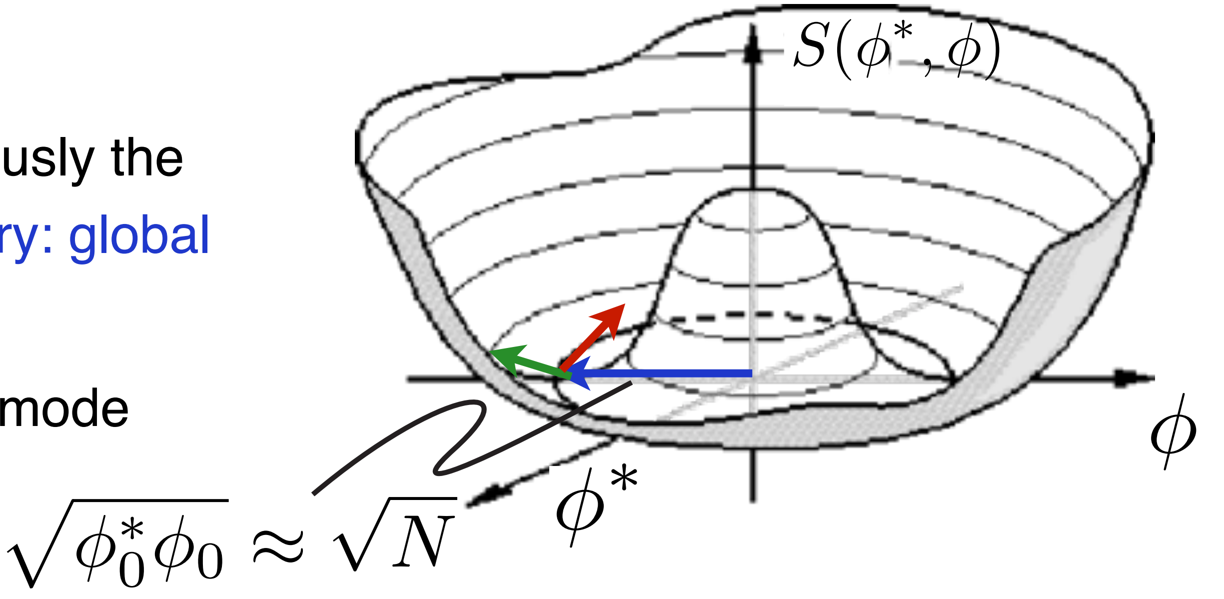
$$S(\phi^*, \phi) = V/T(-\mu\phi^*\phi + \tfrac{g}{2}(\phi^*\phi)^2)$$

- homogeneous GPE or equilibrium condition:

$$0 = \frac{\partial S}{\partial \phi} = \big(-\mu + g\phi^*\phi\big)\phi \qquad \Rightarrow -\mu = -g\phi^*\phi < 0$$

-- negative curvature at origin

- Geometrical interpretation: Mexican hat potential
  - for the ground state, the system chooses spontaneously the direction: spontaneous symmetry breaking (symmetry: global phase rotations U(1))
  - Radial (amplitude) excitations: cost energy, gapped mode
  - angular (phase) excitations: no energy cost due to degeneracy, gapless Goldstone mode



- Next steps:

➡ The radial (amplitude) and angular (phase) excitations can be identified explicitly in the quadratic fluctuations. En route of showing this, recover Bogoliubov theory

➡ The Goldstone mode is not an artifact of Mean Field but will be established as an exact property

Quadratic Fluctuations: Recovering Bogoliubov Theory

- We go one step beyond the classical limit and include quadratic fluctuations on top of the mean field
- Expansion of S in powers of $(\delta\varphi^*, \delta\varphi)$ around $(\delta\varphi^*, \delta\varphi) = (0,0)$ yields the approximate effective action (saddle point approximation):

$$\begin{aligned}\Gamma[\phi^*, \phi] \quad &= -\log \int \mathcal{D}(\delta\varphi^*, \delta\varphi) \exp -S[\phi^* + \delta\varphi^*, \phi + \delta\varphi] \\ &\approx S[\phi^*, \phi] - \log \int \mathcal{D}(\delta\varphi^*, \delta\varphi) \exp -\tfrac{1}{2} \int (\delta\varphi, \delta\varphi^*) S^{(2)}[\phi^*, \phi] \begin{pmatrix} \delta\varphi \\ \delta\varphi^* \end{pmatrix}\end{aligned}$$

Here, we have used the field equation $\delta S/\delta(\delta\varphi) = \delta S/\delta\phi = 0$

- We restrict to the homogeneous case $\phi(\tau, \mathbf{x}) = \phi_0$

➡ specify ϕ_0
➡ specify $S^{(2)}$

Quadratic Fluctuations: Recovering Bogoliubov Theory

- Homogenous case:
  - The field equation (in general: GPE) reduces to an equilibrium condition determining the chemical potential (see above)

    $$0 = \frac{\delta S}{\delta \phi}\Big|_{\mathrm{hom.}} = (-\mu + g\phi_0^*\phi_0)\phi_0^*$$

    For small enough T and g, $|\phi_0| \neq 0$ such that at equilibrium

    $$\mu_0 = g\phi_0^*\phi_0.$$

    Coincides with Bogoliubov Theory
  - It is favorable to work in frequency and momentum space. There, the exponent reads explicitly ($Q = (\omega_n, \mathbf{q}), \int_Q = \sum_n T \int \frac{d^3q}{(2\pi)^3}$):

$$S^{(2)}(\phi^*, \phi) \quad = \Big(\frac{\overrightarrow{\delta}}{\delta(\delta\varphi)(-Q)}, \frac{\overrightarrow{\delta}}{\delta(\delta\varphi^*)(Q)}\Big) S \left(\begin{array}{c} \frac{\overleftarrow{\delta}}{\delta(\delta\varphi)(K)} \\ \frac{\overleftarrow{\delta}}{\delta(\delta\varphi^*)(-K)} \end{array} \right) \propto \delta(K-Q) \quad \text{-- diagonal in momentum space}$$

$$\Longrightarrow \quad \frac{1}{2}\int_Q \big(\delta\varphi(-Q), \delta\varphi^*(Q)\big) \left(\begin{array}{cc} g\phi_0^{*2} & -\mathrm{i}\omega_\mathrm{n} + \frac{\mathbf{q}^2}{2\mathrm{M}} - \mu + 2g\phi_0^*\phi_0 \\ \mathrm{i}\omega_\mathrm{n} + \frac{\mathbf{q}^2}{2\mathrm{M}} - \mu + 2g\phi_0^*\phi_0 & g\phi_0^2 \end{array} \right) \left(\begin{array}{c} \delta\varphi(Q) \\ \delta\varphi^*(-Q) \end{array} \right)$$

  - NB: The frequency-independent part of the matrix coincides with Bogoliubov theory
  - This is a quadratic form leading to a Gaussian functional integral. A technique to evaluate it is discussed below

Phase and Amplitude Fluctuations

- We analyze the quadratic action for the boson fluctuations, using $-\mu = g\phi^*\phi$

$$S_F[\delta\varphi^*,\delta\varphi] = \frac{1}{2}\int_Q (\delta\varphi(-Q),\delta\varphi^*(Q)) \begin{pmatrix} g\phi_0^{*2} & -\mathrm{i}\omega_\mathrm{n} + \epsilon_\mathbf{q} + g\phi_0^*\phi_0 \\ \mathrm{i}\omega_\mathrm{n} + \epsilon_\mathbf{q} + g\phi_0^*\phi_0 & g\phi_0^2 \end{pmatrix} \begin{pmatrix} \delta\varphi(Q) \\ \delta\varphi^*(-Q) \end{pmatrix}$$

- We perform a change of basis (real and imaginary parts), NB: signs due to reality $\delta\varphi_i(Q)^* = \delta\varphi_i(-Q)$

$$\delta\varphi_1(Q) = (\delta\varphi^*(-Q) + \delta\varphi(Q))/\sqrt{2}, \quad \delta\varphi_2(Q) = \mathrm{i}(\delta\varphi^*(Q) - \delta\varphi(-Q))/\sqrt{2}$$

- The action in the new coordinates reads ($\rho_0 = \phi_0^*\phi_0$ and we choose ϕ real without loss of generality)

$$S_F[\delta\varphi_1,\delta\varphi_2] = \frac{1}{2}\int_Q (\delta\varphi_1(-Q),\delta\varphi_2(Q)) \begin{pmatrix} \epsilon_\mathbf{q} + 2g\rho_0 & -\omega_\mathrm{n} \\ \omega_\mathrm{n} & \epsilon_\mathbf{q} \end{pmatrix} \begin{pmatrix} \delta\varphi_1(Q) \\ \delta\varphi_2(-Q) \end{pmatrix}$$

- ➡ Phase and amplitude couple asymetrically to the homogenous “gap” term $2g\rho_0$
- ➡ Frequency couples phase and amplitude

Phase and Amplitude Fluctuations

- Action in terms of real fields:

$$S_F[\delta\varphi_1,\delta\varphi_2] = \frac{1}{2}\int_Q (\delta\varphi_1(-Q),\delta\varphi_2(Q)) \overbrace{\begin{pmatrix} \epsilon_{\mathbf{q}}+2g\rho_0 & -\omega_{\mathrm{n}} \\ \omega_{\mathrm{n}} & \epsilon_{\mathbf{q}} \end{pmatrix}}^{\equiv G^{-1}(\omega_n,\mathbf{q})} \begin{pmatrix} \delta\varphi_1(Q) \\ \delta\varphi_2(-Q) \end{pmatrix}$$

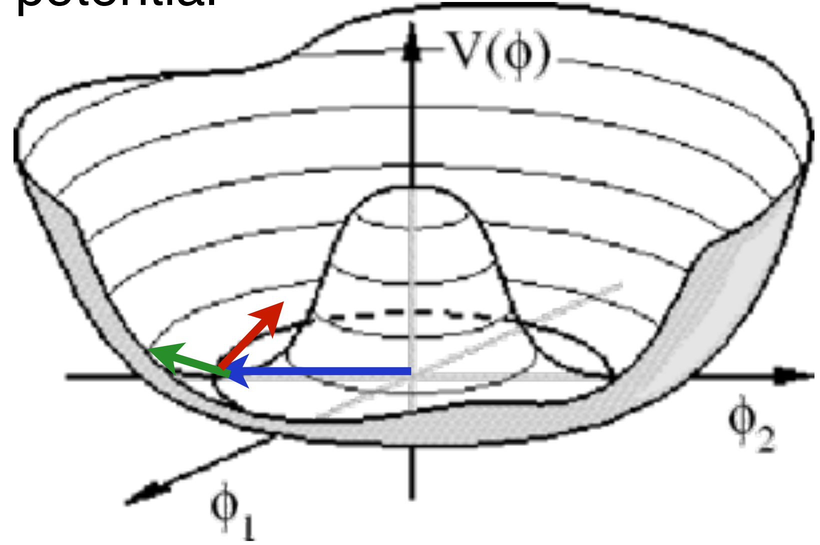
inverse Green's function

- Discussion:
  - Real part corresponds to amplitude fluctuations (see figure) and is gapped (massive) with $2g\rho_0$
  - Imaginary part corresponds to phase fluctuations and is gapless (massless)
  - The dispersion relation obtains from the coupled equations of motion for the fluctuations (analytically continued to real continuous frequencies $E = \mathrm{i}\omega_n$)

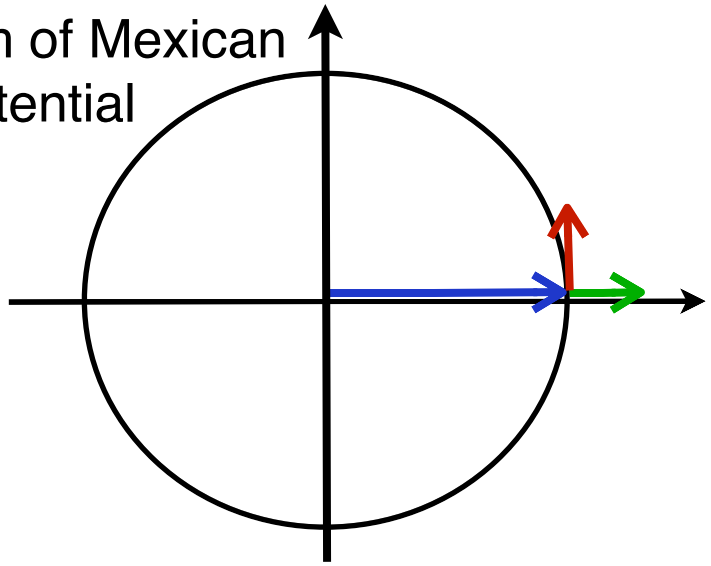
$$\det G^{-1}(\mathrm{E}=\mathrm{i}\omega,\mathbf{q}) \overset{!}{=} 0 \quad \Rightarrow E_{\mathbf{q}} = \sqrt{\epsilon_{\mathbf{q}}(\epsilon_{\mathbf{q}}+2g\rho_0)}$$

reproduces the Bogoliubov excitation spectrum with $E_{\mathbf{q}} \approx c|\mathbf{q}|$, $c = \sqrt{g\rho_0/M}$ for $\mathbf{q} \to 0$

Mexican hat potential



Bottom of Mexican hat potential



Phase-Only Action

- If we are interested in the physics at very low momenta/energies $E \ll g\rho_0$, we can integrate out the amplitude mode:

$$\int \mathcal{D}\delta\varphi_1 \mathcal{D}\delta\varphi_2 \exp -S_F[\delta\varphi_1, \delta\varphi_2] = \mathcal{N} \int \mathcal{D}\delta\varphi_2 \exp -S_{ph}[\delta\varphi_2]$$

- This is done by completing the square in the exponent. The phase-only action reads

$$S_{ph}[\delta\varphi_2] = \tfrac{1}{4g\rho_0} \int_Q \delta\varphi_2(Q)(\omega^2 + c^2\mathbf{q}^2)\delta\varphi_2(-Q)$$

- Discussion:
- This action has a relativistic dispersion $E^2 = c^2\mathbf{q}^2$ (analytic continuation), with speed of sound $c = \sqrt{g\rho_0/M}$
- The speed of sound is also obtained from the limit $\mathbf{q} \to 0$ on the full dispersion relation. Now, we have found the interpretation of the linear dispersion in terms of phase fluctuations

- Conceptually, the low momentum dispersion can be obtained by diagonalization (cf. Bogoliubov operator approach) or by integrating out the fast/gapped modes (renormalization). The low frequency result is the same.
  - ➡ diagonalization keeps the full information of the spectrum, but may be intractable for interacting problems
  - ➡ renormalization drops high momentum information partially, but may be rather efficient for interacting problems

Phase-Only Action

- If we are interested in the physics at very low momenta/energies $E \ll g\rho_0$, we can integrate out the amplitude mode:

$$\int \mathcal{D}\delta\varphi_1 \mathcal{D}\delta\varphi_2 \exp - S_F[\delta\varphi_1, \delta\varphi_2] = \mathcal{N} \int \mathcal{D}\delta\varphi_2 \exp - S_{ph}[\delta\varphi_2]$$

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- The speed of sound is also obtained from the limit $\mathbf{q} \to 0$ on the full dispersion relation. Now, we have found the interpretation of the linear dispersion in terms of phase fluctuations
- The gapless nature of the phase-only action is protected by U(1) symmetry:
  - U(1) transformation with generator θ acts on amplitude and phase components as:

$$\delta\varphi_1 \to \delta\varphi_1, \quad \delta\varphi_2 \to \delta\varphi_2 + \theta$$

  - U(1) invariance: phase action contains derivative terms only. Indeed:

$$S_{ph} = -\int_X \delta\varphi_2(X)(\partial_\tau^2 + \nabla^2)\delta\varphi_2(X) = \int_X [(\partial_\tau\delta\varphi_2(X))^2 + (\nabla\delta\varphi_2(X))^2]$$

➡ More generally, symmetry constrains most general form of the effective action

Goldstone's Theorem

- The gapless nature of low energy excitation is not accidental but an exact property of the theory
- This is expressed in Goldstone's theorem: Assume a theory which is invariant under continuous global symmetry transformations. If the symmetry is spontaneously broken, then there are gapless excitations, the Goldstone modes.
- Discussion:
  - Does not prove the existence of symmetry breaking, but makes statement in case of
  - For an $O(N)$ symmetry, there are $N-1$ Goldstone modes
  - In our case, we have $U(1) \simeq O(2)$ and thus one Goldstone mode (phase)
  - The proof is straightforward using the effective action formalism

Proof of Goldstone's Theorem

- The exact field equation for the full effective action is $\delta\Gamma/\delta\phi(\tau,\mathbf{x}) = \delta\Gamma/\delta\phi^*(\tau,\mathbf{x}) = 0$. In the homogeneous limit, simplification $\partial\Gamma/\partial\phi = \partial\Gamma/\partial\phi^* = 0$
- Explicitly for $U(1)$ invariance: In the homogeneous limit, dependence of Γ restricted to the invariant $\rho = \phi^*\phi$: $\Gamma = \Gamma[\rho]$
- Field parametrization: $\phi = (\phi_1 + \mathrm{i}\phi_2)/\sqrt{2}$, $\phi^* = (\phi_1 - \mathrm{i}\phi_2)/\sqrt{2}$. I.e. $\rho = \frac{1}{2}(\phi_1^2 + \phi_2^2)$
- Equilibrium: choose real expectation value such that $\phi_1 = \phi_{1,0} + \delta\phi_1, \phi_2 = \delta\phi_2$. Spontaneous symmetry breaking: $\phi_{1,0} \neq 0$
- Consider field equation for ϕ_1,

$$0 = \frac{\partial\Gamma}{\partial\phi_1}\Big|_{\mathrm{eq}} = \phi_{1,0}\frac{\partial\Gamma}{\partial\rho}\Big|_{\mathrm{eq}} \quad \Rightarrow \quad \frac{\partial\Gamma}{\partial\rho}\Big|_{\mathrm{eq}} = 0$$

- consider mass term of ϕ_2:

$$m_2^2 \equiv \frac{\partial^2\Gamma}{\partial\phi_2^2}\Big|_{\mathrm{eq}} = \left(\frac{\partial^2\rho}{\partial\phi_2^2}\frac{\partial\Gamma}{\partial\rho} + \left(\frac{\partial\rho}{\partial\phi_2}\right)^2\frac{\partial^2\Gamma}{\partial\rho^2}\right)\Big|_{\mathrm{eq}} = \frac{\partial\Gamma}{\partial\rho}\Big|_{\mathrm{eq}} = 0$$

  I.e. for a symmetry broken spontaneously in the real direction, the imaginary part of the field is massless
- Goldstone's theorem is a relation of first and second derivatives of the homogenous part of the full effective action

Limiting cases of the Effective Action Functional Integral

- Often, reference is made to the “classical limit”

- There are actually (at least) three incarnations of what can be meant by this:

  1. The true classical limit $\hbar \to 0$
  2. The high temperature limit, where quantum fluctuations are unimportant $T \to \infty$
  3. The “semiclassical limit” equivalent to the Gross-Pitaevski approximation $N \to \infty$

- We now investigate these three ordering principles comparatively

1. Classical Limit for the Effective Action

- Here we study $\hbar \to 0$
- We restore the dimension for the action:

$$[S] = [\tau] \cdot [E] = [\tau] \cdot [\hbar\omega] = [\hbar]$$

- Effective Action:

$$\exp - \frac{\Gamma[\phi^*, \phi]}{\hbar} = \int \mathcal{D}(\delta\varphi^*, \delta\varphi) \exp - \frac{S[\phi^* + \delta\varphi^*, \phi + \delta\varphi]}{\hbar}$$

- In the classical limit $\hbar \to 0$ but fixed Γ, the exponential distribution is sharply peaked around the field configuration for which the classical action in the exponent is minimal.
- This is the case for the "classical" field configuration $\phi(\tau, \mathbf{x})$, determined by the classical action (extremum) variational principle $\delta S / \delta \phi(\tau, \mathbf{x}) = 0$
- With this insight, we can expand the classical action in the functional integral in the fluctuation $(\delta\varphi^*, \delta\varphi)$, and keep only the zero order term
- Thus, in the classical limit we have

$$\boxed{\Gamma[\phi^*, \phi] = S[\phi^*, \phi]}$$

- Discussion:
  - This limit is exact (unlike, e.g., the semiclassical limit below)
  - The problem remains nonlinear ("classical" means absence of fluctuations from the classical path/field configuration)
  - It is, however, less clear where this is indeed sensibly realized: For complex bosons, it would still allow for phase coherence and full temporal dynamics

2. High Temperature Limit

- Here we study $T \to \infty$
- In this limit, the field cannot evolve in imaginary time:

$$\varphi(\tau, \mathbf{x}) \approx [\text{const. in } \tau] \equiv \varphi(\mathbf{x})$$

- Implications: we may set

$$\partial_\tau \varphi(\tau, \mathbf{x}) \to 0 \qquad \int_0^\beta d\tau \to \beta$$

$$\boxed{\Rightarrow S \to \beta(H[\varphi] - \mu N[\varphi])}$$

  ➡ in this limit, classical statistical mechanics is recovered

  β can be absorbed into the couplings of H

- Discussion:
  - This limit is exact (unlike, e.g., the semiclassical limit below) and clearly realized in nature.
  - The problem remains nonlinear and keeps all spatial fluctuations.
  - Temporal fluctuations are suppressed completely (quantum fluctuations <-> temporal fluctuations). We cannot decide what the quantum dynamics of the system was originally.

2. High Temperature Limit and Dimensional Reduction

- In this limit, we cannot decide whether the original quantum dynamics was generated by

$$\int_{-\beta/2}^{\beta/2} d\tau[\varphi^*\partial_\tau\varphi] \qquad \text{or} \qquad \int_{-\beta/2}^{\beta/2} d\tau[\partial_\tau\varphi^*\partial_\tau\varphi]$$

non-relativistic dynamics (GP)

relativistic dynamics

or: phase dynamics described by real field, see above!

- For double time derivative, time and space derivatives appear symmetrically

➡ quantum and classical statistical problem are closely related (NB: for Euclidean actions, i.e. imaginary times, i.e. statistical problems!)

$$\int_{-\beta/2}^{\beta/2} d\tau d^dx[\partial_\tau\varphi^*\partial_\tau\varphi + c\nabla\varphi^*\nabla\varphi + m^2\varphi^*\varphi + \frac{g}{2}(\varphi^*\varphi)^2]$$

$$\overset{\beta\to\infty}{\to} \int d^{\boxed{d+1}}x[\partial_\mu\varphi^*\partial_\mu\varphi + m^2\varphi^*\varphi + \frac{g}{2}(\varphi^*\varphi)^2]$$

➡ relativistic d-dimensional quantum statistical problem is in one-to-one correspondence to (d+1)-dimensional classical statistical problem

➡ in other words, high temperatures lead to effective dimensional reduction

➡ non-relativistic dynamics is richer than relativistic one (true quantum criticality, Berry phases, ...)

3. “Semiclassical limit” and Validity of Bogoliubov Theory

- The ordering principle of the semiclassical approximation has been traced to the existence of a macroscopic (extensive) condensate. On the level of the functional integral:

$$\exp -\frac{\Gamma[\phi^*,\phi]}{\hbar} = \int \mathcal{D}(\delta\varphi^*,\delta\varphi)\exp -\frac{S[\phi^*+\delta\varphi^*,\phi+\delta\varphi]}{\hbar}$$

$$\phi\sim N^{1/2}\sim V^{1/2}, \quad \delta\varphi\sim N^0$$

the ordering principle is not $\hbar\to 0$

the ordering principle is only approximate

- Obviously, Bogoliubov theory breaks down if no condensate exists. This situation appears for

$$d=1 \quad \text{all } T$$

$$d=2, \quad T>0$$

Mermin-Wagner theorem plus dimensional reduction: see below

- In these cases, immediate need for nonperturbative approaches such as (functional) RG (Castellani& ’04, Wetterich & ‘08,’09; Kopietz & ’08,’10; Dupuis ’09)

- even in d=3, or d=2,T=0, one should be suspicious since in the range of small momenta the power counting is questionable:

$$n_{\mathbf{q}} = \int_\omega \langle\delta\varphi^*_Q\delta\varphi_Q\rangle \sim 1/E_{\mathbf{q}}\sim 1/|\mathbf{q}|$$

divergent occupation number

$$\to \delta\varphi\sim 1/|\mathbf{q}|^{1/2} \quad ?!$$

Validity of Bogoliubov Theory

- We study perturbative corrections to the self-energy for weakly interacting bosons (zero temperature): The full quadratic part of the effective action is ($Q = (\omega, \mathbf{q})$)

$$\Gamma = \frac{1}{2}\int_Q (\varphi(-Q), \varphi^*(Q)) \begin{pmatrix} \boxed{\Sigma_{an}(Q)} & -\mathrm{i}\omega + \frac{\mathbf{q}^2}{2\mathrm{M}} - \mu + \Sigma_n(Q) \\ \mathrm{i}\omega + \frac{\mathbf{q}^2}{2\mathrm{M}} - \mu + \boxed{\Sigma_n(Q)} & \Sigma_{an}(Q) \end{pmatrix} \begin{pmatrix} \varphi(Q) \\ \varphi^*(-Q) \end{pmatrix}$$

- We may view Bogoliubov Theory as the zero order self energies

$$\Sigma_n^{(0)}(Q) = 2g\rho_0, \quad \Sigma_{an}^{(0)}(Q) = g\rho_0 \qquad\qquad \rho_0 = \phi_0^*\phi_0$$

- The leading pertrubative corrections are shown diagrammatically. The second diagram has in IR divergence (log in d=3, poly in d<3)

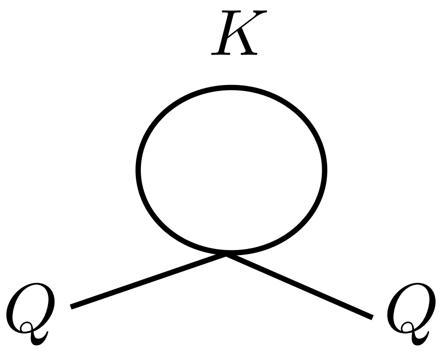
$$\Sigma_n^{(1)}(Q) \sim \Sigma_{an}^{(1)}(Q) \sim -g^2\rho_0 \int_K G_{22}(K)G_{22}(Q-K), \quad G_{22}(Q) = \frac{2g\rho_0}{\omega^2 + c^2\mathbf{q}^2}$$

gapless phase propagator

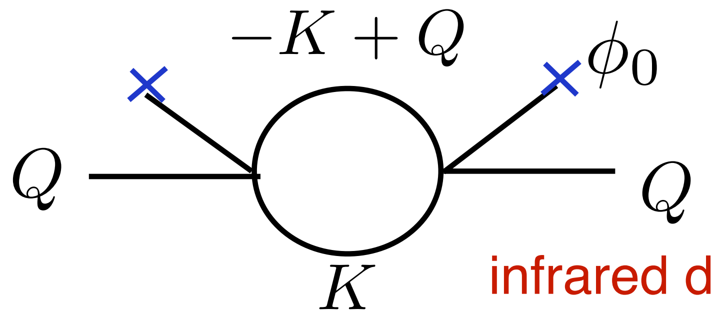
- Perturbation theory breaks down for

$$|\Sigma_{n,an}^{(0)}(Q)| \approx |\Sigma_{n,an}^{(1)}(Q)|$$

first and second order perturbation theory



infrared regular



infrared divergent!

Ginzburg Scale: Breakdown of Bogoliubov Theory

- Due to the gapless Goldstone fluctuations, Bogoliubov theory breaks down at sufficiently small momenta/long wavelength:

- Perturbation theory breaks down for

$$|\Sigma^{(0)}_{n,an}(Q)| \approx |\Sigma^{(1)}_{n,an}(Q)|$$

from which we deduce the scale where the superfluid becomes nonperturbative/strongly correlated

$$\boxed{p_{np} = p_h \cdot \begin{cases} \tilde{g}^{\frac{d}{2(3-d)}} & \text{if} \quad d < 3 \\ \exp(-\frac{1}{\kappa \tilde{g}^{3/2}}) & \text{if} \quad d = 3 \end{cases}}$$

p_{np} Ginzburg scale

p_h healing scale

- The dimensionless ratio $\tilde{g}$ expresses the ratio of interaction versus kinetic energy in the nonrelativistic superfluid ($[g] = d - 2$):

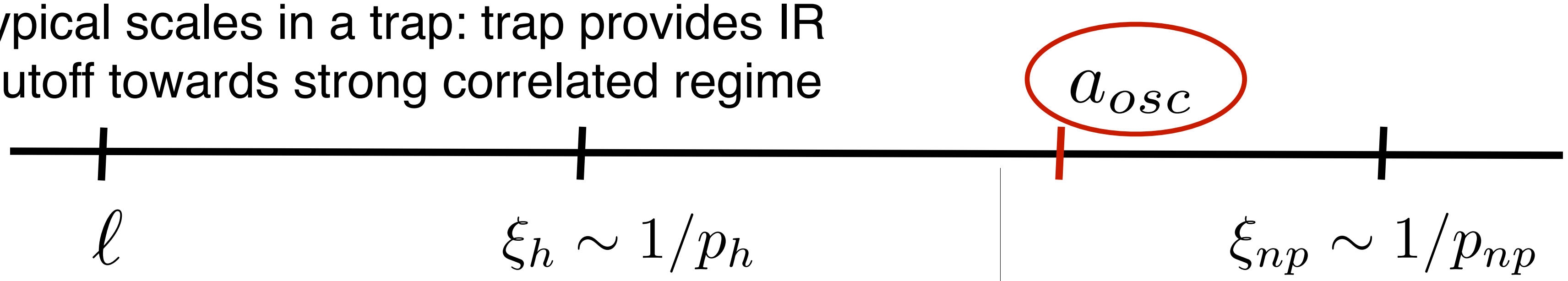
$$\tilde{g} = \frac{E_{pot}}{E_{kin}} = \frac{g\rho_0}{1/(M\ell^2)} = gM\rho_0^{1-2/d} \sim (p_h \ell)^2$$

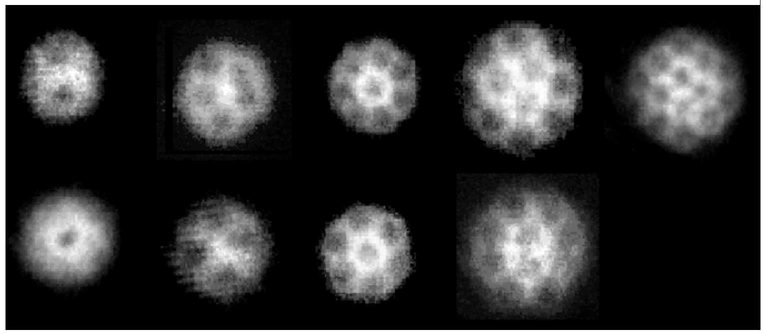
where $\ell \sim n^{-1/d}$ is the mean interparticle distance and $n \approx \rho_0$ in the weakly interacting condensate

Physical meaning: Weakly and Strongly correlated Superfluids

- Thus, superfluids can be classified according to:
  - weakly correlated if $\tilde{g} \ll 1 \Rightarrow p_{np} \ll p_h \ll \ell^{-1}$. Bogoliubov theory is valid for a large part of the spectrum, namely for momenta $|\mathbf{q}| \gtrsim p_{np}$. This is the case in typical traps.
  - strongly correlated if $\tilde{g} \gtrsim 1 \Rightarrow p_{np} \approx p_h \approx \ell^{-1}$. Bogoliubov theory breaks down. This may happen on the lattice close to the Mott insulator – superfluid phase transition.

- Comparison to the typical length scales of ultracold experiments:


typical scales in a trap: trap provides IR cutoff towards strong correlated regime



visualization of the scales

ξ_h -- vortex size

a_{osc} -- extent of cloud

➡ This explains the validity of Bogoliubov theory for (continuum) interacting Bose gases

Parenthesis: Multidimensional Gaussian Integrals

- The equilibrium functional integral is defined as the continuum limit of a multidimensional integral over an exponential distribution
- An analytically tractable class of such integrals are of the Gaussian type, i.e. the exponent is quadratic in the integration variable
- Consider a multidimensional Gaussian integral for a real vector variable $\mathbf{m}$ and positive semidefinite matrix $\mathbf{A}$

$$Z_G = \int \prod_{i=1}^{N} dm_i \exp -\tfrac{1}{2}\mathbf{m}^{\mathbf{T}}\mathbf{A}\mathbf{m} = \int \prod_{i=1}^{N} dm_i \exp -\tfrac{1}{2}\mathbf{m}'^{\mathbf{T}}\mathbf{D}\mathbf{m}' = \prod_{i=1}^{N}(2\pi\lambda_i^{-1})^{1/2} = \det[\mathbf{A}/(2\pi)]^{-1/2}$$

- Remarks:
  - In the second equality, we have performed a diagonalization to the matrix $\mathbf{D} = \lambda_i\delta_{ij}\ \mathbf{m}' = \mathbf{U}\mathbf{m}, \mathbf{D} = \mathbf{U}\mathbf{A}\mathbf{U}^{-1}$
  - We can then do each one dimensional Gaussian integral separately
  - And use the invariance of the determinant under choice of basis

additional material

Parenthesis: Multidimensional Gaussian Integrals

- We note the important relation for a Gaussian free energy (using invariance of tr under choice of basis),

$$\boxed{W_G = \log Z_G = \log \det[\mathbf{A}/(2\pi)]^{-1/2} = -\frac{1}{2}\mathrm{tr}\log \mathbf{A} + \mathrm{const.}}$$

- For a fermionic Gaussian free energy (Grassmann variables), one obtains in contrast

$$\boxed{W_G^{(F)} = \log Z_G^{(F)} = \log \det[\mathbf{A}/(2\pi)]^{+1/2} = +\frac{1}{2}\mathrm{tr}\log \mathbf{A} + \mathrm{const.}}$$

additional material

Saddle Point Effective Potential

- We con now formulate the homogenous saddle point approximation for the effective action. Due to homogeneity, we switch to the effective potential

$$\mathcal{U}[\phi^*,\phi] \equiv \frac{\Gamma[\phi^*,\phi]}{V/T}$$

with quantization volume $V/T = \int d\tau \int d^3x$

- We obtain, with abbreviation $\rho_0 = \phi_0^*\phi_0$ (we can choose ϕ_0 real so also $\phi_0^*\phi_0^* = \phi_0\phi_0 = \rho_0$)

$$\begin{aligned}
\mathcal{U}[\phi_0^*,\phi_0;\mu;T] \quad &\approx -\mu\rho_0 + \tfrac{g}{2}{\rho_0}^2 + \tfrac{1}{2}\mathrm{tr}\log S^{(2)} \\
&= -\mu\rho_0 + \tfrac{g}{2}\rho_0^2 + T\textstyle\sum_n \int \tfrac{d^3q}{(2\pi)^3} \log\det{}_{2\times 2}\begin{pmatrix} g\rho_0 & -\mathrm{i}\omega_n + \epsilon_{\mathbf{q}} - \mu + 2g\rho_0 \\ \mathrm{i}\omega_n + \epsilon_{\mathbf{q}} - \mu + 2g\rho_0 & g\rho_0 \end{pmatrix} \\
&= -\mu\rho_0 + \tfrac{g}{2}\rho_0^2 + T\int \tfrac{d^3q}{(2\pi)^3}\log\left(e^{\sqrt{(\epsilon_{\mathbf{q}}-\mu+2g\rho_0)^2-(g\rho_0)^2})/2T} - e^{-\sqrt{(\epsilon_{\mathbf{q}}-\mu+2g\rho_0)^2-(g\rho_0)^2})/2T}\right) + \mathrm{const}
\end{aligned}$$

tr runs over all indices: frequency/ momentum and the indices of the 2×2 matrix accounting for the complex boson. We use $2\log\sinh x = \sum_n \log(1 + x^2/(n\pi)^2)$, $\sinh x = (\exp x - \exp(-x))/2$. The (infinite) constant is irrelevant for thermodynamics.

additional material

Equation of State

- Effective Potential:

$$\mathcal{U}[\phi_0^*, \phi_0; \mu; T] \quad = -\mu\rho_0 + \tfrac{g}{2}\rho_0^2 + T\int \tfrac{d^3q}{(2\pi)^3} \log\left(e^{\sqrt{(\epsilon_{\mathbf{q}}-\mu+2g\rho_0)^2-(g\rho_0)^2)}/2T} - e^{-\sqrt{(\epsilon_{\mathbf{q}}-\mu+2g\rho_0)^2-(g\rho_0)^2)}/2T}\right)$$

- Discussion:
  - High temperature limit $T \to \infty$: $\rho_0 = 0, \mu < 0$. $\mathcal{U}[0,0;\mu;T] \approx T\int \frac{d^3q}{(2\pi)^3} \log\left(1 - e^{-(\epsilon_{\mathbf{q}}-\mu)/T}\right) + \mathrm{const.}'$
  - Zero temperature limit $T \to 0$: $\mathcal{U}[\phi_0^*, \phi_0; \mu; T] \approx \frac{1}{2}\int \frac{d^3q}{(2\pi)^3} \sqrt{(\epsilon_{\mathbf{q}} - \mu + 2g\rho_0)^2 - (g\rho_0)^2)}$We can make connection to Bogoliubov theory (next slide)
  - NB: Though it seems that this theory interpolates well between low and high temperatures, it becomes problematic close to the finite temperature BEC phase transition

- The equation of state, i.e. the explicit expression for the density, can be obtained from the effective potential
- Using the functional integral representation,

$$n = \lim_{\tau\to 0, \mathbf{x}\to 0} \langle \hat{\phi}^*(\tau, \mathbf{x})\hat{\phi}(0, \mathbf{0})\rangle = -\partial\mathcal{U}/\partial\mu, \;\; \hat{\phi}(\tau, \mathbf{x}) = \phi(\tau, \mathbf{x}) + \delta\varphi(\tau, \mathbf{x})$$

NB: This relation follows also using thermodynamics

Recovering the Bogoliubov Theory

- We calculate the equation of state explicitly
- Within the saddle point approximation and the equilibrium value $\mu = g\rho_0$, we find

$$n = \phi_0^* \phi_0 + \frac{1}{2} \int \frac{d^3 q}{(2\pi)^3} \frac{2g\rho_0}{\sqrt{2g\rho_0(\epsilon_{\mathbf{q}} + g\rho_0)}}$$

- Discussion:
  - Diverges linearly at high momenta
  - This is because the functional integral does not respect normal ordering. Note, for bosonic fields ϕ and operators a, $\langle \phi^* \phi \rangle = \frac{1}{2}\langle \phi^* \phi + \phi \phi^* \rangle = \frac{1}{2}\langle a^\dagger a + a a^\dagger \rangle = \langle a^\dagger a \rangle + \frac{1}{2}$. For each momentum mode:

$$\begin{aligned} n &= \phi_0^* \phi_0 + \int \frac{d^3 q}{(2\pi)^3} \langle a^\dagger_{\mathbf{q}} a_{\mathbf{q}} \rangle = \phi_0^* \phi_0 + \int \frac{d^3 q}{(2\pi)^3} \big(\langle \delta\varphi^*_{\mathbf{q}} \delta\varphi_{\mathbf{q}} \rangle - \tfrac{1}{2} \big) \\ &= \phi_0^* \phi_0 + \frac{1}{2} \int \frac{d^3 q}{(2\pi)^3} \Big(\frac{2g\rho_0}{\sqrt{2g\rho_0(\epsilon_{\mathbf{q}} + g\rho_0)}} - 1 \Big) = \phi_0^* \phi_0 + \int \frac{d^3 q}{(2\pi)^3} v^2_{\mathbf{q}} \end{aligned}$$

The Bogoliubov result is reproduced

Condensation - Superfluidity - Off-diagonal Long-Range Order

- Three cornerstones:

Bose Condensation
Statistical property

Superfluidity
Response property

Off-diagonal long range order
Correlation property

- strong fluctuations may overwrite statistics
- Dimensional dependence of long range order
- Mermin-Wagner-Theorem

Condensation vs. Superfluidity

- real time atom action

$\mu = g\rho_0, \quad \rho_0 = \phi_0^*\phi_0$

$$S[\varphi] = \int_X \left\{\varphi^*\left(\mathrm{i}\partial_t + \frac{\nabla^2}{2M} + \mu\right)\varphi - \frac{g}{2}(\varphi^*\varphi)^2\right\}$$

$$\approx V/T(g\rho_0^2/2) + \frac{1}{2}\int_X (\delta\varphi_1, \delta\varphi_2)\begin{pmatrix} \frac{\nabla^2}{2M} - 2g\rho_0 & -\partial_t \\ \partial_t & \frac{\nabla^2}{2M} \end{pmatrix}\begin{pmatrix} \delta\varphi_1 \\ \delta\varphi_2 \end{pmatrix}$$

- imprint plane wave onto the field:

$$\varphi(t,\vec{x}) \to \varphi'(t,\vec{x}) = e^{\mathrm{i}(\vec{p}\cdot\vec{x} - Et)}\varphi(t,\vec{x})$$

- decompose

$$\varphi(t,\vec{x}) = \phi_0 + \delta\varphi(t,\vec{x})$$

ground state: condensate

fluctuation: test stability

- transformed ground state carries superfluid current:

$$\vec{j} = \frac{\mathrm{i}}{2M}[\nabla\phi_0^{'*}(t,\vec{x})\phi_0'(t,\vec{x}) - \phi_0^{'*}(t,\vec{x})\nabla\phi_0'(t,\vec{x})] = \phi_0^*\phi_0\frac{\vec{p}}{M} = \vec{v}\rho_0$$

current velocity

current density

➡ study stability of this state carrying supercurrent

Condensation vs. Superfluidity

➡ study stability of this state carrying supercurrent

- Transformation of the action

$$S[\varphi] \to S[\varphi] + \int_X \varphi^* \Big(E - \mathrm{i}\vec{v}\cdot\nabla - \frac{\vec{p}^2}{2M} \Big) \varphi .$$

choose zero of
energy by

$$E = \vec{p}^2/2M$$

$$\approx V/T(g\rho_0^2/2) - \frac{1}{2}\int_Q (\delta\varphi_1, \delta\varphi_2) \begin{pmatrix} \frac{\mathbf{q}^2}{2M} + 2g\rho_0 & \boxed{-\mathrm{i}(\omega + \vec{v}\cdot\vec{q})} \\ \boxed{\mathrm{i}(\omega + \vec{v}\cdot\vec{q})} & \frac{\mathbf{q}^2}{2M} \end{pmatrix} \begin{pmatrix} \delta\varphi_1 \\ \delta\varphi_2 \end{pmatrix}$$

- Transformation of excitation energy (zeros of fluctuation matrix determinant)

$$E_q \to E'_q = E_q - \vec{v}\cdot\vec{q} \geq E_q - |\vec{v}||\vec{q}| \overset{!}{>} 0$$

- For a dynamically stable situation, need

$$E'_q \overset{!}{>} 0 \qquad\qquad v_{\mathrm{crit}} = \frac{E_q}{|\vec{q}|}$$

➡ coincides with result from Landau argument

➡ makes more explicit the connection to supercurrent/superfluid flow

Condensation vs. Off-Diagonal Long-Range Order

- How do we measure long range order?

  - strict definition
$$\boxed{\lim_{t,\mathbf{x}\to\infty}\langle\varphi^*(t,\mathbf{x})\varphi(0,\mathbf{0})\rangle \neq 0}$$

  - remark: “off-diagonal” in position space and time (diagonal: $\mathbf{x} = t = 0$)

  - This is realized to full extent in the presence of condensate. Decompose

$$\lim_{t,\mathbf{x}\to\infty}\langle\varphi^*(t,\mathbf{x})\varphi(0,\mathbf{0})\rangle = \lim_{t,\mathbf{x}\to\infty}\langle\delta\varphi^*(t,\mathbf{x})\delta\varphi(0,\mathbf{0})\rangle + \phi_0^*\phi_0$$

connected two-point function

condensate expectation value $\phi_0 = \langle\varphi(t,\mathbf{x})\rangle$

  - Connected two-point function decays for local Hamiltonians:
    condensation <=> perfect long range order

- We will see:

  - Fluctuations can degrade perfect long range order down to “quasi-long range order”. The latter can exist in the absence of condensation.
  - general statements on the degree of quasi-long range order are available just depending on the dimensionality of the system (Mermin-Wagner-Theorem)

Condensation vs. Off-Diagonal Long-Range Order

- We study the long distance behavior of the two-point correlation (stat mech context: imaginary time)

$$\mathcal{C}_2(\tau,\mathbf{x}) = \langle \varphi^*(\tau,\mathbf{x})\varphi(0,\mathbf{0})\rangle \text{ for } \tau,\mathbf{x}\to\infty$$

- Phase-amplitude representation

$$\varphi(\tau,\mathbf{x}) = r(\tau,\mathbf{x})e^{\mathrm{i}\theta(\tau,\mathbf{x})} \approx \sqrt{n}e^{\mathrm{i}\theta(\tau,\mathbf{x})}$$

- remarks:
  - neglect gapped amplitude (here: density) fluctuations
  - taking into account non-perturbative curvature effects of the phase fluctuations mandatory here

- simplification:

$$\mathcal{C}_2(\tau,\mathbf{x}) \approx n\langle e^{\mathrm{i}[\theta(\tau,\mathbf{x})-\theta(0,\mathbf{0})]}\rangle$$

- useful formula (valid for Gaussian distributed variables):

$$\boxed{\langle e^{\mathrm{i}\alpha\phi(X)}\rangle = e^{-\alpha^2\langle\phi(X)^2\rangle/2}}$$

- proof: see lecture

Condensation vs. Off-Diagonal Long-Range Order

- evaluate the correlation function:

$$\mathcal{C}_2(\tau,\mathbf{x}) \approx n e^{-\langle\theta^2(0,\mathbf{0})-\theta(\tau,\mathbf{x})\theta(0,\mathbf{0})\rangle}$$

- with the universal low energy form of the euclidean (imaginary time) phase action

$$S_{ph} = \int_Q \theta(Q) G^{-1}(Q)\theta(Q) + \ldots \qquad G^{-1}(Q) = \underbrace{\kappa}_{\text{value determined by high energy physics}}(\omega^2 + c^2\mathbf{q}^2) = \kappa Q^2$$

  - c = 1 WLOG (redefinition of momentum)
  - space and time appear symmetrically in euclidean action
  - remember: exactly gapless

- we calculate the correlator

$$\langle\theta^2(0) - \theta(X)\theta(0)\rangle = \int_Q [1 - e^{\mathrm{i}QX}]G(Q) = \int d^D\mathbf{q}[1 - e^{\mathrm{i}QX}]G(Q)$$

$$\xrightarrow{X\to\infty} \frac{1}{\kappa}\begin{cases} \frac{1}{S_D(D-2)}\Lambda^{D-2} & D > 2 \\ \frac{1}{2\pi}\log\Lambda'|X| & D = 2 \\ \frac{1}{2\pi}|X| & D = 1 \end{cases}$$

$\Lambda' = \Lambda e^{\gamma}, \gamma \approx 0.116$

$\Lambda \sim 1/a$ lattice spacing

- where (dimensional reduction NB: consideration holds for nonrelativistic matter)

$$T = 0: \quad Q = (\omega, \mathbf{q}) \;\Rightarrow\; D = d + 1$$

$$T > 0: \quad Q \approx (0, \mathbf{q}) \;\Rightarrow\; D = d$$

higher Matsubara modes are gapped,
do not contribute to long wavelength behavior

Condensation vs. Off-Diagonal Long-Range Order

- discussion

$$\langle \theta^2(0) - \theta(X)\theta(0) \rangle \xrightarrow{X\to\infty} \frac{1}{\kappa} \begin{cases} \frac{1}{S_d(d-2)} \Lambda^{d-2} & D > 2 \\ \frac{1}{2\pi} \log \Lambda' |X| & D = 2 \\ \frac{1}{2\pi} |X| & D = 1 \end{cases}$$

- spatial correlations at finite temperature in various dimensions:
  - d = 3:

$$\mathcal{C}_2(\mathbf{x}) \xrightarrow{|\mathbf{x}|\to\infty} \text{const.}$$

➡ represents true long range order with SSB as physical origin

  - d = 1:

$$\mathcal{C}_2(\mathbf{x}) \xrightarrow{|\mathbf{x}|\to\infty} n e^{-|\mathbf{x}|/(2\kappa)} .$$

➡ exponential decay, i.e. only short range correlations: disordered state, no SSB

Condensation vs. Off-Diagonal Long-Range Order

- discussion

$$\langle \theta^2(0) - \theta(X)\theta(0)\rangle \xrightarrow{X\to\infty} \frac{1}{\kappa}\begin{cases} \frac{1}{S_d(d-2)}\Lambda^{d-2} & D>2 \\ \frac{1}{2\pi}\log \Lambda' |X| & D=2 \\ \frac{1}{2\pi}|X| & D=1 \end{cases}$$

- spatial correlations at finite temperature in various dimensions:
  - d = 2:

$$\mathcal{C}_2(\mathbf{x}) \xrightarrow{|\mathbf{x}|\to\infty} n(\Lambda'|\mathbf{x}|)^{-\frac{1}{2\pi\kappa}}$$

➡ slow algebraic/ power law decay, but no homogeneous order parameter: Quasi-long-range order

- remarks:
  - at finite temperature $\kappa = \kappa'\beta$, with weakly T-dependent κ'
    - T -> 0: LRO re-established (cf. dimensional reduction)
    - T -> infty: correlations eventually decay faster than any algebraic power, i.e. disordered phase is reached
  - at finite T, there is a phase transition which connects the disordered and quasi-LRO phase (Kosterlitz-Thouless-transition) without breaking the symmetry
  - i.e., (quasi)-LRO can exist without condensation
  - The quasi-LRO phase is robustly critical (algebraic decay)

Summary

- Mermin-Wagner-Theorem:

  In systems with continuous symmetries, there is no true long-range order in spatial dimensions smaller two and finite temperature

- comments
  - d = 2 is called lower critical dimension
  - at T = 0, the lower critical dimension is d = 1
  - physically, LRO is spoiled by phase fluctuations which are of arbitrarily long wavelength as protected by phase rotation symmetry, in conjunction with small phase space in d=2
  - This statement is not truly a mathematical theorem. For example, collective effects can modify the effective dispersion

$$\omega^2 \sim \mathbf{q}^{2-\eta}$$

with η an "anomalous dimension". In that case, the discussion is more subtle.

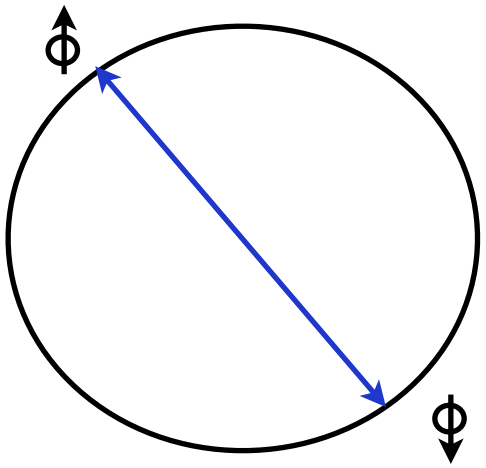
Summary: Weakly interacting Bosons

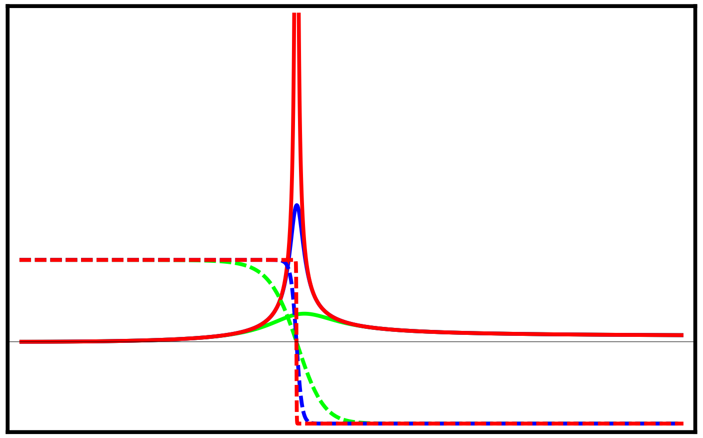
- We have applied the effective action formalism to weakly interacting bosons
- Important concepts:
    - Classical Limit(s) and Gross-Pitaevski Theory
    - Spontaneous symmetry breaking
    - Phase/ amplitude fluctuations and Bogoliubov theory
    - Goldstone’s theorem
    - condensation vs. superfluidity and supercurrent instability
    - condensation vs. ODRLO and Mermin-Wagner theorem
- These concepts can be applied to many other physical situations.
- We now use the effective action formalism to analyze weakly interacting fermions

Weakly Interacting Fermions

$$\langle \psi_\uparrow \rangle = \langle \psi_\downarrow \rangle = 0$$

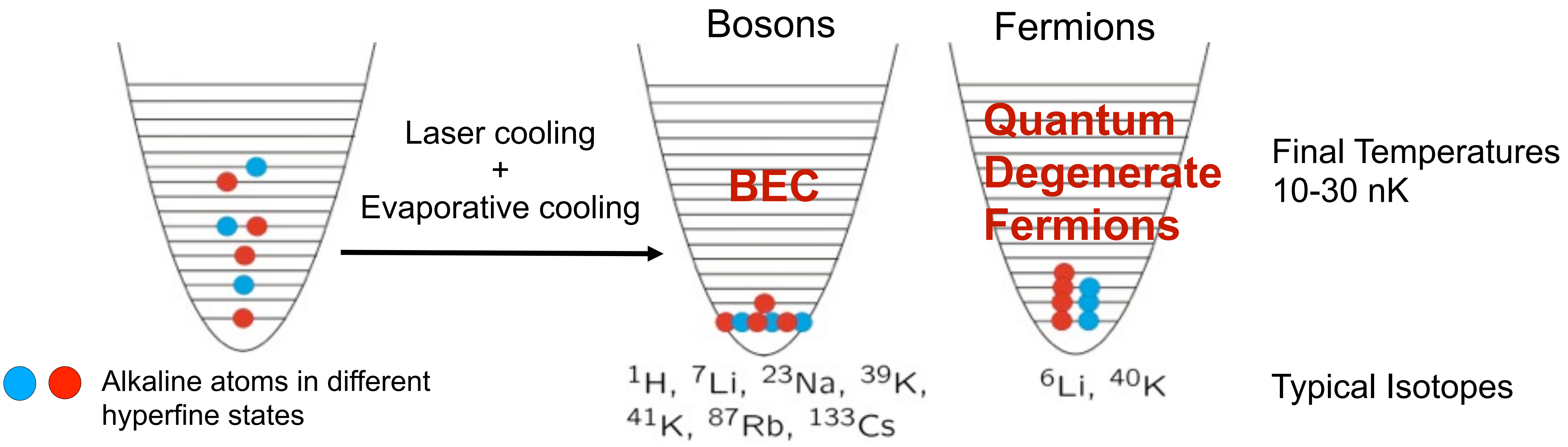
$$\langle \psi_\uparrow \psi_\downarrow \rangle \neq 0$$





Degenerate Bose vs. Fermi Gases

- Bosons: commutator $[b(\mathbf{x}), b^\dagger(\mathbf{y})] = \delta(\mathbf{x}-\mathbf{y}),\ [b(\mathbf{x}), b(\mathbf{y})] = [b^\dagger(\mathbf{x}), b^\dagger(\mathbf{y})] = 0$
- Bose-Einstein distribution: $n_{\mathbf{q}} = (\exp(\frac{\epsilon_{\mathbf{q}}-\mu}{T}) - 1)^{-1}$, $\epsilon_{\mathbf{q}} = \frac{\mathbf{q}^2}{2M}$, $\mu \leq 0$
- Fermions: Pauli principle $c_\sigma^{\dagger\,2} = 0$, anticommutator $\{c_\sigma(\mathbf{x}), c_{\sigma'}^\dagger(\mathbf{y})\} = \delta_{\sigma,\sigma'}\delta(\mathbf{x}-\mathbf{y}),\ \{c_\sigma(\mathbf{x}), c_{\sigma'}(\mathbf{y})\} = \{c_\sigma^\dagger(\mathbf{x}), c_{\sigma'}^\dagger(\mathbf{y})\} = 0$
- Fermi-Dirac distribution: $n_{\mathbf{q}} = (\exp(\frac{\epsilon_{\mathbf{q}}-\mu}{T}) + 1)^{-1}$, $\epsilon_{\mathbf{q}} = \frac{\mathbf{q}^2}{2M}$, $\mu > 0$
- real space picture:



Bosons

Fermions

Laser cooling
+
Evaporative cooling

BEC

Quantum Degenerate Fermions

Final Temperatures
10-30 nK

● ● Alkaline atoms in different hyperfine states

^{1}H, ^{7}Li, ^{23}Na, ^{39}K, ^{41}K, ^{87}Rb, ^{133}Cs

^{6}Li, ^{40}K

Typical Isotopes

- Alkaline atoms (bosons and fermions) can be prepared in the quantum degenerate regime, using laser cooling and evaporative cooling
- The fermion spin is realized with two hyperfine states

Free Fermions and Fermi Momentum

- Collection of some useful formulae and abbreviations for 3D two-component fermions:
- The equation of state for free fermions at zero temperature:

$$n = 2\int \frac{d^3q}{(2\pi)^3}\left(\exp\left(\frac{\epsilon_{\mathbf{q}}-\mu}{T}\right)+1\right)^{-1} \xrightarrow{T\to 0} 2\int \frac{d^3q}{(2\pi)^3}\theta(\epsilon_{\mathbf{q}}-\mu) = \frac{(2M\mu)^{3/2}}{3\pi^2} \equiv \frac{k_{\mathrm{F}}^3}{3\pi^2}$$

two spin states

- The Fermi momentum k_F is defined as the momentum scale associated to the chemical potential of free fermions at T = 0

$$k_{\mathrm{F}} \equiv (2M\mu^{(\mathrm{free})}_{T=0})^{1/2}$$

- The Fermi momentum is a measure for the total density of a fermion system:
  - It is a measure for the mean interparticle spacing $d = (3\pi^2)^{1/3}k_{\mathrm{F}}^{-1}$
  - It is temperature and interaction independent
  - In contrast, the chemical potential is a function of temperature and interactions

- The associated energy and temperature scales are the Fermi energy and the Fermi temperature

$$\epsilon_{\mathrm{F}} = \frac{k_{\mathrm{F}}^2}{2M}, \quad T_{\mathrm{F}} = \frac{\epsilon_{\mathrm{F}}}{k_{\mathrm{B}}}$$

Physical Picture for Weakly Attractive Fermions

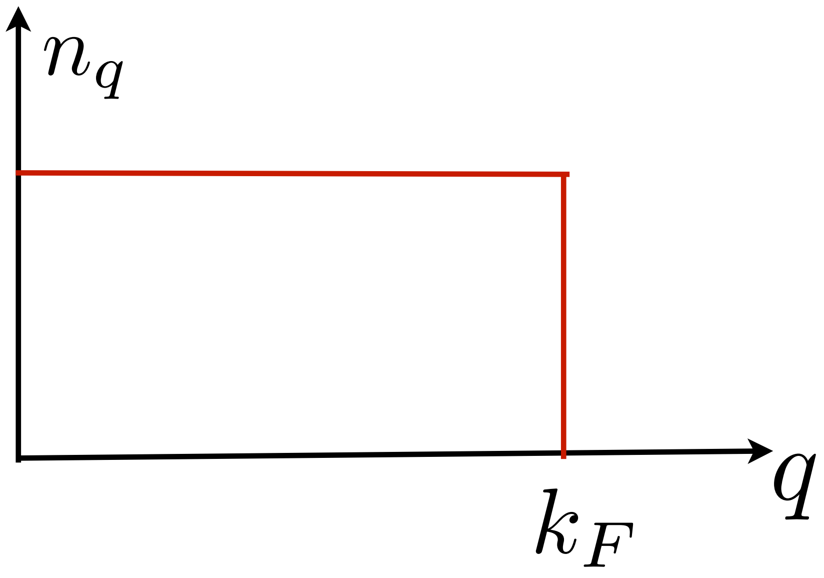
- The low temperature physics of fermions is governed by the Pauli principle

  (1) Expression of a Fermi sphere in momentum space

  (2) Absence of fermion condensation: $\langle \psi_\sigma \rangle = 0 \quad \sigma = \uparrow, \downarrow$

  (3) Local s-wave interactions of fermions are only possible for more than one spin state (ultracold atoms: hyperfine states)

Fermi distribution at low T



- Now we allow for weak 2-body s-wave attraction between 2 spin states of fermions

$$a < 0$$

attractive scattering length

$$|ak_{\mathrm{F}}| \sim |a/d| \ll 1$$

weakness/diluteness condition

- A small interaction scale will not be able to substantially modify the Fermi sphere. This is the key to BCS theory

Physical Picture for Weakly Attractive Fermions

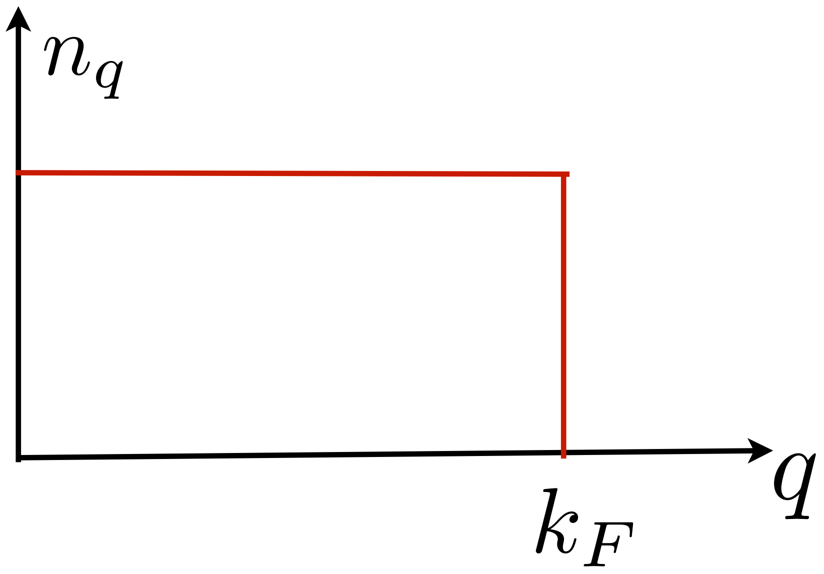
$$|ak_{\mathrm{F}}| \sim |a/d| \ll 1$$

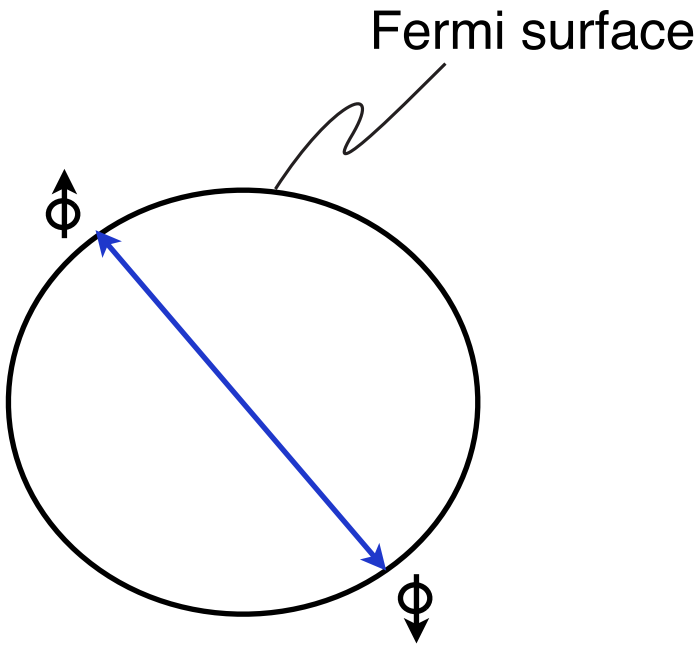
- A small interaction scale will not be able to substantially modify the Fermi sphere
- However, pairing of fermions with momenta close to the Fermi surface is possible: “Cooper pairs”:
  - These fermions attract each other with strength a
  - The total energy of the system is lowered when
    - bosonic pairs with zero cm energy (total momentum zero) form: local in momentum space
    - These pairs condense, i.e. occupy a single quantum state macroscopically:

$$\boxed{\langle \psi_\uparrow \psi_\downarrow \rangle \neq 0}$$

- Comments:
  - Distinguish pairing correlation from Bose condensation $\langle \varphi \rangle \neq 0$
  - But: in both cases, spontaneous breaking of U(1) symmetry

Fermi distribution at low T





Cooper pairing: Local in momentum space

Fermionic Path Integral I: Grassmann variables

- Agenda: Construct Path integral by writing partition sum in coherent state basis
- Remember complex bosons: Bosonic operators and commutation relations replaced by commuting c-numbers
- Fermionic operators fulfill anticommutation relations. They will be replaced by anticommuting objects: Grassmann variables η_i

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- Defining properties:
  - anti-commutativity $\{\eta_i, \eta_j\} = 0$ $\Rightarrow \eta_i^2 = 0$
  - add to and multiply with complex numbers according to

$$a + b_i\eta_i + b_j\eta_j , \quad a, b_i, b_j \in \mathbf{C}$$

  - anti-commutativity with fermion operators

$$\{\eta_i, a_j\} = \{\eta_i, a_j^\dagger\} = 0$$

  - adjoint $\bar{\eta}_i$ with

$$\{\eta_i, \bar{\eta}_j\} = \{\bar{\eta}_i, \bar{\eta}_j\} = 0$$

Fermionic Path Integral I: Grassmann variables

Motivations/proofs:
blackboard

- Grassmann calculus
  - Differentiation

$$\partial_{\eta_i}\eta_j = \delta_{ij}$$

NB: anticommutativity of Grassmann derivative, e.g.

$$\partial_{\eta_i}\eta_j\eta_i = -\eta_j\delta_{ij}$$

  - Functions of Grassmann variables: Taylor expansion terminates

$$F(\eta) = F(0) + \partial_\eta F(0)\eta$$

NB: $F(0), \partial_\eta F(0) \in \mathbf{C}$

  - Integration

$$\int d\eta = 0, \quad \int d\eta\eta = 1$$

NB: constructed to reproduce structural properties of c-number integrals (eg. translation invariance)

  - Implication: Grassmann differentiation and integration have the same effect:

$$\int d\eta F(\eta) = \partial_\eta F(\eta)$$

  - Gaussian Integral:

NB: up to (conventional) factors of pi, inverse of result for complex bosons

$$\int d\bar{\eta}d\eta e^{-\bar{\eta}a\eta} = a$$

one-dimensional

$$\int d\bar{\eta}d\eta e^{-\bar{\eta}^T A\eta} = \det A$$

multi-dimensional

Fermionic Path Integral II: Coherent states

proofs: blackboard

- construct eigenstates to fermion annihilation operator:

$$a_i|\eta\rangle = \eta_i|\eta\rangle$$

- explicit form:

vacuum $a_i|0\rangle = 0$

$$|\eta\rangle = e^{-\sum_i \eta_i a_i^\dagger}|0\rangle = (1 - \sum_i \eta_i a_i^\dagger)|0\rangle$$

- adjoint (defines $\bar{\eta}_i$)

$$\langle\bar{\eta}| = \langle 0|e^{-\sum_i a_i \bar{\eta}_i} = \langle 0|e^{\sum_i \bar{\eta}_i a_i}$$

- completeness relation

$$\int \prod_i d\bar{\eta}_i d\eta_i e^{-\sum_i \bar{\eta}_i \eta_i}|\eta\rangle\langle\bar{\eta}| = \mathbf{1}_{\mathrm{Fock}}$$

Fermionic Path Integral III: List of Changes

proofs: blackboard

- Key identity: $\langle n|\eta\rangle\langle\bar\eta|n\rangle = \langle-\bar\eta|n\rangle\langle n|\eta\rangle$

NB: counterintuitive sign compared boson case

- Rewrite partition sum

$$Z = \sum_{\{n\}\in\text{Fock space}} \langle n|e^{-\beta(\hat H-\mu\hat N)}|n\rangle$$

$$= \int \mathcal{D}(\bar\psi,\psi)e^{-\sum_i \bar\psi_i\bar\psi}\sum_n \langle n|\psi\rangle\langle\bar\psi|e^{-\beta(\hat H-\mu\hat N)}|n\rangle$$

$$= \int \mathcal{D}(\bar\psi,\psi)e^{-\sum_i \bar\psi_i\bar\psi}\langle-\bar\psi|e^{-\beta(\hat H-\mu\hat N)}|\psi\rangle$$

- break up into N segments. Use: (i) exponential is bilinear in Grassmann variables, (ii) at the end of the ``time'' interval, fermion field returns to its opposite (anti-periodic bc's)

$$Z = \int_{\psi(\beta)=-\psi(0)} \mathcal{D}(\bar\psi,\psi)e^{-S[\bar\psi,\psi]}$$

$$S[\bar\psi,\psi] = \int_0^\beta d\tau\{\bar\psi\partial_\tau\psi + H[\bar\psi,\psi] - \mu N[\bar\psi,\psi]\}$$

Action for weakly interacting fermions

NB: from now on, we use notations
for the conjugate field: $\bar{\psi} \equiv \psi^*$

- Two-component fermions are described by a spinor

$$\psi(\tau, \mathbf{x}) = \begin{pmatrix} \psi_\uparrow(\tau, \mathbf{x}) \\ \psi_\downarrow(\tau, \mathbf{x}) \end{pmatrix}, \quad \psi^\dagger(\tau, \mathbf{x}) = (\psi^*_\uparrow(\tau, \mathbf{x}), \psi^*_\uparrow(\tau, \mathbf{x}))$$

The components are Grassmann variables, i.e. they anticommute $\{\psi_\sigma(\tau.\mathbf{x}), \psi_{\sigma'}(\tau'.\mathbf{x}')\} = \{\psi^*_\sigma(\tau.\mathbf{x}), \psi^*_{\sigma'}(\tau'.\mathbf{x}')\}$ $\{\psi_\sigma(\tau.\mathbf{x}), \psi^*_{\sigma'}(\tau'.\mathbf{x}')\} = 0$ (reflecting anticommutation relations for fermionic operators)

- The kinetic (single particle) term describes nonrelativistic propagation:

$$S_{\text{kin}} = \sum_{\sigma,\sigma'} \int d\tau dx [\psi_\sigma(\tau, x)(\partial_\tau - \frac{\triangle}{2M} - \mu)\delta_{\sigma\sigma'}\psi_{\sigma'}(\tau, x)] = \int_0^\beta d\tau dx [\psi^\dagger(\tau, x)(\partial_\tau - \frac{\triangle}{2M} - \mu)\psi(\tau, x)]$$

However, unlike bosons $\mu > 0$ to ensure a fixed particle number

- Local s-wave two-body density-density interactions between the two spin states are described by

$$S_{\text{int}} = \frac{g}{2} \int_0^\beta d\tau dx [\psi^\dagger(\tau, x)\psi(\tau, x)]^2$$

The precise relation of the coupling constant $g < 0$ to the scattering length a is discussed below

- Validity: as for bosons, in particular, $a \ll d \sim k^{-1}{}_{\text{F}}$
- Symmetries: as for the boson action, supplemented by global $SU(2)$ spin rotation invariance

Cooper Pairing and Hubbard-Stratonovich Transformation

- We perform a Hubbard Stratonovich transformation, which makes the expected pairing of the fermions ($\langle\psi_\uparrow\psi_\downarrow\rangle = \frac{1}{2}\langle\psi^T\epsilon\psi\rangle \neq 0$) explict. There are 3 steps:
  1. Rearrange the fermion fields into local singlets, to make the pairing explicit (Fierz transformation)

$$(\psi^\dagger\psi)^2 = (\psi^\dagger\delta\psi)^2 = -\tfrac{1}{2}(\psi^\dagger\epsilon\psi^*)(\psi^T\epsilon\psi), \quad \varepsilon = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

  2. Introduce a properly written factor of unity into the fermionic functional integral $Z = \int \mathcal{D}\psi \exp -(S_{\text{kin}} + S_{\text{int}})$, (note $\left(\psi^T\epsilon\psi\right)^\dagger = -\psi^\dagger\epsilon\psi^*$; we use $X = (\tau, \mathbf{x}), \int_X = \int d\tau\mathbf{x}, \int\mathcal{D}\psi = \int\mathcal{D}(\psi^*,\psi)$)

$$\mathbf{1} \quad = \mathcal{N}\int\mathcal{D}\varphi \exp -\int_X m^2(\varphi^* + \tfrac{h}{2m^2}\psi^\dagger\epsilon\psi^*)(\varphi - \tfrac{h}{2m^2}\psi^T\epsilon\psi)$$

     The parameters m^2, h are real and $m^2 > 0$ to make the Gaussian integral convergent but otherwise arbitrary. The resulting partition function is ($D = \partial_\tau - \frac{\triangle}{2M} - \mu$)

$$Z = \mathcal{N}\int\mathcal{D}\psi)D\varphi \exp -\int_X \left[\psi^\dagger D\psi + m^2\varphi^*\varphi + \tfrac{h}{2}(\varphi\psi^\dagger\epsilon\psi^* - \varphi^*\psi^T\epsilon\psi) - \tfrac{1}{4}(g + \tfrac{h^2}{m^2})(\psi^\dagger\epsilon\psi^*)(\psi^T\epsilon\psi)\right]$$

  3. For attractive interaction $g < 0$, we can now choose the parameters such that $g = -\frac{h^2}{m^2}$
     - Then we get rid of the fermion interaction term
     - Only this ratio is physical. We can redefine $\varphi \to h\varphi$ and get

$$Z = \mathcal{N}\int\mathcal{D}\psi\mathcal{D}\varphi \exp -S_{\text{HS}}, \quad S_{\text{HS}}[\psi,\varphi] = \int_X \left[\psi^\dagger D\psi + \tfrac{1}{|g|}\varphi^*\varphi + \tfrac{1}{2}(\varphi\psi^\dagger\epsilon\psi^* - \varphi^*\psi^T\epsilon\psi)\right]$$

Cooper Pairing and Hubbard-Stratonovich Transformation

- We discuss the Hubbard-Stratonovich action

$$S_{\mathrm{HS}}[\psi,\varphi] = \int_X \left[\psi^\dagger D\psi + \tfrac{1}{|g|}\varphi^*\varphi + \tfrac{1}{2}(\varphi\psi^\dagger\epsilon\psi^* - \varphi^*\psi^T\epsilon\psi)\right]$$

- The interacting fermion theory is mapped into a coupled fermion-boson theory.
- The boson field represents Cooper pairs, $\phi \sim \psi_\uparrow\psi_\downarrow$. A nonzero expectation value $\phi = \langle\varphi\rangle \neq 0$ breaks the $U(1)$ symmetry and describes Cooper pair condensation
- The theory is quadratic in the fermions. We introduce Nambu-Gorkov fields $\Psi^T = (\psi^T, \psi^\dagger)$ to make this explicit,

$$S_{\mathrm{HS}} = \frac{1}{2}\int_X \left[\Psi^T S^{(2)}[\varphi]\Psi + \tfrac{1}{|g|}\varphi^*\varphi\right], \quad S^{(2)}[\varphi] = \begin{pmatrix} -\varphi^*\epsilon & -D^\dagger\delta \\ D\delta & \varphi\epsilon \end{pmatrix}$$

  They can be eliminated by Gaussian integration. However, the result is an interacting boson theory due to the dependence $S^{(2)}[\varphi]$
- The BCS approximation consists in neglecting the fluctuations of the bosonic Cooper pair field: Mean field approximation for the boson dofs

BCS Effective Action

- We implement the above strategy on the effective action for homogeneneous classical field configurations, [1]

$$\Gamma[\psi_{\rm cl},\phi], \qquad = -\log\int\mathcal{D}\delta\psi\mathcal{D}\delta\varphi\exp -S_{\rm HS}[\psi_{\rm cl}+\delta\psi,\phi+\delta\varphi]$$

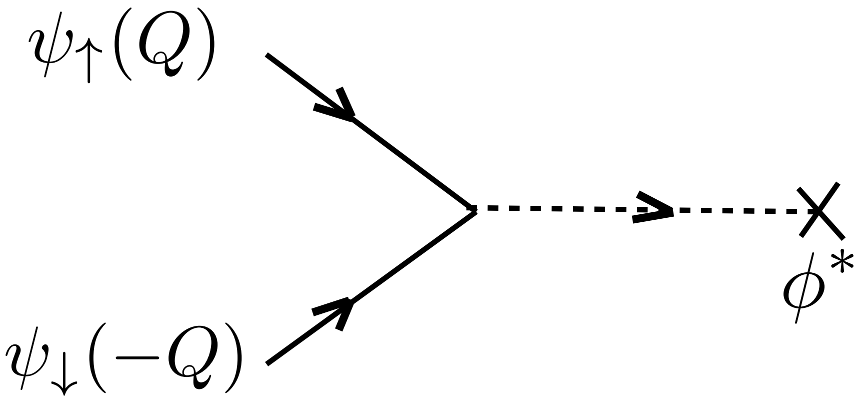
$$= \frac{V}{T}\frac{1}{|g|}\phi^*\phi - \log\int\mathcal{D}\delta\psi\exp -S_{\rm HS}[\delta\psi,\phi]/(V/T)$$

- Due to the approximation on φ, $S_{\rm HS}$ is now truly quadratic, in the background of a classical field ϕ. It is useful to switch to momentum space where

$$S_{\rm HS}[\delta\psi,\phi] \quad = \frac{1}{2}\int_Q \Psi^T(-Q)S^{(2)}[\phi]\Psi(Q),$$

$$S^{(2)}[\phi] \quad = \begin{pmatrix} -\phi^*\epsilon & -(-\mathrm{i}\omega_n+\epsilon_{\mathbf{q}}-\mu)\delta \\ (\mathrm{i}\omega_n+\epsilon_{\mathbf{q}}-\mu)\delta & \phi\epsilon \end{pmatrix}, \quad \Psi(Q) = \begin{pmatrix} \psi(Q) \\ \psi^*(-Q) \end{pmatrix}$$

- NB: the classical field couples $\phi\psi^*_\uparrow(Q)\psi^*_\downarrow(-Q)$. Interpretation similar to Bogoliubov theory: creation of fermions with opposite momenta out of the Cooper pair condensate



annihilation process of two oppositely directed fermions into the pair condensate

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[1]
- The fermion field expectation takes the physical value $\psi_{\rm cl}=0$ but serves to carry out successive derivatives to generate the 1PI correlation functions

BCS Effective Action

- Evaluation of the Grassmann Gaussian integral ($2 \log \cosh x = \sum_n \log(1 + x^2/((n+1/2)\pi)^2)$)

$$\begin{aligned}\Gamma[\psi_{\text{cl}}, \phi]/(V/T) &= \tfrac{1}{|g|}\phi^*\phi - \tfrac{1}{2}\text{tr} \log S^{(2)}[\phi] \\ &= \tfrac{1}{|g|}\phi^*\phi - 2T \int \tfrac{d^3\mathbf{q}}{(2\pi)^3} \log \cosh(E_{\mathbf{q}}/2T) + \text{const.} \\ E_{\mathbf{q}} &= \sqrt{(\epsilon_{\mathbf{q}} - \mu)^2 + \phi^*\phi}\end{aligned}$$

- NB: The homogeneous BCS effective action depends on the chemical potential μ and on the $U(1)$ invariant combination $\rho = \phi^*\phi$, $\Gamma = \Gamma[\mu, \rho]$

- we now derive two physical conditions from this effective BCS potential:
  - the equation of state
  - the condition for the transition into the BCS condensed phase
- we will face problems at high momenta and provide the cure: UV renormalization

The Equation of State

- The explicit expression for the density is obtained from

$$n_\Lambda = -\frac{\partial \mathcal{U}}{\partial \mu} = -\int \tfrac{d^3\mathbf{q}}{(2\pi)^3} \tanh(E_\mathbf{q}/2T) \qquad\qquad \mathcal{U} = \Gamma/(V/T)$$

  Again, the expression is UV divergent, here $\sim \Lambda^3$

- Using $\tanh(x/2) = 1 - 2(\exp x + 1)^{-1}$, we split the integral into a physical (depending on μ and ρ) and an unphysical contribution:

$$n_\Lambda = 2\left(\int \tfrac{d^3\mathbf{q}}{(2\pi)^3} \frac{1}{e^{E_\mathbf{q}/T}+1} - \int \tfrac{d^3\mathbf{q}}{(2\pi)^3} \tfrac{1}{2}\right)$$

  The overall factor of two counts the degenerate spin states

- Interpretation:
  - First term: involves the Fermi-Dirac distribution. The physical density is

$$n = 2\int \tfrac{d^3\mathbf{q}}{(2\pi)^3} \frac{1}{e^{E_\mathbf{q}/T}+1}$$

  - Second term: Unobservable zero-point energy shift due to the fact that the functional integral does not respect operator ordering: consider single fermion mode field ψ and associated operator c ($\{c, c^\dagger\} = 1$),

$$\langle \psi^* \psi \rangle = \tfrac{1}{2}\langle \psi^*\psi - \psi\psi^* \rangle = \tfrac{1}{2}\langle c^\dagger c - c c^\dagger \rangle = \langle c^\dagger c \rangle - \tfrac{1}{2}$$

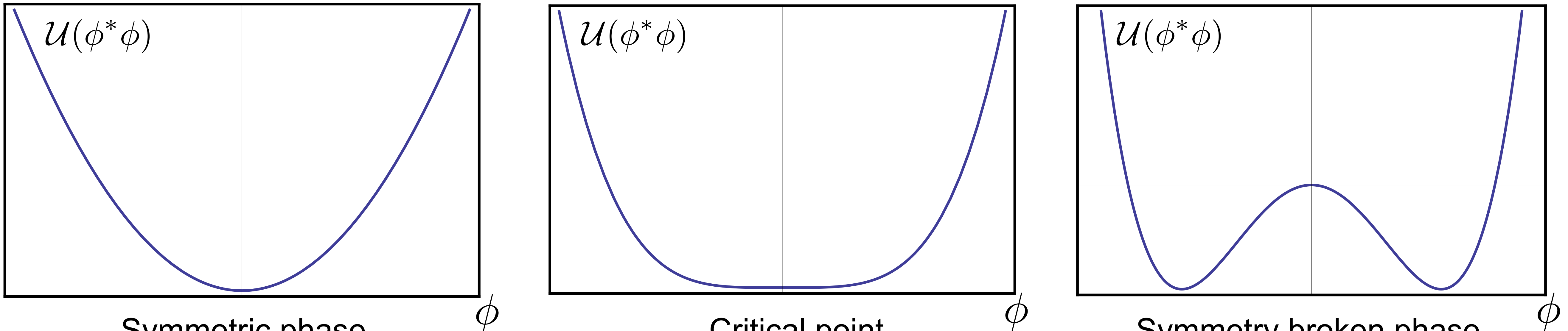
Spontaneous Symmetry Breaking

- The phase transition towards a state with macroscopic Cooper pairing at low T can be obtained from analyzing symmetry breaking patterns
- Study the field equation/ equilibrium condition for the effective potential $\mathcal{U}[\mu,\rho] = \Gamma[\mu,\rho]/(V/T)$,

$$\frac{\partial \mathcal{U}}{\partial \phi^*} = \phi \cdot \frac{\partial \mathcal{U}}{\partial \rho} \overset{!}{=} 0$$

- There are three possibilities:
  1. Spontaneously symmetry broken phase: $\phi, \phi^* \neq 0, \quad \frac{\partial \mathcal{U}}{\partial \rho} = 0$
  2. “Symmetric” phase: $\phi = \phi^* = 0, \quad \frac{\partial \mathcal{U}}{\partial \rho} \neq 0$
  3. Critical point: $\phi = \phi^* = 0, \quad \frac{\partial \mathcal{U}}{\partial \rho} = 0$
- NB: in the symmetry broken phase, $\frac{\partial \mathcal{U}}{\partial \rho} = 0$ signals the vanishing mass of the Golstone mode

Cuts through potential landscape for U(1) symmetric theory



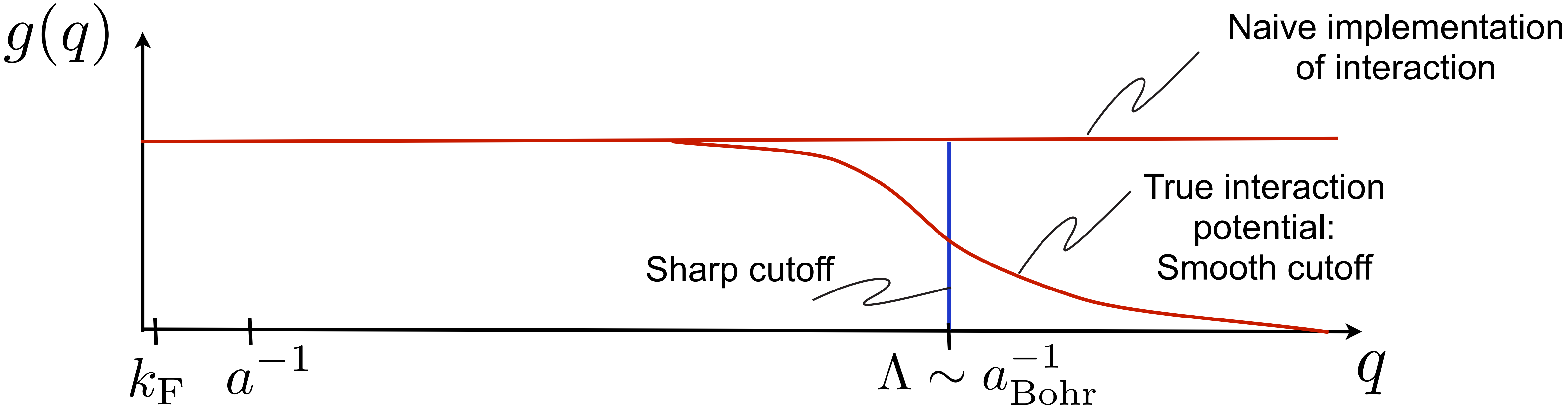
Symmetric phase   Critical point   Symmetry broken phase

Critical Temperature and a Problem at Large Momenta

- We focus on the critical point for the Cooper instability first, i.e. we study $\frac{\partial \mathcal{U}}{\partial \rho}\big|_{\rho=0} = 0$. Explicitly:

$$0 = -\frac{1}{g} - \frac{1}{2}\int \frac{d^3q}{(2\pi)^3} \frac{1}{\epsilon_{\mathbf{q}} - \mu} \tanh\left(\frac{\epsilon_{\mathbf{q}} - \mu)}{2T}\right) = \frac{1}{|g|} - \frac{1}{4\pi^2}\int dq \frac{q^2}{q^2/(2M) - \mu} \tanh\left(\frac{q^2/(2M) - \mu)}{2T}\right)$$

- The integral is linearly divergent, as the integrand tends to 1 for large momenta $q \to \infty$: "Ultraviolet divergence"
- This is because we have assumed spatially local interactions, i.e. constant in momentum space up to arbitrarily large momenta
- In reality, this is not the case. There is a (smooth) momentum cutoff at large momenta. Details of the precise cutoff function should not matter (cf. discussion of effective theories above)



Ultraviolet Renormalization

- The problem is cured by a proper ultraviolet (UV) renormalization procedure:
  - Introduce a (sharp) UV cutoff Λ in the momentum space integral (UV regularization)
  - Interpret g as “bare” coupling with cutoff dependence, $g = g_\Lambda$
  - Trade the bare coupling for a physical observable: Require that $\partial\mathcal{U}/\partial\rho$ performed in vacuum ($\mu = 0\,(n=0),\ T=0, \rho=0$) produce the physical inverse scattering length (UV renormalization):

$$\left.\frac{\partial\mathcal{U}}{\partial\rho}\right|_{\mathrm{vac}} = -\frac{1}{g_\Lambda} - \frac{1}{4\pi^2}\int^{\Lambda} dq \frac{q^2}{q^2/(2M)} = -\frac{1}{g_\Lambda} - \frac{M\Lambda}{2\pi^2} \overset{!}{=} -\frac{1}{g_p} = -\frac{M}{4\pi a}$$

NB: The relation between g_Λ and a is not perturbative; a more systematic treatment uses $g_\Lambda(q) = g_\Lambda\theta(\Lambda - q)$ and interprets the above equation as a resummed loop equation; the relation between a physical fermionic two-body coupling g_p and a scattering lenght is $a = Mg_p/(4\pi)$

- The renormalized equation for the critical temperature reads

$$0 = -\frac{1}{a} - \frac{2}{\pi}\int dq \left[\frac{q^2}{q^2 - 2M\mu}\tanh\left(\frac{q^2/(2M) - \mu)}{2T}\right) - 1\right]$$

bosons: 8pi;
bosons indistinguishable,
fermions distinguishable
(spin)

It will be analyzed below

BCS Equations for the Critical Temperature

- We have derived two equations governing the thermodynamics of weakly interacting fermions:
  - The equation of state

$$\boxed{n = 2\int \frac{d^3\mathbf{q}}{(2\pi)^3} \frac{1}{e^{(\epsilon_{\mathbf{q}}-\mu)/T}+1}}$$

  - The equation for the critical temperature

$$\boxed{0 = -\frac{1}{a} - \frac{2}{\pi}\int dq \left[\frac{q^2}{q^2-2M\mu}\tanh\left(\frac{q^2/(2M)-\mu)}{2T}\right) - 1\right]}$$

- Given μ we could solve the second equation. For $T/T_{\mathrm{F}} \ll 1$, the corrections to the chemical potential from $\epsilon_{\mathrm{F}} = \mu(T=a=0)$ are negligible. We therefore work with $\mu \approx \epsilon_{\mathrm{F}}$

The Critical Temperature

- We rescale momenta and energies as $\tilde{q} = q/k_\mathrm{F}, \tilde{E} = E/\epsilon_\mathrm{F}$. The dimensionless critical temperature is determined from

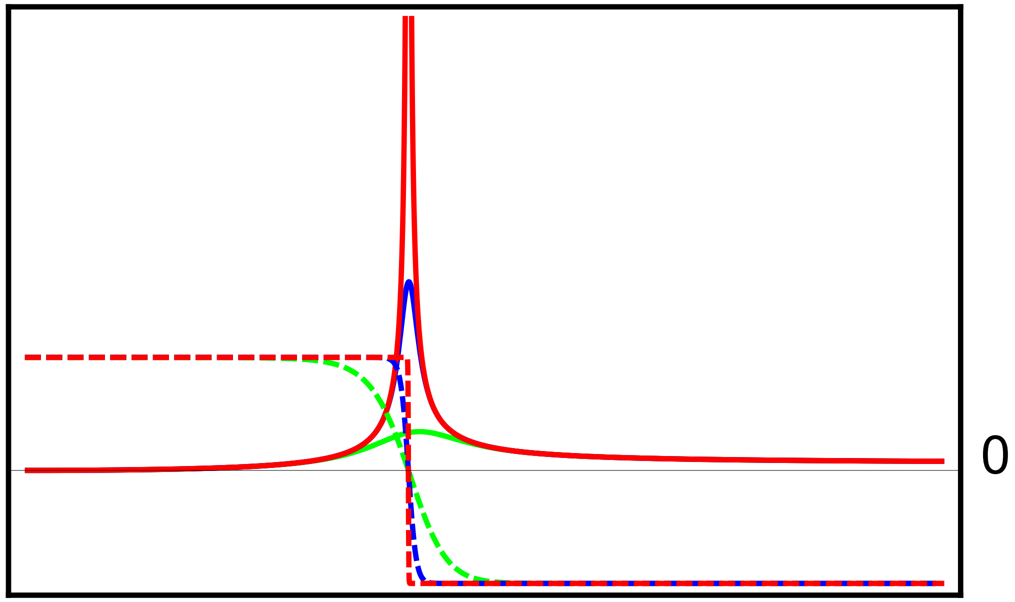
$$0 = \frac{1}{|ak_\mathrm{F}|} - \frac{2}{\pi} \int d\tilde{q} \left[\frac{\tilde{q}^2}{\tilde{q}^2 - 1} \tanh\left(\frac{\tilde{q}^2 - 1)}{2\tilde{T}} \right) - 1 \right]$$

- For $\tilde{T} \to 0$, the integral develops a logarithmic divergence at the Fermi surface where $\tilde{q} = 1$. Thus, the equation has a solution for arbitrarily weak interaction a if T is lowered sufficiently
- This establishes the BCS transition with critical temperature

$$\boxed{\frac{T_\mathrm{c}}{\epsilon_\mathrm{F}} = \frac{8\gamma}{\pi e^2} e^{-\frac{\pi}{2|ak_\mathrm{F}|}}}$$

The exponential dependence reflects the log divergence. The prefactor is ≈ 0.61 with the Euler constant $\gamma \approx 1.78$

- For $T < T_\mathrm{c}$ a gap $\rho > 0$ develops to cure the log divergence



divergent part of the integrand,
and distribution function (dashed)

green: $\tilde{T} = 0.1$

blue: $\tilde{T} = 0.01$

red: $\tilde{T} = 0.001$

BCS Equations for the Gap at Zero Temperature

- We have derived two equations governing the thermodynamics of weakly interacting fermions at $T = 0$:
  - The equation of state

$$\boxed{n = 2\int \frac{d^3\mathbf{q}}{(2\pi)^3}\frac{1}{e^{E_\mathbf{q}/T}+1}}$$

  - The dimensionless equation for the gap $\rho = \phi^*\phi$ (from $\partial\mathcal{U}/\partial\rho = 0$ in the presence of symmetry breaking $\rho \neq 0$ and $T = 0$)

$$\boxed{0 = \frac{1}{|ak_\mathrm{F}|} - \frac{2}{\pi}\int d\tilde{q}\left[\frac{\tilde{q}^2}{\tilde{E}_\mathbf{q}} - 1\right]}$$

with $E_\mathbf{q} = \sqrt{(\epsilon_\mathbf{q} - \mu)^2 + \rho}$

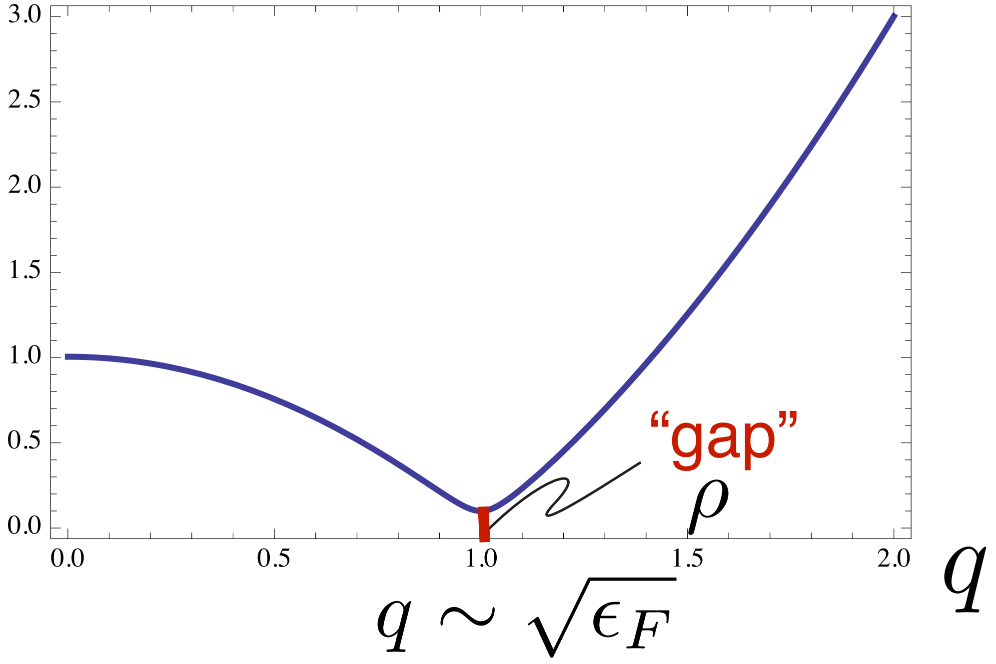
- The scale T is exchanged for the scale ρ, wich now regularizes the log divergence. Again, for $\rho/T_\mathrm{F} \ll 1$, the corrections to the chemical potential from $\epsilon_\mathrm{F} = \mu(T = a = 0)$ are negligible. We therefore work with $\mu \approx \epsilon_\mathrm{F}$
- This establishes the BCS gap at zero temperature ($\pi/\gamma \approx 1.76$)

$$\boxed{\frac{\rho(T=0)}{\epsilon_\mathrm{F}} = \frac{8}{e^2}\,e^{-\frac{\pi}{2|ak_\mathrm{F}|}} = \frac{\pi}{\gamma}\frac{T_\mathrm{c}}{\epsilon_\mathrm{F}}}$$

Fermion Gap and Superfluidity

- Below the critical temperature, a “gap” opens up
- This means that single fermion excitations are suppressed even very close to the Fermi surface (unlike the behavior above T_c). The spectrum is given by

$$E_{\mathbf{q}} = \left[\left(\frac{q^2}{2M} - \mu\right)^2 + \rho\right]^{1/2}$$



- The suppression of single fermion excitations is responsible for superfluidity:
  - The low lying modes are bosonic phonons with linear dispersion
  - This ensures superfluidity according to Landau’s criterion

Summary: Weakly Interacting Fermions

- We have derived BCS theory within the effective action formalism
  - Condensation of the fermion field is impossible due to Pauli's principle, but a second order pairing correlation can develop.
  - The BCS mechanism builds on two cornerstones:
    - the sharpness of the Fermi surface, guaranteed by $ak_{\mathrm{F}} \ll 1$
    - Cooper pairing of fermions close to the Fermi surface with opposite momenta
  - Pairing is introduced in the functional integral by a Hubbard-Stratonovich transformation, mapping the purely fermionic to a fermion-boson theory
  - BCS theory integrates out the quadratic fermions and treats the bosons classically
  - The exponential dependence of critical temperature and gap at zero temperature persists to arbitrarily small interactions. It can be traced to a logarithmic divergence at the Fermi surface.
  - Like the condensation amplitude for bosons, the pairing correlation breaks the U(1) symmetry. The finite gap prevents single fermion excitations and leads to superfluidity

Experimental (Ir)relevance of Weakly Interacting Atomic Fermions

- We compare the critical temperatures for a noninteracting BEC and weakly attractive fermions
    - Free bosons of mass M undergo condensation at $n\lambda_{dB} = \zeta(3/2), \quad \lambda_{dB} = (2\pi/(MT))^{1/2}$
    - Rewrite by using definitions from fermions $n = k_{\rm F}^3/(3\pi^2), \quad \epsilon_{\rm F} = k_{\rm F}^2/(2M)$

$$\frac{T_{\rm c}^{(\rm BEC)}}{\epsilon_{\rm F}} = 4\pi(3\pi^2\zeta(3/2))^{-2/3} \approx 0.69 = \mathcal{O}(1)$$

    - In contrast, the BCS critical temperature is exponentially small for $ak_{\rm F} \ll 1$

$$\frac{T_{\rm c}^{(\rm BCS)}}{\epsilon_{\rm F}} = \frac{8\gamma}{\pi e^2}\, e^{-\frac{\pi}{2|ak_{\rm F}|}} \approx 0.61 e^{-\frac{\pi}{2|ak_{\rm F}|}}$$

- additionally, cooling of degenerate fermions is experimentally more challenging due to Pauli blocking

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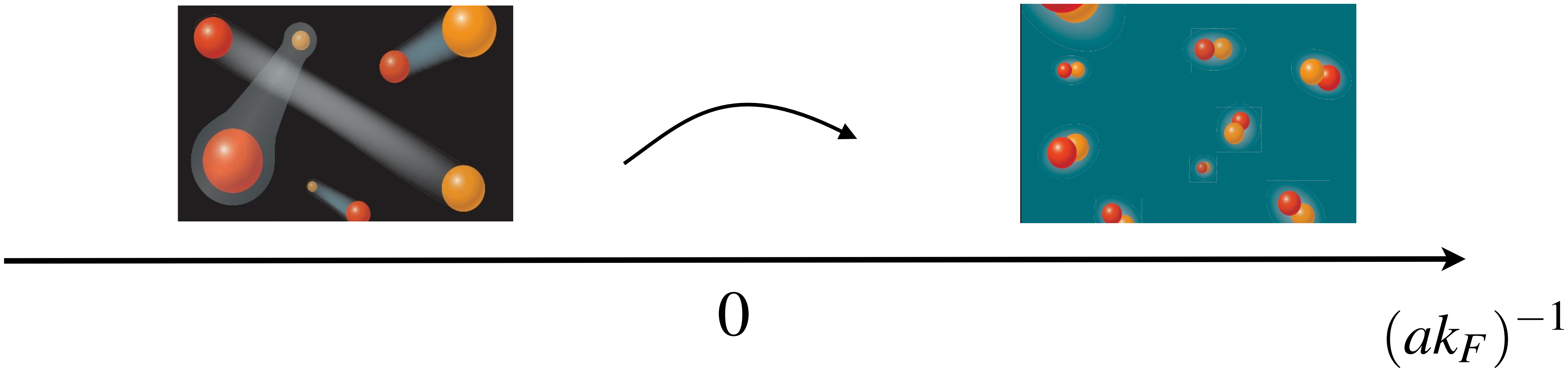
- On the other hand, note a (formal) exponential increase of T_c for rising $ak_{\rm F}$ i.e. towards strong interactions
- Q: What is the fate of the exponential increase in T_c for rising $ak_{\rm F}$
- A: BCS-BEC crossover

Strong Interactions
and
the BCS-BEC Crossover



0

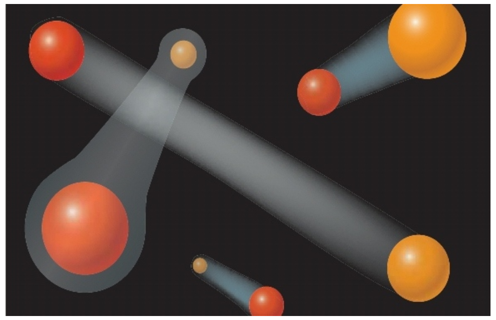
$(ak_F)^{-1}$

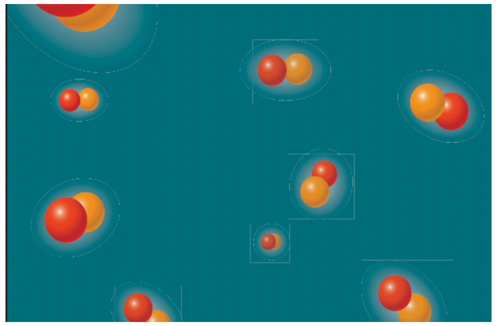
Physical picture: BCS-BEC Crossover

- We have discussed two cornerstones for quantum condensation phenomena:

  - fermions with attractive interactions
    - ➡ BCS superfluidity at low T
  - weakly interacting bosons
    - ➡ Bose-Einstein Condensate (BEC) at low T

bosons could be realized as
tightly bound molecules
(“effective theory”)





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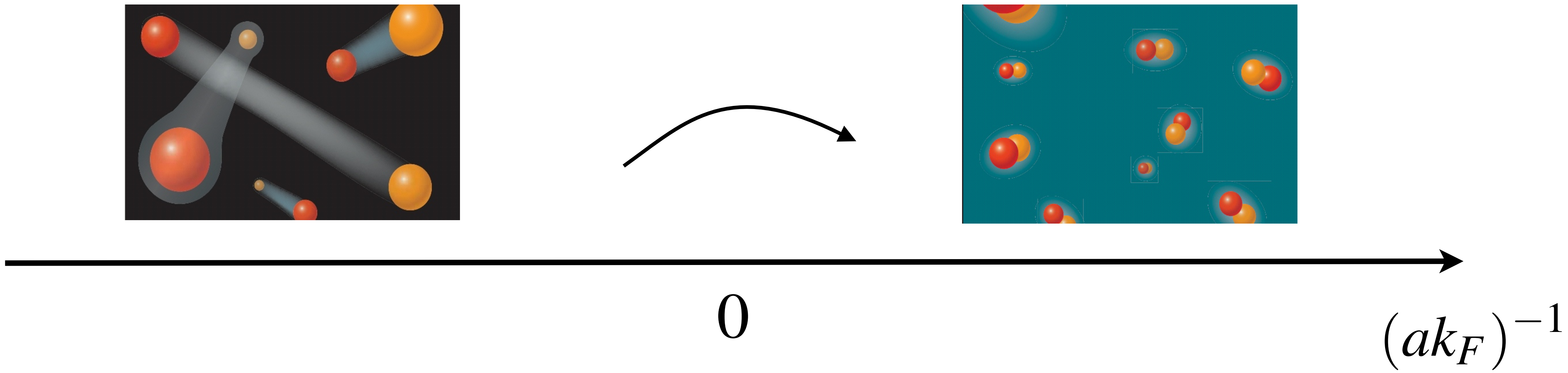


- There is an experimental knob to connect these scenarios: Feshbach resonances

  - microscopically, the phenomenon is due to a bound state formation at the resonance $\frac{1}{ak_{\mathrm{F}}} = 0$
  - from a many-body perspective, the phenomenon is understood as
    - Localization in position space
    - Delocalization in momentum space

➡ In the strongly interacting regime, no simple ordering principle is known:
Challenge for Many-Body methods

Microscopic Origin: Feshbach Resonances

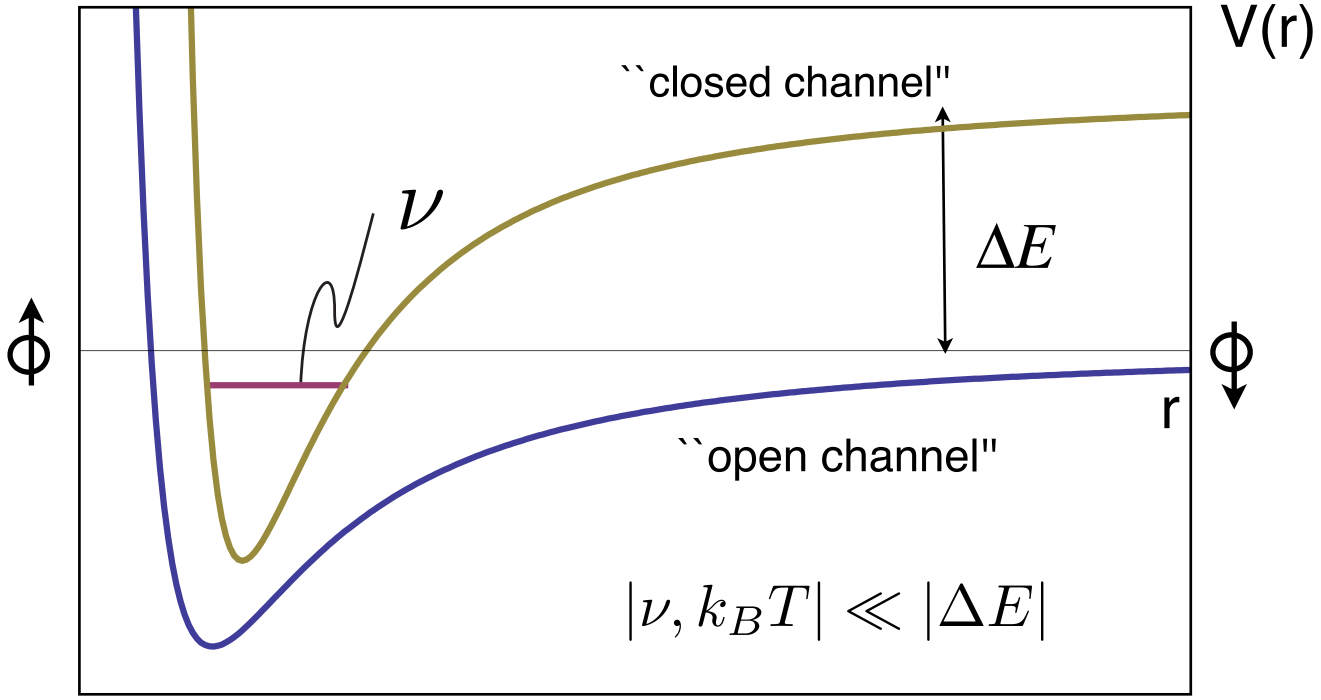
- Start from fermions: (Euclidean) Action

fermion field:
two hyperfine states

$$\psi = \begin{pmatrix} \psi_\uparrow \\ \psi_\downarrow \end{pmatrix}$$

$$S_\psi[\psi] = \int d\tau d^3x \big(\psi^\dagger(\partial_\tau - \frac{\triangle}{2M})\psi + \frac{\lambda_\psi}{2}(\psi^\dagger\psi)^2\big)$$

- Consider a second interaction channel with bound state close to scattering threshold V=0, detuned by ν



examples: $^6\mathrm{Li}, ^{40}\mathrm{K}$

- Detuning ν can be controlled with magnetic field

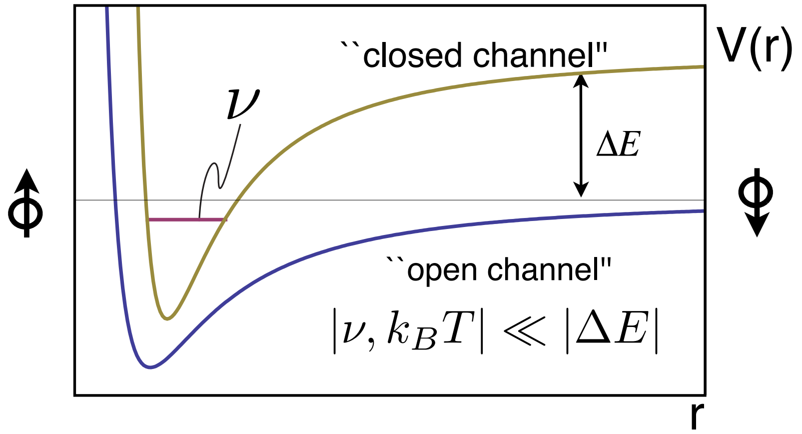
$$\nu(B) = \mu_B(B - B_0)$$

magnetic moment

resonance position

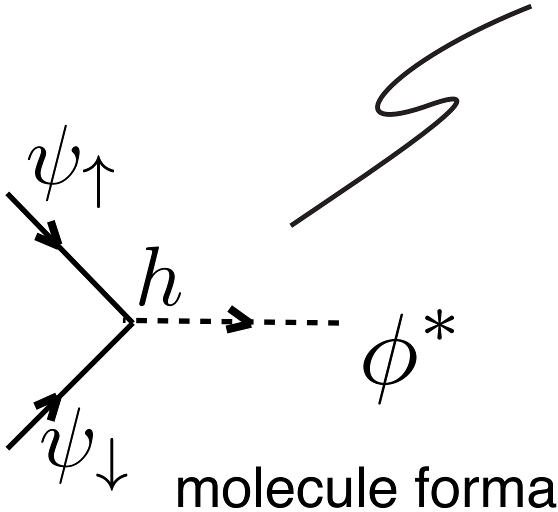
Microscopic Origin: Feshbach Resonances

- Effective Model to describe this situation:
  Interconversion of two fermions into a molecule



bosonic molecule field:
$$S_\phi[\phi] = \int d\tau d^d x \phi^* (\partial_\tau - \frac{\triangle}{4M} + \boxed{\nu})\phi$$

interconversion:
Feshbach, Yukawa term
$$S_F[\psi, \phi] = -\boxed{h} \int d\tau d^d x (\phi^* \psi_\uparrow \psi_\downarrow - \phi \psi_\uparrow^* \psi_\downarrow^*)$$



molecule formation

- NB: cf. BCS Cooper pairing with condensate amplitude:

$$\phi_0^* = \text{const.}$$

- Now we allow for dynamic bosonic degrees of freedom

$$\phi^*(\tau, \mathbf{x}) \quad \text{or} \quad \phi^*(\omega, \mathbf{q})$$

- Parameters:
  - (background scattering in open channel) λ_ψ
  - Feshbach coupling: width of resonance h
  - detuning: distance from resonance ν

Relation to a strongly interacting theory

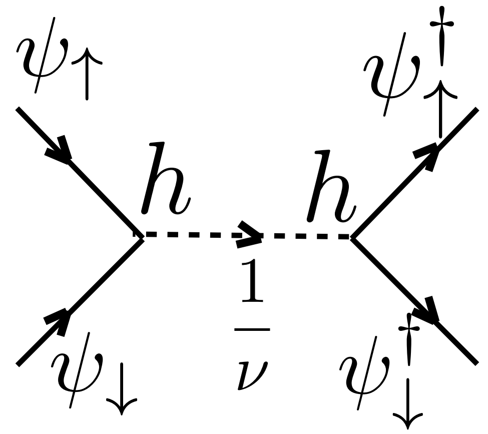
- Total action: $S = S_\psi + S_\phi + S_F[\psi, \phi]$
- Field equations:

$$\frac{\delta S}{\delta \phi^*} = 0 \qquad \Rightarrow (\partial_t - \frac{\triangle}{4M} + \nu)\phi = h\psi_\uparrow\psi_\downarrow$$

$$\Rightarrow \phi = \frac{h}{\partial_t - \frac{\triangle}{4M} + \nu}\psi_\uparrow\psi_\downarrow$$

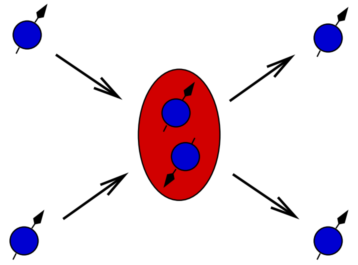
- Formally solve for ϕ, ϕ^*, and insert solution into the Feshbach term

$$S = S_\psi + \int d\tau d^3x\, \psi_\uparrow\psi_\downarrow \frac{h^2}{\cancel{\partial_t - \frac{\triangle}{2M}} + \nu} \psi_\uparrow^\dagger \psi_\downarrow^\dagger$$



- take constrained "broad resonance" limit:
  pointlike interactions

$$h \to \infty, \qquad \frac{h^2}{\nu} \to \text{const.}$$



$$S \to S_\psi + \frac{h^2}{\nu} \int d\tau d^3x\, \psi_\uparrow^\dagger \psi_\downarrow^\dagger \psi_\uparrow \psi_\downarrow = S_\psi - \frac{1}{2}\frac{h^2}{\nu} \int d\tau d^3x\, (\psi^\dagger\psi)^2$$

Relation to a strongly interacting theory

- pointlike/broad resonance limit: The action takes the form

$$S[\psi] = \int d\tau d^d x \big(\psi^\dagger(\partial_t - \frac{\triangle}{2M})\psi + \frac{\lambda_\psi^{\text{eff}}}{2}(\psi^\dagger\psi)^2\big)$$

$$\lambda_\psi^{\text{eff}} = \lambda_\psi - \boxed{\frac{h^2}{\nu(B)}}$$

effective fermionic interaction

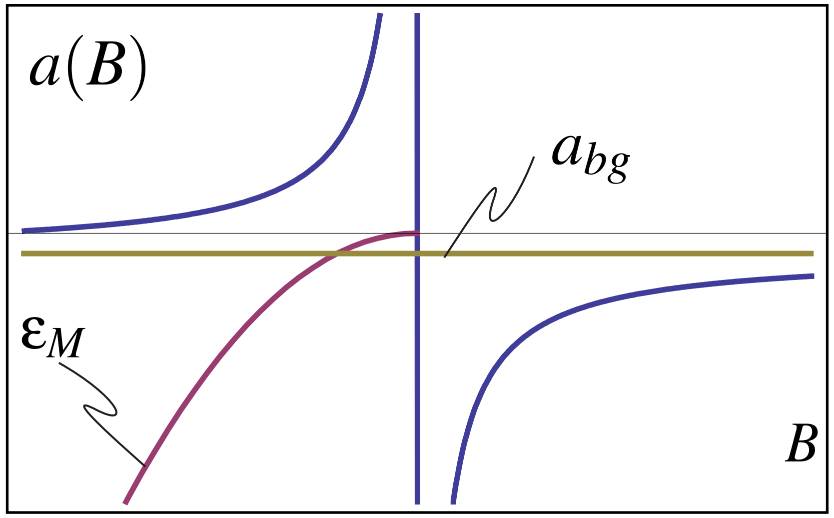
$$a = \frac{4\pi\lambda_\psi^{\text{eff}}}{M}$$

scattering length (nonidentical fermions)

- remember $\nu(B) = \mu_B(B - B_0)$

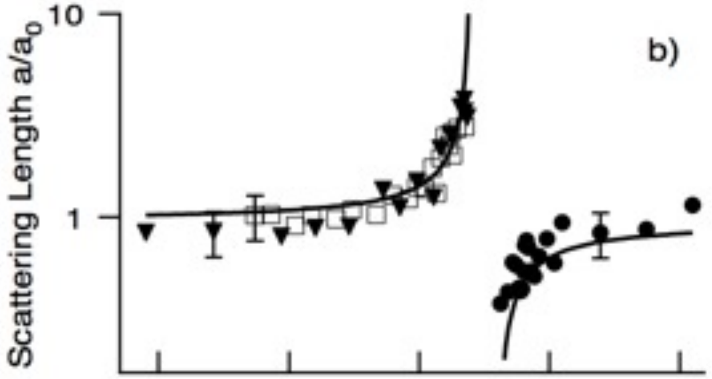
  ➡ resonant (divergent) interaction at B_0

- in the following, we shall ignore the background scattering for simplicity



scattering length a and binding energy

observation of divergent scattering length
Ketterle Group, MIT (1999)
bosonic sodium



Regimes in the BCS-BEC Crossover

- Compare the scattering length to the mean interparticle spacing $d = (3\pi^2 n)^{-1/3}$

  ➡ three regimes

$a < 0,\ \vert a/d\vert \ll 1$	weakly interacting (dilute) fermions
$\vert a/d\vert \gtrsim 1$	strong interactions, dense
$a > 0,\ \vert a/d\vert \ll 1$	molecular bound states: dilute bosons ➡ see below!

- We identify the inverse scattering length as an adequate "crossover parameter"

$$a^{-1}(B) = -\frac{M\nu(B)}{4\pi h^2}$$

since the Feshbach resonance is located at the zero crossing of the detuning $\nu(B)$

- Cf. microscopic justification: a/d > 1 does not invalidate the microscopic Hamiltonian (as could be suspected from the discussion of weakly interacting gases). The relevant ratio for the validity is $r_{vdW}/d, r_{vdW}/\lambda_{dB} \ll 1$. Feshbach resonances violate the generic relation $r_{vdW}/a \approx 1$: "anomalously large scattering length"

Evaluation Strategy: Effective Action

- So far: microscopic physics of few scattering particles
- Quantize the many-body theory via functional integral for the effective action
  - ➡ Consider S, the classical action:

$$S[\chi] \qquad\qquad \frac{\delta S[\chi]}{\delta \chi} = 0$$

  - ➡ The effective action is given by

$$\Gamma[\chi] = -\log \int \mathcal{D}\delta\chi \exp -S[\chi + \delta\chi] \qquad\qquad \frac{\delta \Gamma[\chi]}{\delta \chi} = 0$$

- Result:
  - Effective action includes all quantum and statistical fluctuations by integrating over all possible paths
  - Leverages over the intuition from classical physics:
    - symmetries
    - action principle, field equation
  - Lends itself for powerful modern field theory techniques

Integrating out the fermions

- For practical purposes, the Feshbach type action is favorable:
  - the potential bosonic bound state is already explicit
  - NB: can be seen as result of Hubbard-Stratonovich transformation of fermionic theory
  - for simplicity restrict to broad resonance limit, no background coupling

- This theory is quadratic in the fermions

$$S[\psi] = \int d\tau d^3x (\psi^\dagger(\partial_t - \frac{\triangle}{2M} - \mu)\psi + (\nu - 2\mu)\phi^*\phi - h(\phi^*\psi_\uparrow\psi_\downarrow + \phi\psi^*_\uparrow\psi^*_\downarrow)$$

$$= \frac{1}{2}\int_Q (\Psi^T, \Phi^T) \begin{pmatrix} S^{(2)}_{FF} & 0 \\ 0 & S^{(2)}_{BB} \end{pmatrix} \begin{pmatrix} \Psi \\ \Phi \end{pmatrix}$$

Nambu-Gorkov fields

$$\Psi = \begin{pmatrix} \psi \\ \psi^* \end{pmatrix}$$

$$\Phi = \begin{pmatrix} \phi \\ \phi^* \end{pmatrix}$$

Fourier transform

spin indices

$$S^{(2)}_{FF}[\phi] = \begin{pmatrix} -\epsilon_{\alpha\beta} h\phi^* & -P_F(-Q)\delta_{\alpha\beta} \\ P_F(Q)\delta_{\alpha\beta} & \epsilon_{\alpha\beta} h\phi \end{pmatrix} \qquad S^{(2)}_{BB} = \begin{pmatrix} 0 & \nu - 2\mu \\ \nu - 2\mu & 0 \end{pmatrix}$$

$$P_F(Q) = \mathrm{i}\,\omega + \frac{q^2}{2M} - \mu$$

- Inverse propagator matrix depends on the fluctuating bosonic field

boson carries two atoms

- fermions can be integrated out
- the result is a (nontrivial) purely bosonic theory, to be analyzed subsequently

Gaussian Integral for Fermions

- Effective Action:

$\Psi_0 = 0$ (Pauli principle)

$$\Gamma[\Psi_0, \Phi_0] = -\log \int \mathcal{D}\delta\Psi \mathcal{D}\delta\Phi \exp - S[\Psi_0 + \delta\Psi, \Phi_0 + \delta\Phi]$$

$$= -\log \int \mathcal{D}\delta\Phi \exp - S_{\text{int}}[\Phi_0 + \delta\Phi]$$

composite field expectation value
(condensation for $\Phi_0 \neq 0$)

with intermediate action

$$S_{\text{int}}[\Phi] = S_{\phi}^{(cl)}[\Phi] - \frac{1}{2} \log\det S_{FF}^{(2)}[\Phi] = S_{\phi}^{(cl)}[\Phi] - \frac{1}{2} \mathrm{Tr} \log S_{FF}^{(2)}[\Phi].$$

$$\int (\nu - 2\mu)\phi^*\phi$$

- The Tr Log term features arbitrary powers of Φ (compatible with symmetries)

➡ This gives rise to an effective bosonic theory (Hertz-Millis approach)

Effective Quadratic Theory for Bosons

- Integrating out the fermions yields bosonic theory: Interpretation?
- Progress can be made by expansion in fluctuation field powers:

$$-\frac{1}{2}\mathrm{Tr}\log\left(\mathcal{P}_F+\mathcal{F}\right) \quad = \quad -\frac{1}{2}\mathrm{Tr}\log\mathcal{P}_F-\frac{1}{2}\mathrm{Tr}\mathcal{P}_F^{-1}\mathcal{F}+\frac{1}{4}\mathrm{Tr}(\mathcal{P}_F^{-1}\mathcal{F})^2+\dots$$

$$= S_{FF}^{(2)}[\Phi].$$

$\mathcal{O}(\delta\Phi)$ $\qquad$ $\mathcal{O}(\delta\Phi^2)$

- $\mathcal{P}_F$ depends on the condensate $\quad \Phi_0$
- $\mathcal{F}$ is the “fluctuation matrix” $\quad \sim \delta\Phi$

vanishes due to field equation

- Good qualitative understanding at arbitrary temperature: Truncate after quadratic term
- Yields effective Bogoliubov theory for boson fluctuations

$$S_{\mathrm{Bog}}=\frac{1}{4}\mathrm{Tr}(\mathcal{P}_F^{-1}\mathcal{F})^2=\frac{1}{2}\int_K(\delta\phi(-K),\delta\phi^*(K))\begin{pmatrix}\lambda_\phi(K)\phi_0^*\phi_0^* & P_\phi(K)\\ P_\phi(-K) & \lambda_\phi(K)\phi_0\phi_0\end{pmatrix}\begin{pmatrix}\delta\phi(K)\\ \delta\phi^*(-K)\end{pmatrix}$$

- The coefficients are given by the classical + fluctuation contributions, e.g.

$K=(\omega,\mathbf{k})$

frequency and momentum

$$P_\phi(K)=\nu-h^2\int_Q\frac{P_F(-Q-K)P_F(Q)}{P_F^{|2|}(Q)P_F^{|2|}(Q+K)} \quad = \mathrm{i}Z_\phi\omega+\tfrac{A_\phi}{4M}\mathbf{k}^2+m_\phi^2+\dots$$

“mass term”

low energy/derivative expansion

Crossover Effective Potential I

- The steps in summary (and a last one...): Effective Potential

integration of fermion fluctuations

$$\Gamma[\Phi_0] = -\log\int \mathcal{D}\delta\Phi \exp -S_{\mathrm{int}}[\Phi_0+\delta\Phi]$$

quadratic expansion of boson fluctuations

$$= \int_Q \big((\nu-2\mu)\phi_0^*\phi_0 - \tfrac{1}{2}\mathrm{Tr}\log\mathcal{P}_F[\phi_0^*\phi_0]\big) - \log\int \mathcal{D}\delta\Phi \exp -S_{\mathrm{Bog}}[\delta\Phi]$$

integration of quadratic boson fluctuations

$$= V/T\big((-2\mu+\nu)\phi_0^*\phi_0 - \tfrac{1}{2}\mathrm{Tr}\log\mathcal{P}_F[\phi_0^*\phi_0] + \tfrac{1}{2}\mathrm{Tr}\log\mathcal{P}_B[\phi_0^*\phi_0]\big) \equiv V/T\;\mathcal{U}[\phi^*\phi]$$

“classical contribution”:
condensed bosons

fermionic fluctuations

bosonic fluctuations
(approximation)

effective potential:
homogeneous contribution to
effective action

important in regime: BEC BCS BEC

Crossover Effective Potential II

- The Crossover Physics can now be extracted from the Effective Potential

$$\mathcal{U}[\rho;\mu] = (-2\mu+\nu)\rho - \tfrac{1}{2}\mathrm{Tr}\log\mathcal{P}_F[\rho;\mu] + \tfrac{1}{2}\mathrm{Tr}\log\mathcal{P}_B[\rho;\mu] \qquad \rho = \phi_0^*\phi_0$$

perform spin and frequency traces

$$= (\nu-2\mu)\rho - 2T\int\frac{d^3q}{(2\pi)^3}\log\cosh(E_{\mathbf{q}}^{(\mathrm{F})}/2T) + T\int\frac{d^3q}{(2\pi)^3}\log\sinh(E_{\mathbf{q}}^{(\mathrm{B})}/2T)$$

$$E_{\mathbf{q}}^{(\mathrm{F})} = [(\tfrac{q^2}{2M}-\mu)^2 + h^2\rho]^{1/2}$$

- single fermion excitation energies, coefficients from fermionic action

$$E_{\mathbf{q}}^{(\mathrm{B})} = [(A_\phi q^2 + m_\phi^2)^2 + 2\lambda_\phi\rho(A_\phi q^2 + m_\phi^2)]^{1/2}$$

- effective boson excitation energies
- coefficients: integrals from TrLog + derivative expansion
- mu-dependence: mainly $m_\phi^2(\mu)$

- The effective potential depends on μ and ρ
- These quantities will be determined by:
  - The gap equation
  - The equation of state

Self-consistency relations for the solution of the crossover thermodynamics

The Gap Equation and Spontaneous Symmetry Breaking

- field equation for the effective action: $$\frac{\delta\Gamma[\phi_0(x)^*,\phi_0(x)]}{\delta\phi_0(y)} = 0$$

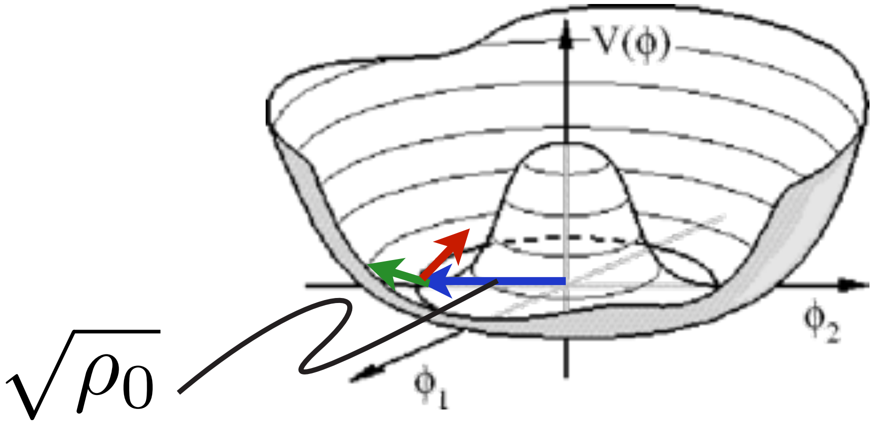
- simplifications:
  - the effective potential depends only on homogeneous field configuration
  - due to U(1) (global phase) symmetry, it only depends on the invariant $\rho = \phi_0^*\phi_0$

$$\frac{\partial\mathcal{U}[\phi_0^*\phi_0]}{\partial\phi_0} = \frac{\partial\mathcal{U}[\rho]}{\partial\rho}\phi_0^* = 0$$

- if the symmetry is broken spontaneously, $\phi_0^* \neq 0$, then we must have

$$\frac{\partial\mathcal{U}[\rho]}{\partial\rho} = 0$$

gap equation (cf. fully analogous treatment in BCS theory)



- NB: This criterion based on symmetry breaking works throughout the whole crossover. At T=0, the symmetry will be broken for any value of scattering length. Therefore, there is no quantum phase transition, but only a crossover phenomenon

The Equation of State

chemical potential

- We would like to consider a situation with fixed density
- Our problem is formulated in the grand canonical ensemble, $S \ni \int dt d^3x(-\mu\psi^\dagger\psi)$

- The density can be obtained from the effective potential:

$$N/V = \lim_{\mathbf{x}\to 0}\langle \delta\psi^\dagger(\mathbf{x})\delta\psi(0)\rangle = \lim_{\mathbf{x}\to 0}\int \mathcal{D}\delta\psi[\delta\psi^\dagger(\mathbf{x})\delta\psi(0)]\exp -S[\psi_0+\delta\psi]/\mathcal{N}$$

$$= -\frac{\partial\mathcal{U}}{\partial\mu}$$

- In our approximation, there are three additive contributions to U. Thus

$$n = 2\phi_0^*\phi_0 + \tfrac{1}{2}\mathrm{Tr}\mathcal{P}_F^{-1} + \mathrm{Tr}\tfrac{1}{2}\mathcal{P}_B^{-1}\frac{\partial m_\phi^2}{\partial\mu}$$

$$= 2\phi_0^*\phi_0 + n_F + n_B$$

effective bosonic propagator

classical bosonic condensate contribution

fermionic (quasiparticle) contribution

~ integral over Fermi distribution

contribution of fermions bound in bosons

~ integral over Bose distribution

in the presence of condensates

➡ definite interpretations only possible in the BCS and BEC limits

The Extended Mean Field Theory of the BCS-BEC Crossover

- The two self-consistency equations from the Effective Potential read
  - The Gap equation

$$0 = \frac{\partial \mathcal{U}}{\partial \rho} = \nu - 2\mu - \frac{h^2}{2} \int \frac{d^3 q}{(2\pi)^3} \left[\frac{1}{E_{\mathbf{q}}^{(\mathrm{F})}} \tanh \frac{E_{\mathbf{q}}^{(\mathrm{F})}}{2T} - \frac{1}{E_{\mathbf{q}}^{(\mathrm{F})}} \Big|_{\phi=\mu=0} \right]$$

NB: Bosonic contribution neglected for simplicity

UV Renormalization: in complete analogy to BCS theory

  - The Equation of State

$$n = -\frac{\partial \mathcal{U}}{\partial \mu} = 2\phi_0^* \phi_0 + n_F + n_B$$

- Solve for μ and ρ

$$a^{-1} = -\frac{M}{4\pi} \frac{\nu}{h^2}$$

- Plot as a function of dimensionless crossover parameter

$$n = \frac{k_F^3}{3\pi^2}$$

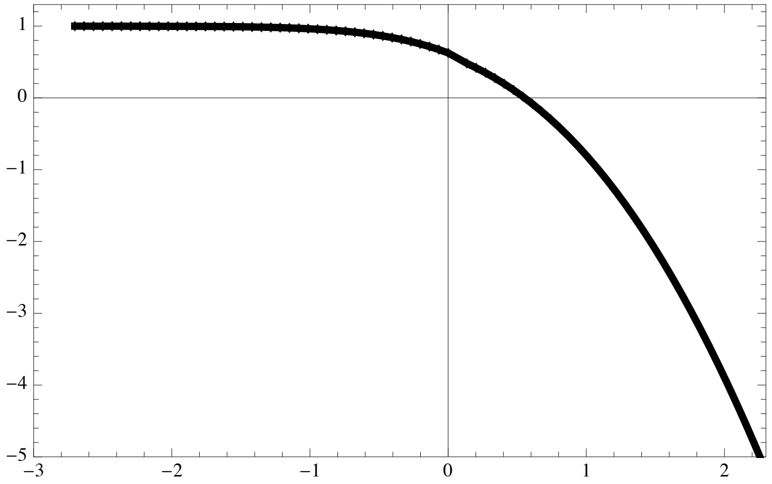
Fermi momentum

$$(a/d)^{-1} = (ak_F)^{-1}$$

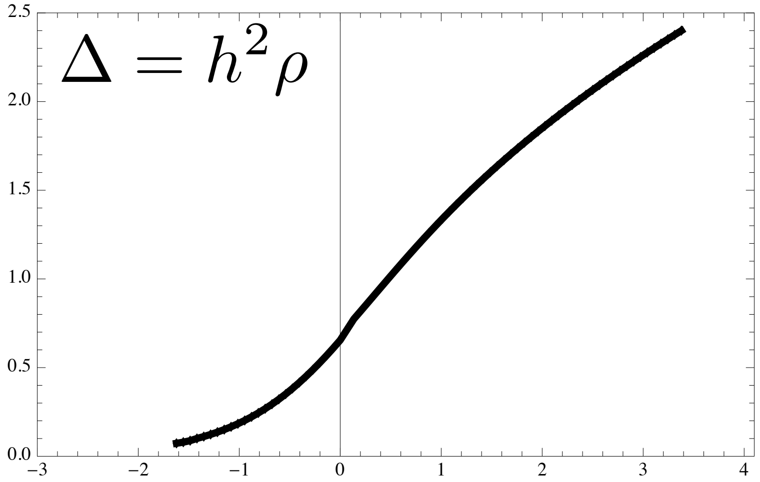
$\frac{\mu}{\epsilon_F}$

$$\epsilon_F = \frac{k_F^2}{2M}$$

Fermi energy



0 $(ak_F)^{-1}$



0 $(ak_F)^{-1}$

➡ What do these solutions tell us?

The Extended Mean Field Theory of the BCS-BEC Crossover

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  - The Gap equation

$$0 = \frac{\partial \mathcal{U}}{\partial \rho} = \nu - 2\mu - \frac{h^2}{2}\int \frac{d^3q}{(2\pi)^3}\Big[\frac{1}{E_{\mathbf{q}}^{(\mathrm{F})}}\tanh\frac{E_{\mathbf{q}}^{(\mathrm{F})}}{2T} - \frac{1}{E_{\mathbf{q}}^{(\mathrm{F})}}\Big|_{\phi=\mu=0}\Big]$$

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UV Renormalization: in complete analogy to BCS theory

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$$n = -\frac{\partial \mathcal{U}}{\partial \mu} = 2\phi_0^*\phi_0 + n_F + n_B$$

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- Plot as a function of dimensionless crossover parameter

$$(a/d)^{-1} = (ak_F)^{-1}$$

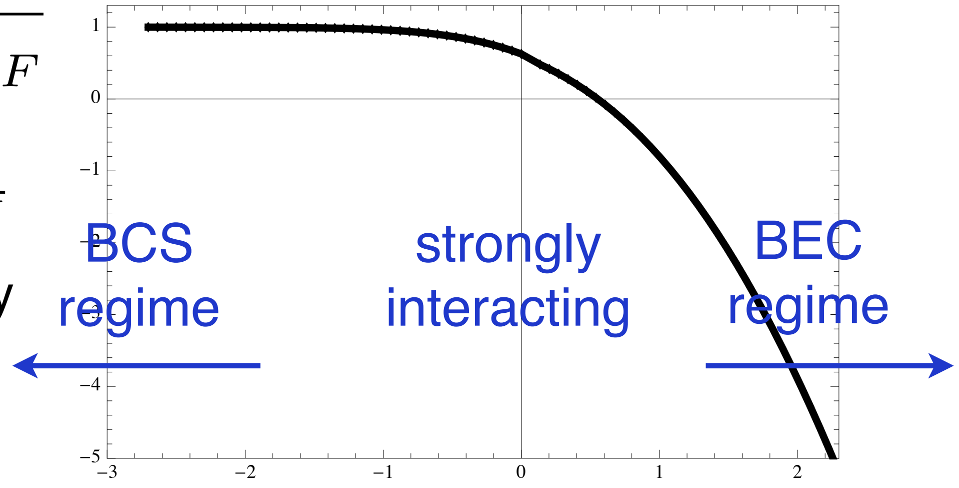
$$n = \frac{k_F^3}{3\pi^2}$$

Fermi momentum

$$\frac{\mu}{\epsilon_F}$$

$$\epsilon_F = \frac{k_F^2}{2M}$$

Fermi energy

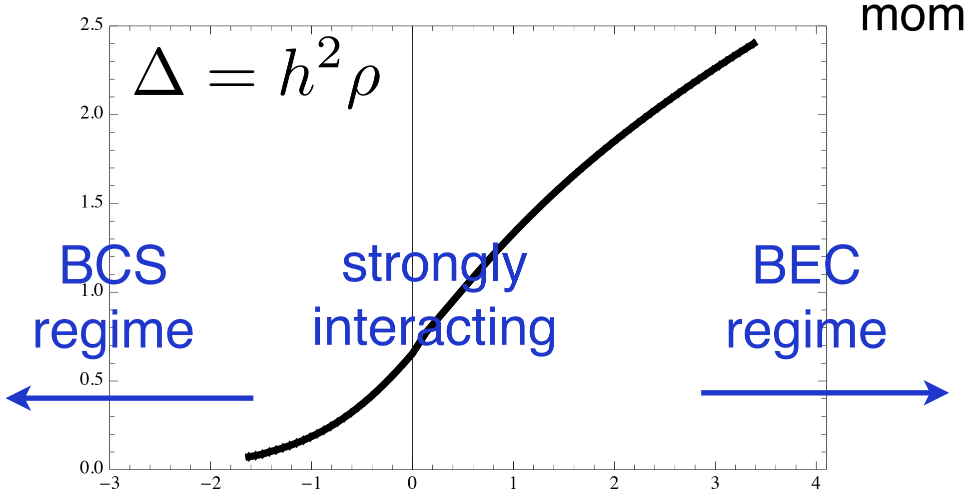


BCS regime

strongly interacting

BEC regime

0 $(ak_F)^{-1}$



$\Delta = h^2\rho$

BCS regime

strongly interacting

BEC regime

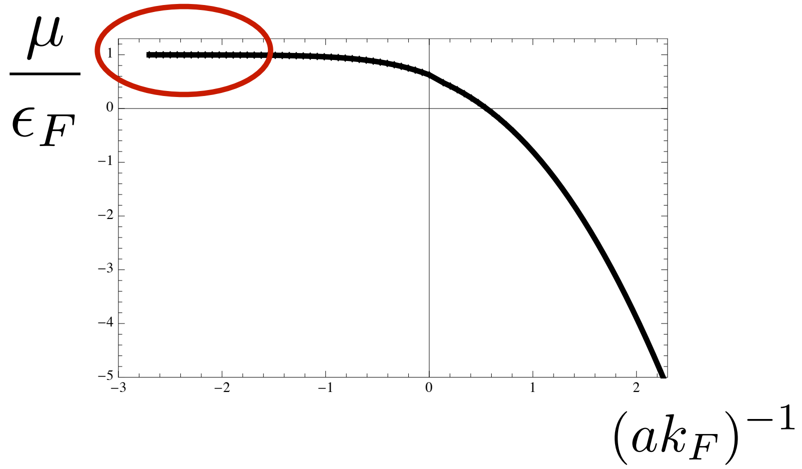
0 $(ak_F)^{-1}$

➡ Discuss the limiting cases!

The limiting cases: BCS limit

- Solution above: $\frac{\mu}{\epsilon_F} \to 1$
  - ➡ Expression of a Fermi surface, weakly interacting fermion gas is approached

BCS regime



- Simplifications
  - ➡ The EoS reduces to

$$n = 2\phi_0^*\phi_0 + n_F + n_B \to n_F$$

  - ➡ The gap equation can be solved analytically

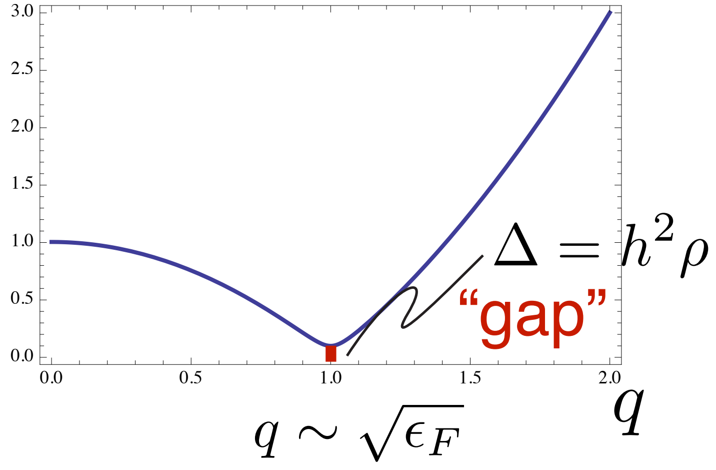
$$0 = \frac{\nu - 2\mu}{h^2} - \frac{1}{2}\int \frac{d^3q}{(2\pi)^3}\Big[\frac{1}{E_{\mathbf{q}}^{(\mathrm{F})}}\tanh\frac{E_{\mathbf{q}}^{(\mathrm{F})}}{2T} - \frac{1}{E_{\mathbf{q}}^{(\mathrm{F})}}\Big|_{\phi=\mu=0}\Big]$$

  - ➡ NB: For broad resonances: $h \to \infty,\ \nu \propto h^2$

$$\frac{\nu - 2\mu}{h^2} \to \frac{\nu}{h^2} = -\frac{4\pi}{M}a^{-1}$$

single fermion excitation spectrum

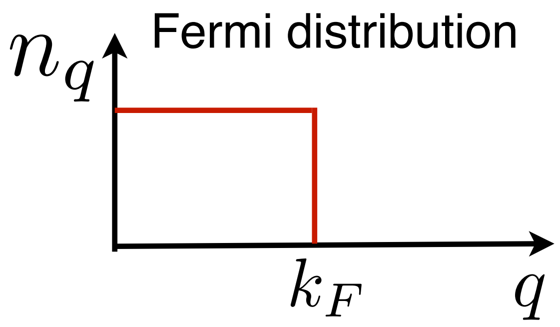
$$E_{\mathbf{q}}^{(\mathrm{F})} = \Big[\big(\frac{\mathbf{q}^2}{2M} - \mu\big)^2 + h^2\rho\Big]^{1/2}$$

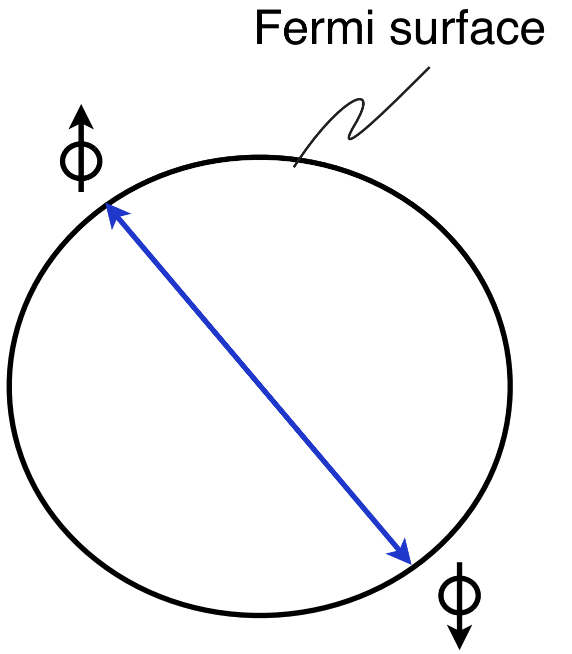


$$0 = -\frac{1}{a} - \frac{M}{8\pi}\int \frac{d^3q}{(2\pi)^3}\Big[\frac{1}{E_{\mathbf{q}}^{(\mathrm{F})}}\tanh\frac{E_{\mathbf{q}}^{(\mathrm{F})}}{2T} - \frac{1}{E_{\mathbf{q}}^{(\mathrm{F})}}\Big|_{\phi=\mu=0}\Big]$$

cf. above: BCS Gap equation reproduced

The limiting cases: BCS limit





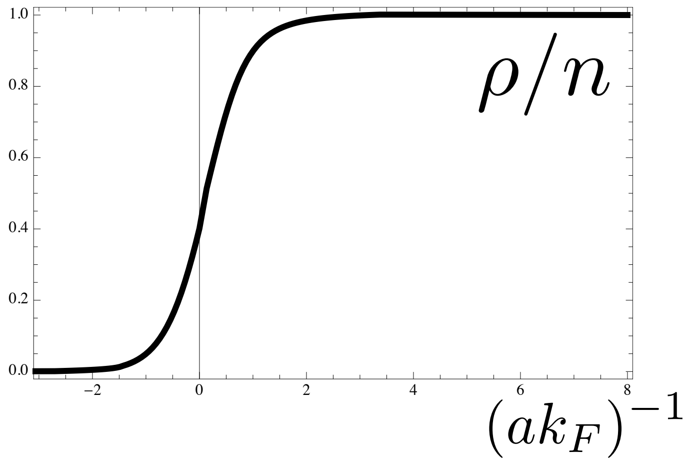
Locality in momentum space

Delocalization in position space

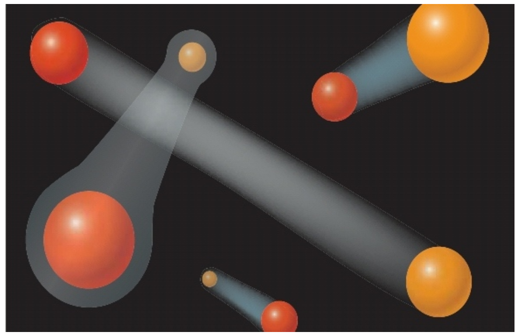
- Interpretations:
  - Strongly expressed Fermi surface
    ➡ Scattering/Pairing highly local in momentum space
  - The result for the gap:

$$\Delta = 0.61\epsilon_F\, e^{-\frac{\pi}{2ak_F}}$$

➡ Condensation is very weakly expressed: only Fermions close to Fermi surface contribute



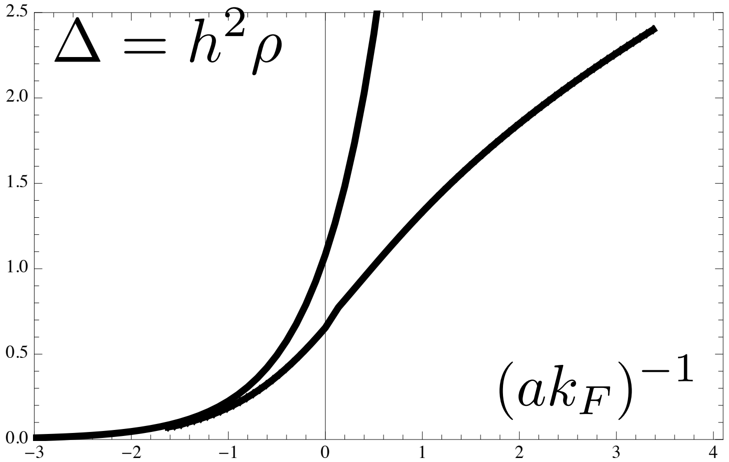
slight cheating here, this plots the renormalized condensate (below)



- Comparison to full result

➡ Strong deviations from BCS result once

$$(ak_F)^{-1} \sim -1$$



The limiting cases: BEC limit

- Solution above: $\frac{\mu}{\epsilon_F} \to -\infty$

➡ Strong gap $-\mu$ develops on the normal $(\psi^\dagger\psi)$ sector of the inverse fermion propagator

➡ However, there is a piece from the anomalous part that is independent of $-\mu$

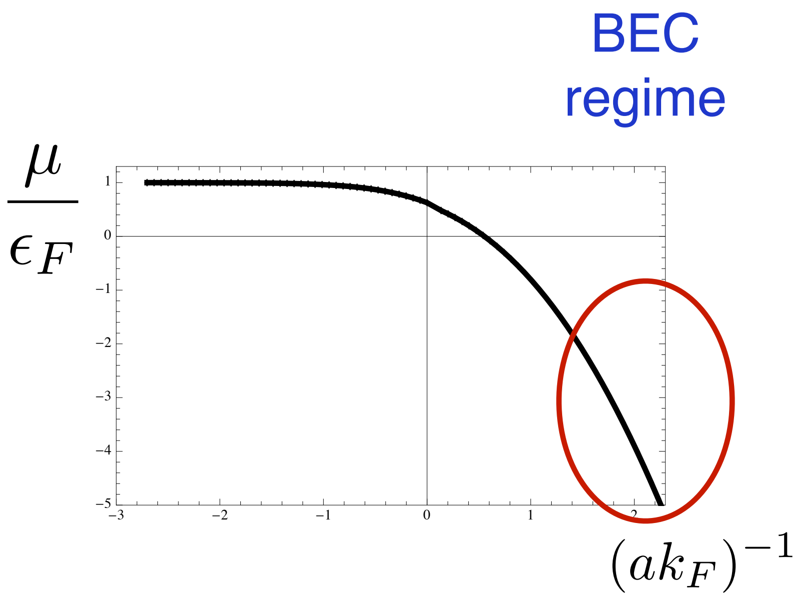
➡ The fermion density can be written

$\psi\psi$

$$n_F = \tfrac{1}{2}\mathrm{Tr}\,\mathcal{P}_F^{-1} \to -\frac{\partial \Delta m_\phi^2}{\partial \mu}\,\phi_0^*\phi_0$$

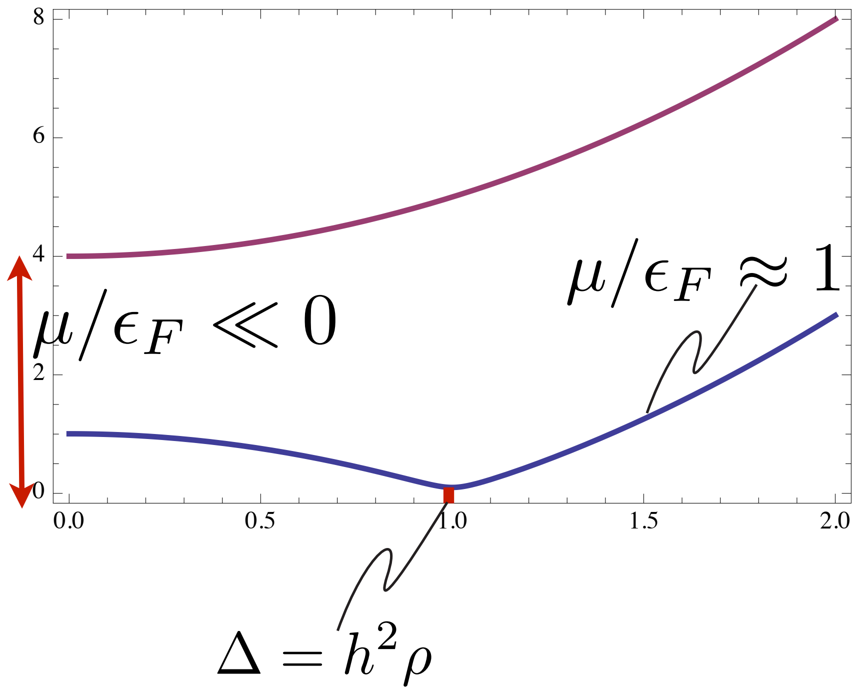
Δm_ϕ^2 is identified as the fluctuation correction to the bosonic mass term

➡ Interpretation?



single Fermion excitation spectrum

$$E_{\mathbf{q}}^{(\mathrm{F})} = \left[\left(\frac{\mathbf{q}^2}{2M} - \mu\right)^2 + h^2\rho\right]^{1/2}$$



Renormalized Condensate

total mass term:
classical + fluctuations

- We consider the equation of state in the BEC regime:

$$n = 2\phi_0^*\phi_0 + n_F + n_B \to (2 - \frac{\partial \Delta m_\phi^2}{\partial \mu})\phi_0^*\phi_0 + n_B = -\frac{\partial m_\phi^2}{\partial \mu}\phi_0^*\phi_0 + n_B$$

- We consider the bosonic density further (T=0):

Bosonic propagator

$$n_B = -\frac{\partial}{\partial\mu}\frac{1}{2}\mathrm{Tr}\log\mathcal{P}_B[\rho;\mu] \approx -\frac{\partial m_\phi^2}{\partial\mu}\mathrm{Tr} \quad \mathcal{P}_B^{-1}[\rho;\mu]$$

- For $\mu \to -\infty$ the bosonic propagator matrix simplifies to

$$\mathcal{P}_B = \begin{pmatrix} \lambda_\phi(K)\phi_0^*\phi_0^* & P_\phi(K) \\ P_\phi(-K) & \lambda_\phi(K)\phi_0\phi_0 \end{pmatrix} \to Z_\phi \begin{pmatrix} 2aZ_\phi\phi_0^*\phi_0^* & \mathrm{i}\omega + \frac{\mathbf{q}^2}{4M} + 2aZ_\phi\phi_0^*\phi_0 \\ -\mathrm{i}\omega + \frac{\mathbf{q}^2}{4M} + 2aZ_\phi\phi_0^*\phi_0 & 2aZ_\phi\phi_0\phi_0 \end{pmatrix}$$

- We observe that the expression

$$Z_\phi := -\frac{1}{2}\frac{\partial m_\phi^2}{\partial\mu}$$

is ubiquitous to all the formulas here

- We introduce a renormalized condensate density as $\boxed{\tilde\phi^*\tilde\phi = Z_\phi\phi_0^*\phi_0^*}$

The limiting cases: BEC limit

- Expressing all quantities in terms of the renormalized condensate gives:
  - Equation of state

$$\boxed{n = 2\tilde{\phi}_0^*\tilde{\phi}_0 + 2\mathrm{Tr}\tilde{\mathcal{P}}_B^{-1} = 2\tilde{\phi}_0^*\tilde{\phi}_0 + 2\tilde{n}_B}$$

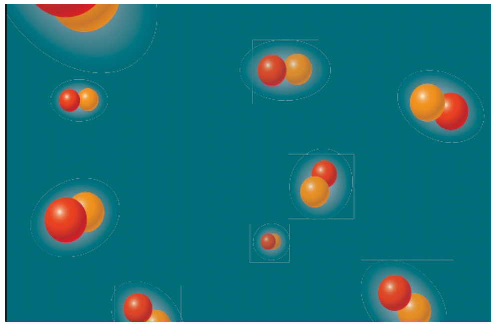
  - with renormalized inverse boson propagator

$$\tilde{\mathcal{P}}_B = \mathcal{P}_B/Z_\phi = \begin{pmatrix} 2a\tilde{\phi}_0^*\tilde{\phi}_0^* & \mathrm{i}\omega + \frac{\mathbf{q}^2}{4M} + 2a\tilde{\phi}_0^*\tilde{\phi}_0 \\ -\mathrm{i}\omega + \frac{\mathbf{q}^2}{4M} + 2a\tilde{\phi}_0^*\tilde{\phi}_0 & 2a\tilde{\phi}_0\tilde{\phi}_0 \end{pmatrix}$$

➡ Reduction to an effective theory of “renormalized” bosonic bound states

- Mass 2M
- Interaction strength 2a
- Atom number 2

Local objects in position space



- All reference to the concrete value of Z is gone in the renormalized quantities
- Macroscopic measurements probe the renormalized quantities
- Microscopic probes can measure Z, but this is beyond the scope here
- NB: While boson mass and atom number follow from symmetry, the interaction strength 2a is an approximation. The exact answer is 0.6a (four-body problem)

Connection to Scattering Physics: Vacuum limit

- Heuristics: Study the gap equation (broad resonance) for $\frac{\mu}{\epsilon_F} \to -\infty$

$$\frac{1}{a} = \sqrt{-\mu \cdot 2M}$$

  - ➡ The density scale k_F (also: temperature) have disappeared from the gap equation:
  - ➡ only two-body physics left!
  - ➡ Very different from BCS limit, cf. $\frac{\Delta}{\epsilon_F} = 0.61\, e^{-\frac{\pi}{2ak_F}}$

Connection to Scattering Physics: Vacuum limit

- More systematically: Project on physical vacuum by

$$\Gamma_{k\to 0}(vak) = \lim_{k_F \to 0} \Gamma_{k\to 0}\big|_{T/\epsilon_F > T_c/\epsilon_F = \text{const.}}$$

  - Diluting procedure: $d \sim k_F^{-1} \to \infty$
  - Getting cold: $T \sim \epsilon_F$

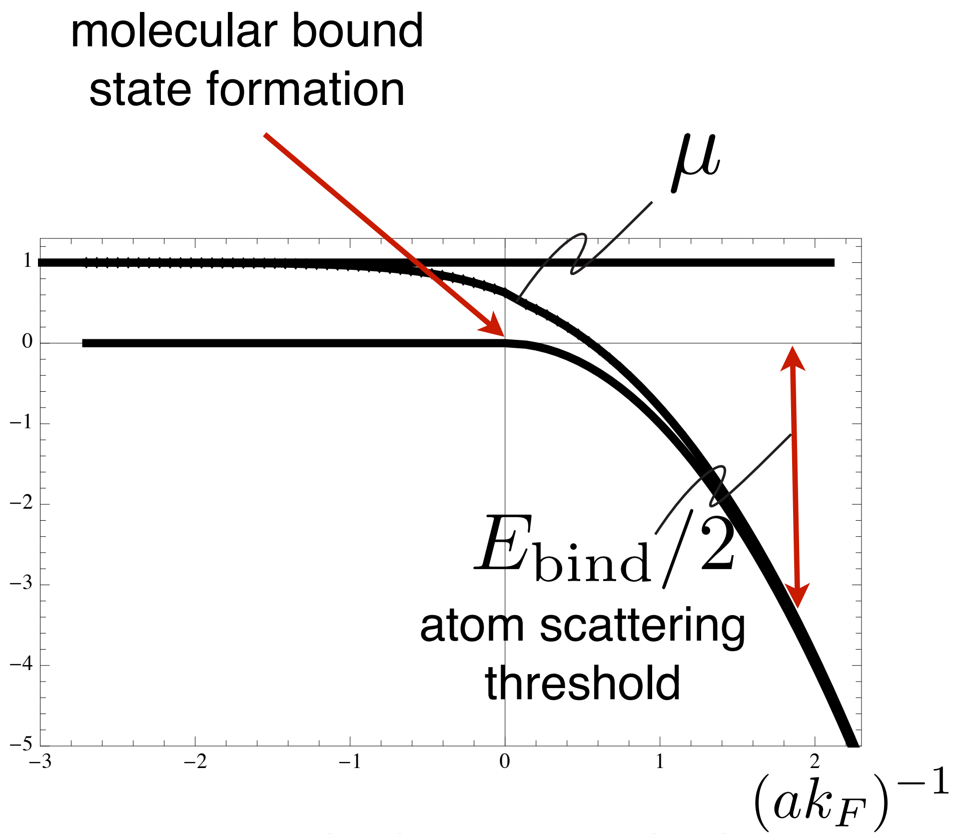
$$n = \frac{k_F^3}{3\pi^2}$$

- The chemical potential plays the role of half the binding energy

$$\boxed{E_{\text{bind}} = -1/(Ma^2)}$$

- Smooth crossover terminates in sharp

  “second order phase transition” in vacuum



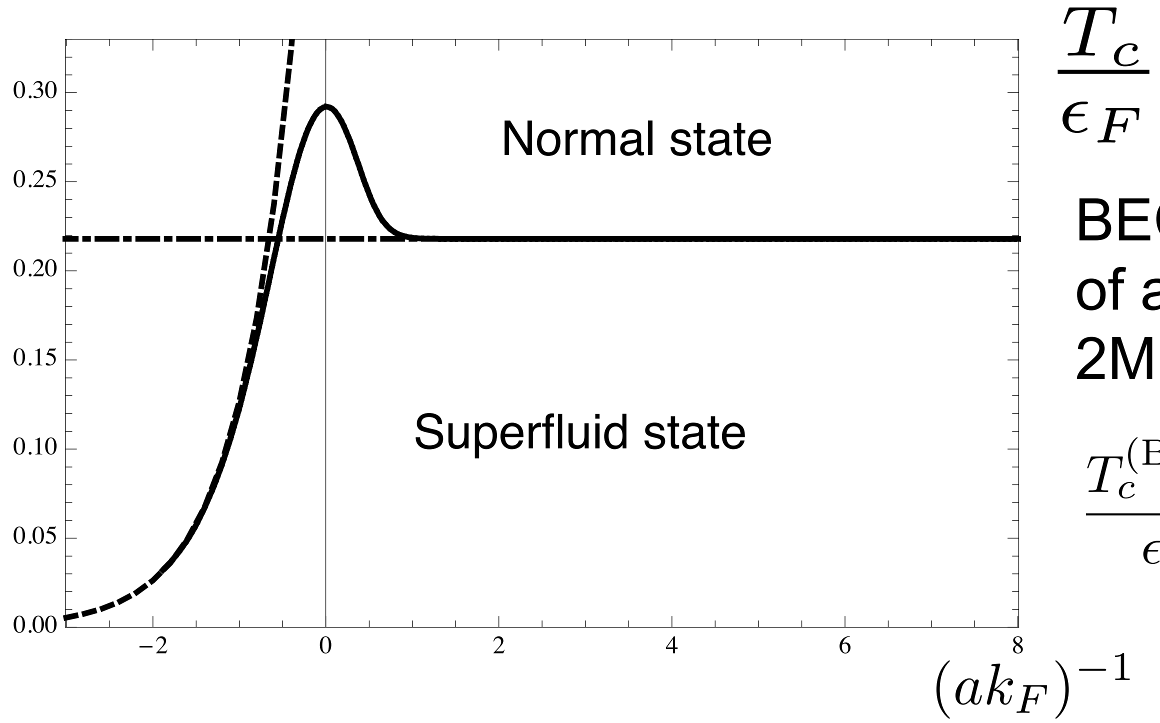
two-body vs. many-body

- NB: Using this vacuum procedure, the above functional integral treatment solves the two-body scattering problem -- as quantum mechanics would do

➡ microscopic origin of the crossover is bound state formation

Finite Temperatures

- So far: Crossover Physics at T=0
- The above formalism is readily applied to finite temperature: Frequency integration -> Matsubara sum
- Finite temperature phase diagram:



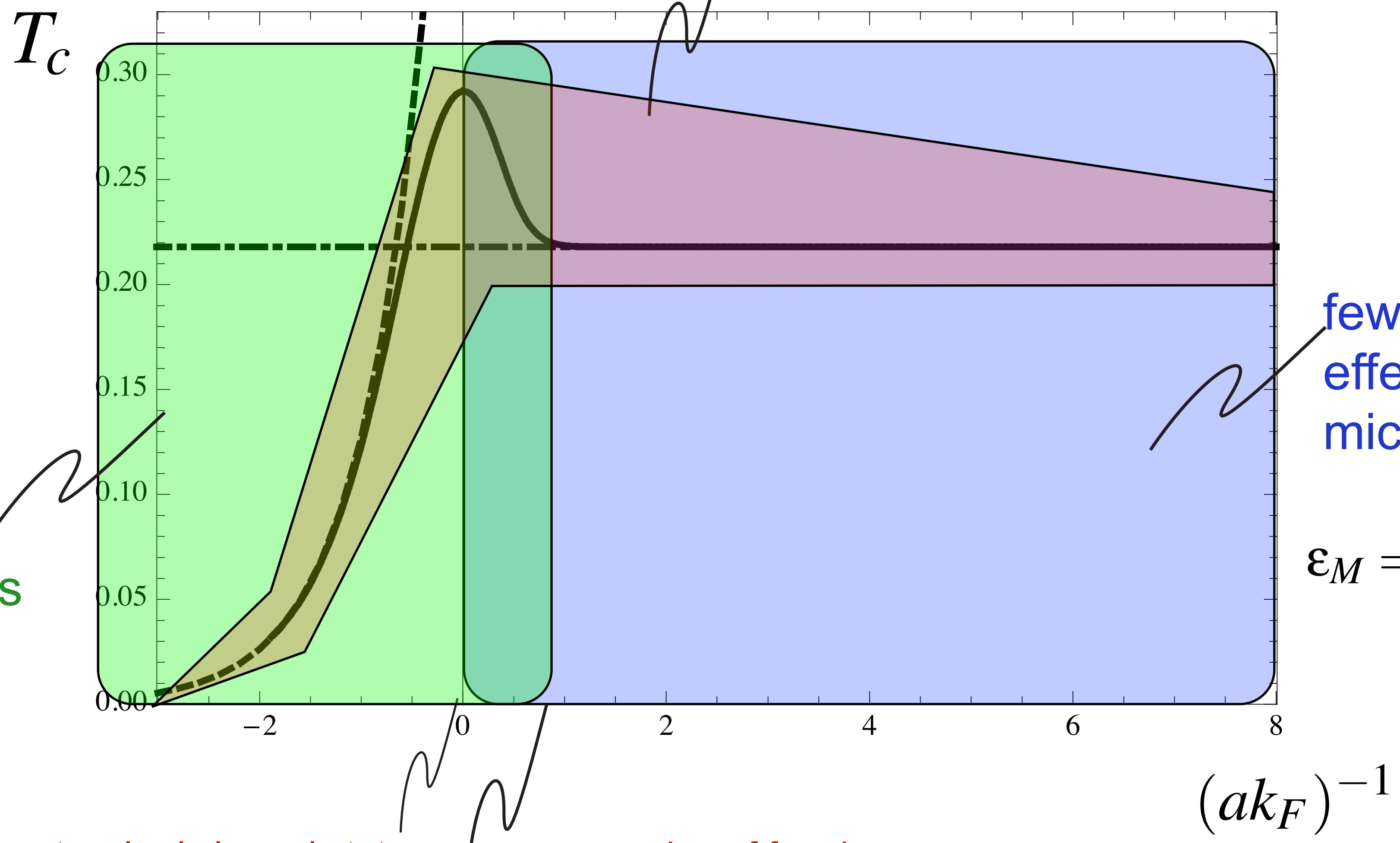
BCS limit:
BCS theory

BEC limit: Free bosons of atom number 2, mass 2M

$$\frac{T_c^{(\mathrm{BEC})}}{\epsilon_\mathrm{F}} = 2\pi(6\pi^2\zeta(3/2))^{-2/3} \approx 0.218$$

Challenges beyond Mean Field

Beyond mean field effects and challenges
at very different scales:



critical behavior:
long distance scales $k_{ld} \gg n^{1/3}, T^{1/2}, \varepsilon_M^{1/2}$

few-body physics of
effective dimers:
microscopic scales

$$\varepsilon_M = -\frac{1}{Ma^2} \gg T, \frac{k_F^2}{2M}$$

Many-Body fermion
physics:
Thermodynamic scales

$$n = \frac{k_F^3}{3\pi^2}, T$$

two-body bound state

zero crossing of fermion
chemical potential

Strategy: Find an interpolation scheme which incorporates known physical effects in the limiting cases
Methods: t-matrix approaches, 2PI Effective Action, Functional RG, ...

Results beyond Mean Field

- Functional RG treatment: connecting micro- and macrophysics, unified treatment of physics on various scales

microscopic

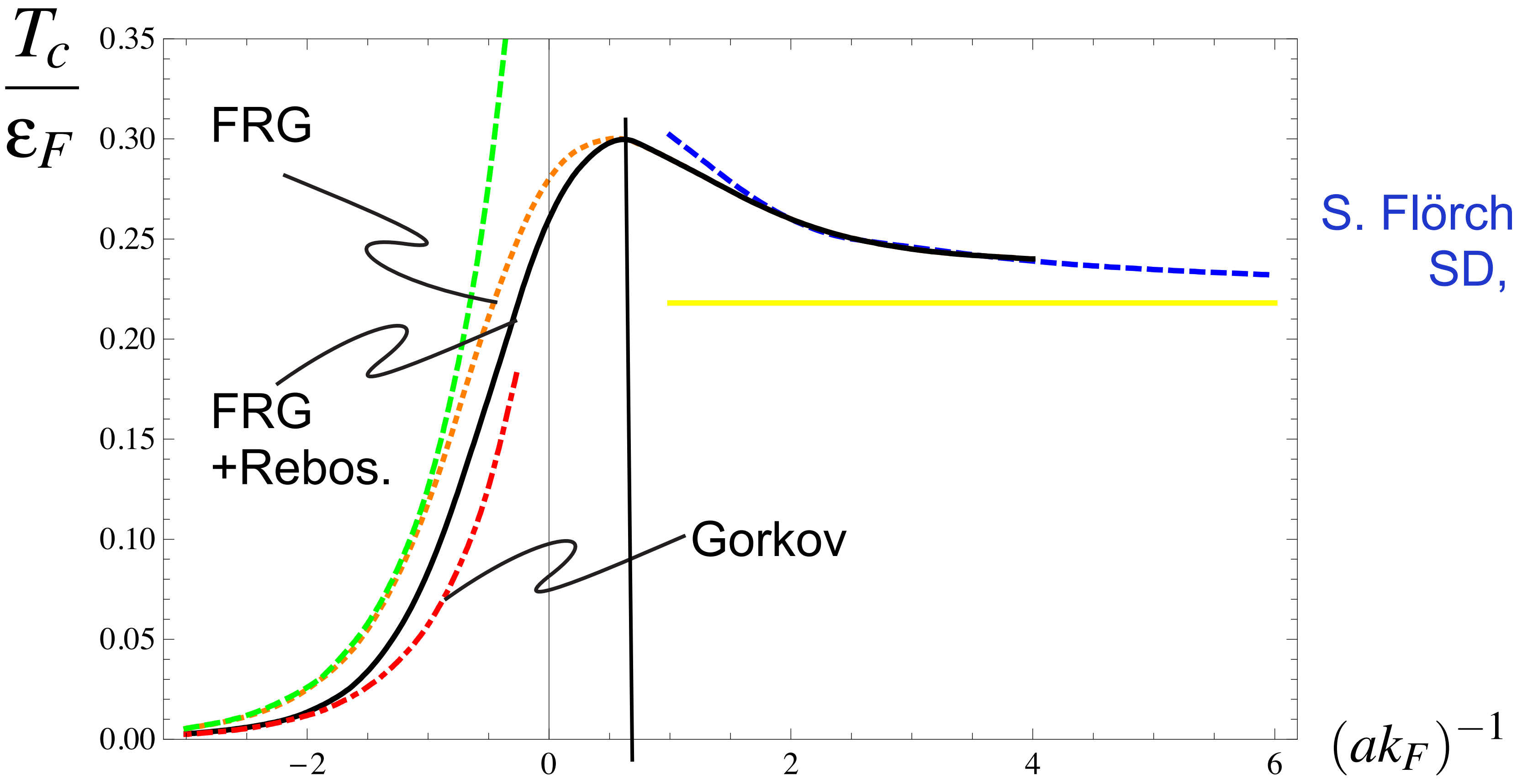
$$\varepsilon_M = -\frac{1}{Ma^2}$$

thermodynamic

$$n = \frac{k_F^3}{3\pi^2}, T$$

long distance

$$k_{ld} \gg n^{1/3}, T^{1/2}, \varepsilon_M^{1/2}$$

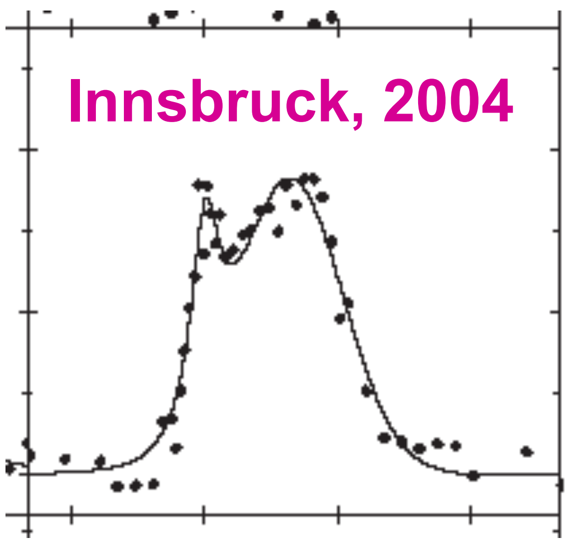


S. Flörchinger, M. Scherer, SD, C. Wetterich

zero crossing of fermion chemical potential

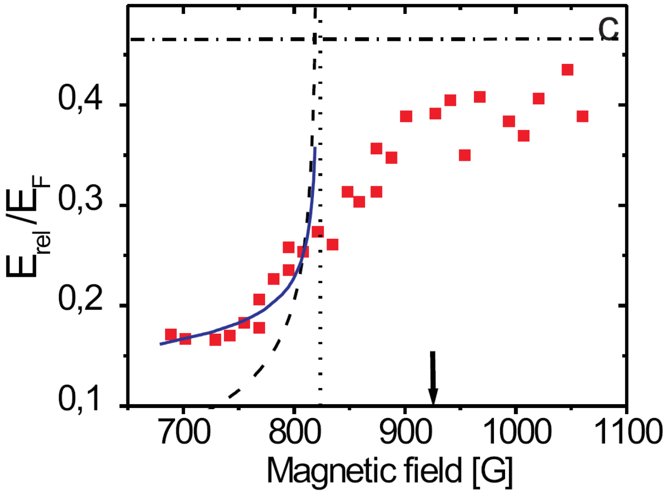
- Accurate treatment of molecular scattering physics in BEC regime
- Accurately reproduce Gorkov effect in the BCS regime from rebosonization procedure
- Long wavelengths: second order phase transition

Experiments in the BCS-BEC Crossover



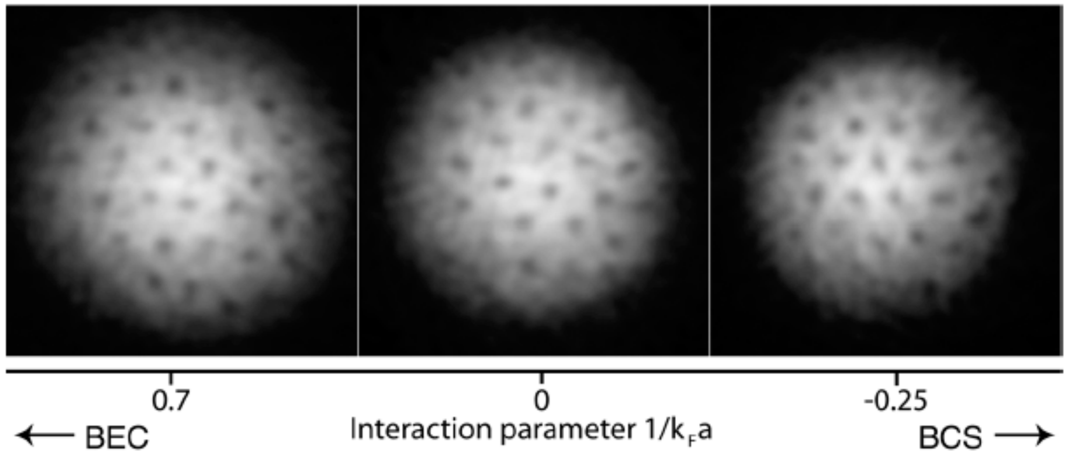
pairing gap

ENS, 2004

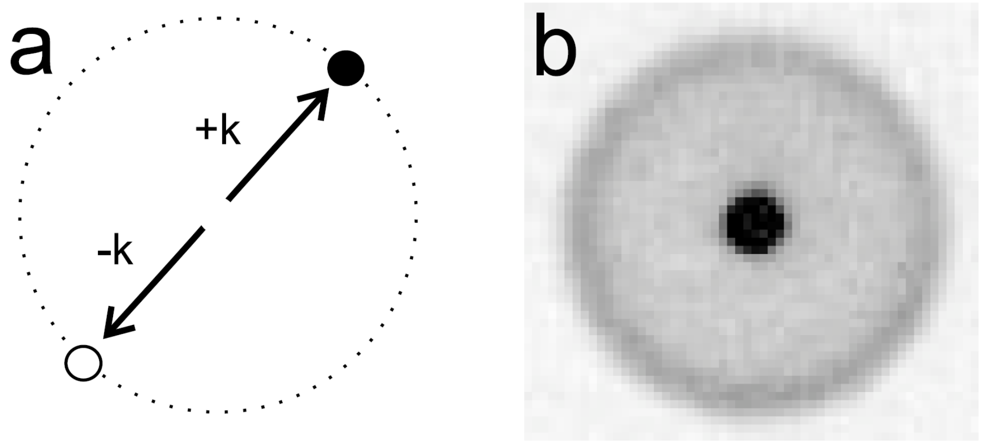


release energy

MIT, 2005 *vortices*

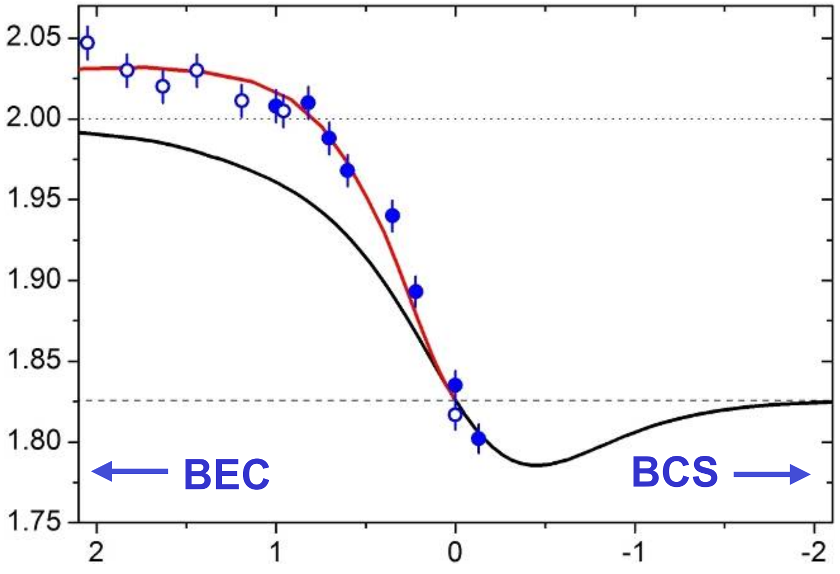


JILA, 2005



pair correlations

Duke ´04, Innsbruck 2004 & `06



collective modes

Summary: BCS-BEC Crossover

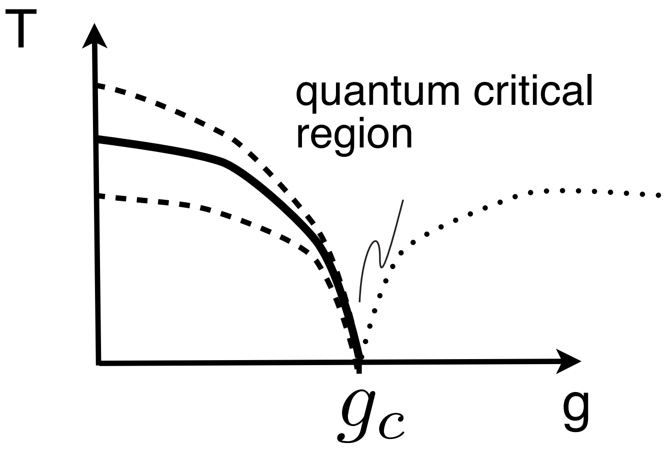
- We have discussed a simple approximation scheme based on the effective action capturing the qualitative features of the BCS-BEC crossover at zero and finite temperatures
  - The BCS-BEC crossover interpolates between the two cornerstones for quantum condensation phenomena, BCS and BEC type superfluidity
  - The microscopic origin is a Feshbach resonance. The divergence of the scattering length is accompanied by the formation of a bosonic bound state. There are three regimes for the many-body physics

$a < 0, \; \lvert ak_{\mathrm{F}} \rvert \ll 1$	weakly interacting (dilute) fermions
$\lvert ak_{\mathrm{F}} \rvert \gtrsim 1$	dense regime, strong interactions
$a > 0, \; \lvert ak_{\mathrm{F}} \rvert \ll 1$	molecular bound states: dilute bosons

  - The crossover from BCS to BEC regimes may be viewed as a localization process in real space, or a delocalization in momentum space
  - Though there are profound quantitiative changes in the thermodynamics, the ground state symmetry properties are unchanged: Crossover instead of quantum phase transition

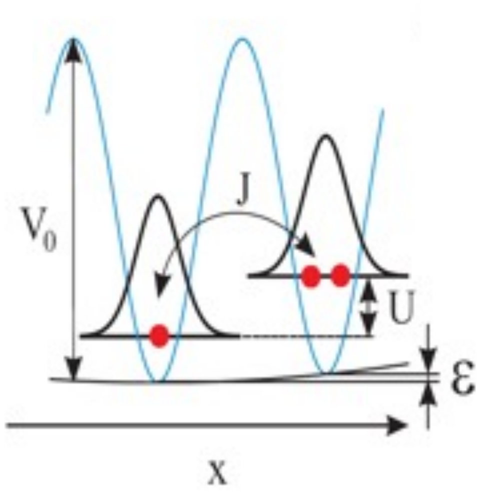
Lattice Systems: Outline

Quantum Phase transitions: General Overview



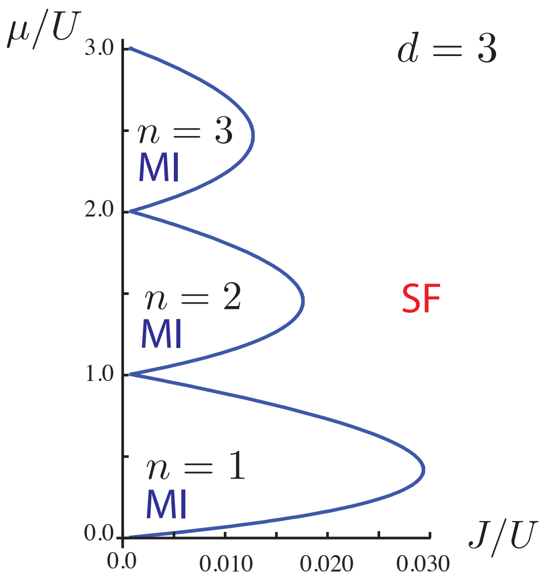
- What is a Quantum Phase transition?
- Example: Mott Insulator -- Superfluid transition

Microscopic derivation of the Bose-Hubbard model



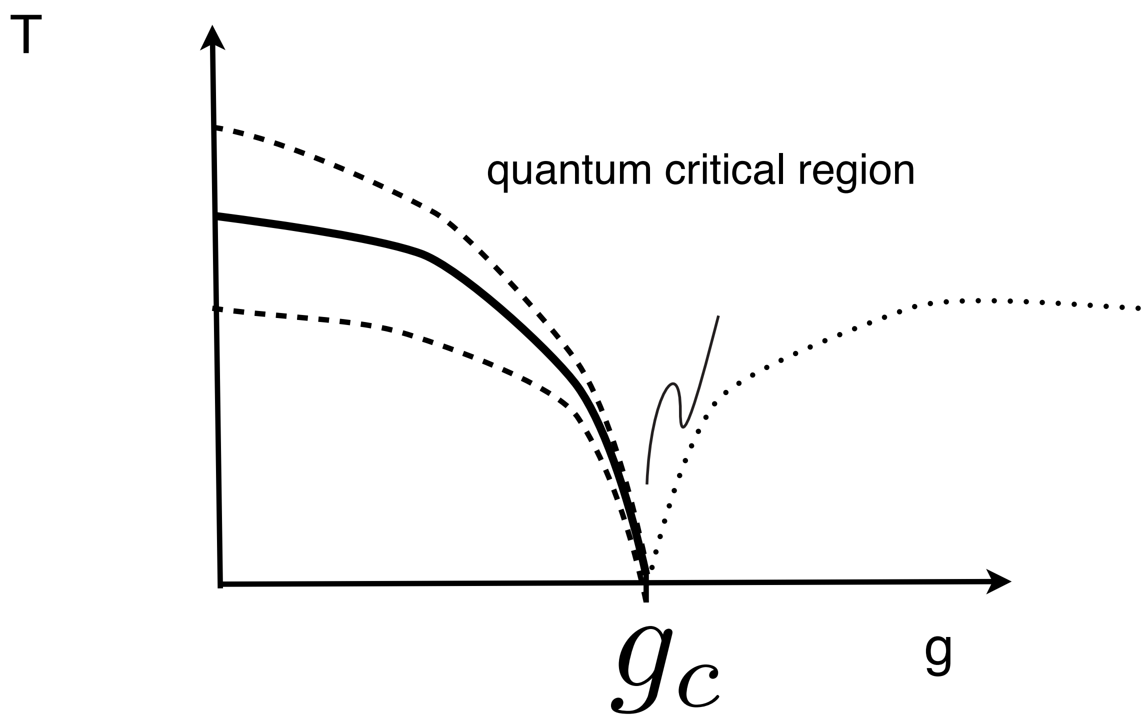
- Atoms in optical potentials
- Periodic potentials, Bloch theorem
- Bose-Hubbard model

Phase diagram of the Bose-Hubbard model



- Basic mean field theory: phase border and limiting cases
- Path integral formulation: excitation spectrum in the Mott phase and bicritical point

Quantum Phase Transitions: General Overview



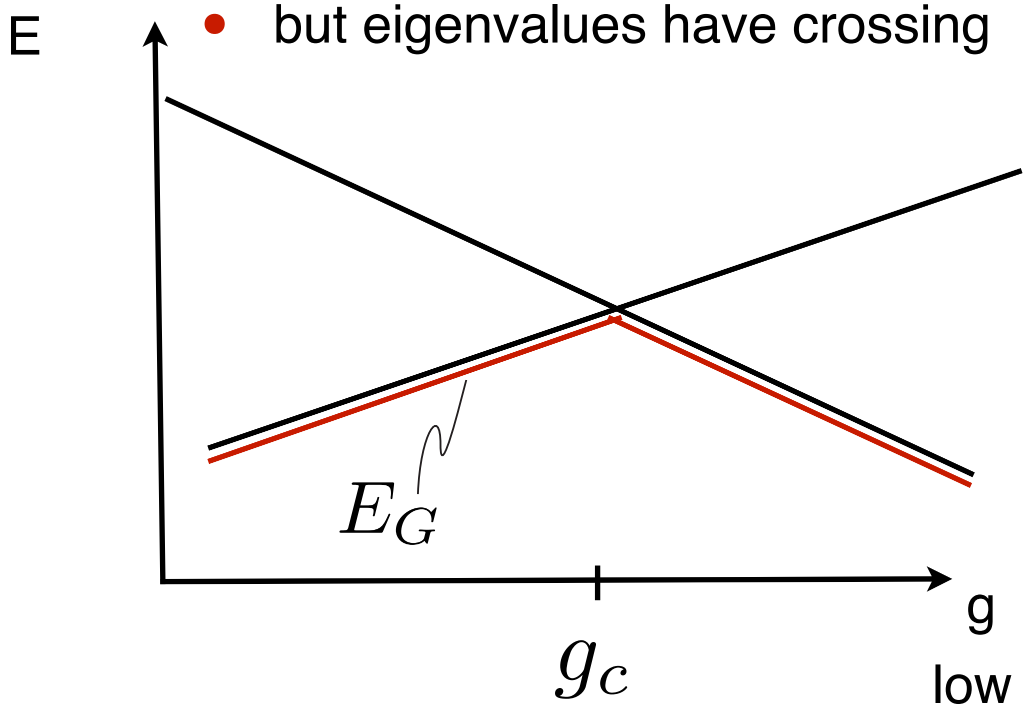
What is a quantum phase transition?

- Consider a Hamiltonian of the form:

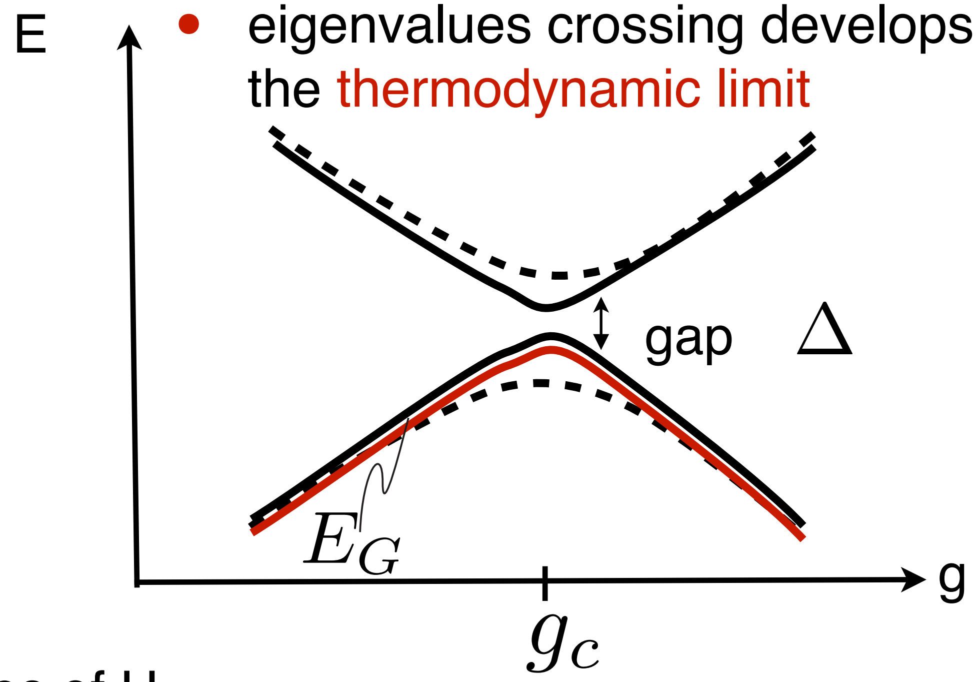
$$H = H_1 + gH_2$$

dimensionless parameter

- Study the ground state behavior of the energy $E(g) = \langle \mathrm{G}|H|G\rangle$
- Quantum phase transition: Nonanalytic dependence of the ground state energy on coupling parameter g
- Two possibilities:
    - parts commute, $[H_1, H_2] = 0$
    - but eigenvalues have crossing
    - parts do not commute, $[H_1, H_2] \neq 0$
    - eigenvalues crossing develops in the thermodynamic limit



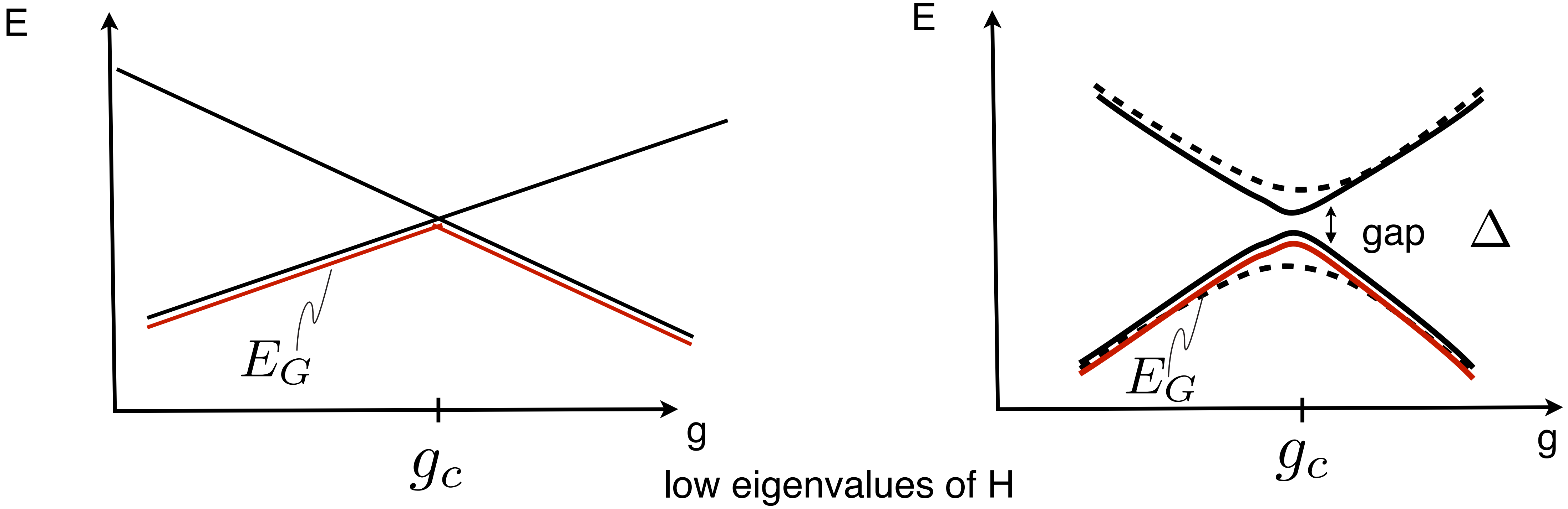
low eigenvalues of H



Literature: Subir Sachdev, Quantum Phase Transitions, Cambridge University Press (1999)

What is a quantum phase transition?

$$H = H_1 + gH_2$$



low eigenvalues of H

- The second possibility is more common and closer to the situation in conventional classical phase transitions in the thermodynamic limit
- The first possibility often occurs only in conjunction with the second (ex: Bose-Hubbard phase diagram)
- The phase transition is usually accompanied by qualitative change in the correlations in the ground state

What is a quantum phase transition?

- We concentrate on second order transitions (as those above)
- characteristic features:
  - vanishing of the energy scale separating ground from excited states (gap) at the transition point
  - universal scaling close to criticality,

critical exponent

$$\Delta \sim J|g - g_c|^{\nu z_d}$$

typical microscopic energy scale (in H)

  - diverging length scale describing the decay of spatial correlations at the transition point

$$\xi^{-1} \sim \Lambda|g - g_c|^{\nu}$$

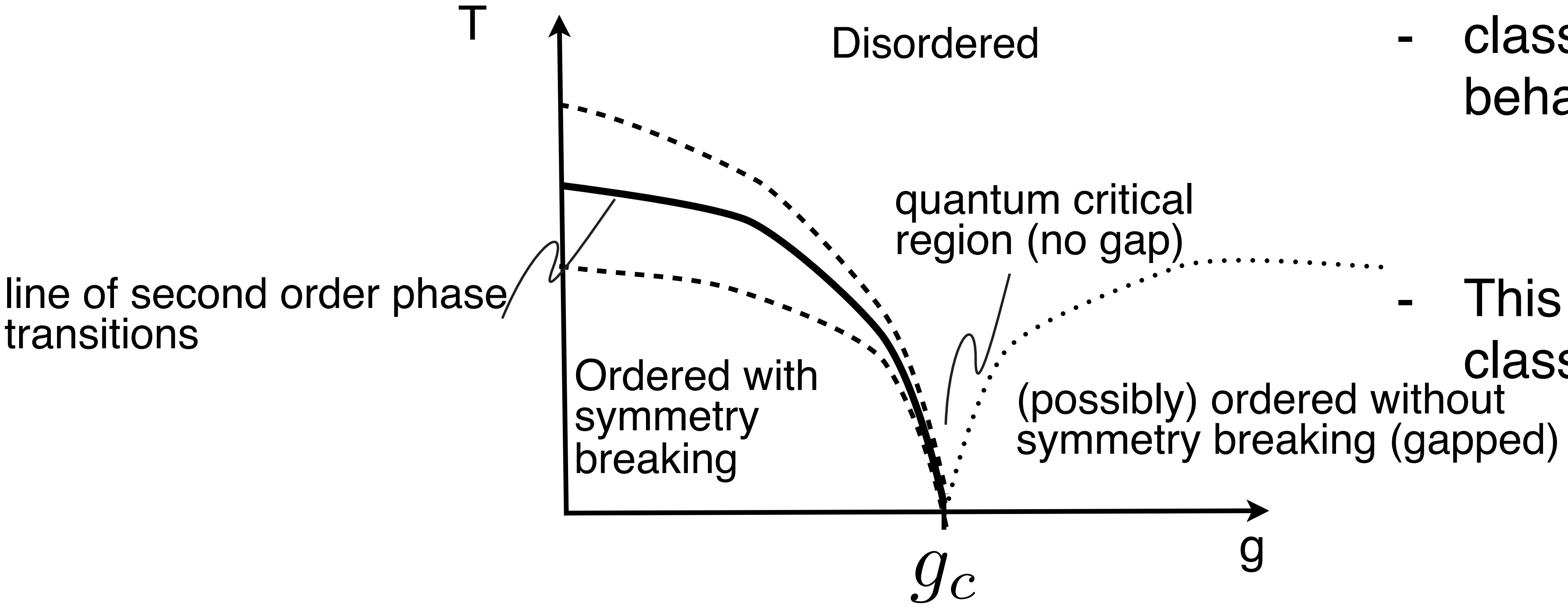
typical microscopic length scale (e.g. lattice spacing)

  - the ratio defines the dynamic critical exponent,

$$\Delta \sim \xi^{-z_d}$$

Quantum vs. Classical Phase Transition

- A quantum phase transition strictly occurs only at zero temperature T=0
- Temperature always sets a minimal energy scale, preventing scaling of Δ
- Generic quantum phase diagram:



- classical description of critical behavior applies if

$$\hbar\omega_{typ} \ll k_B T$$

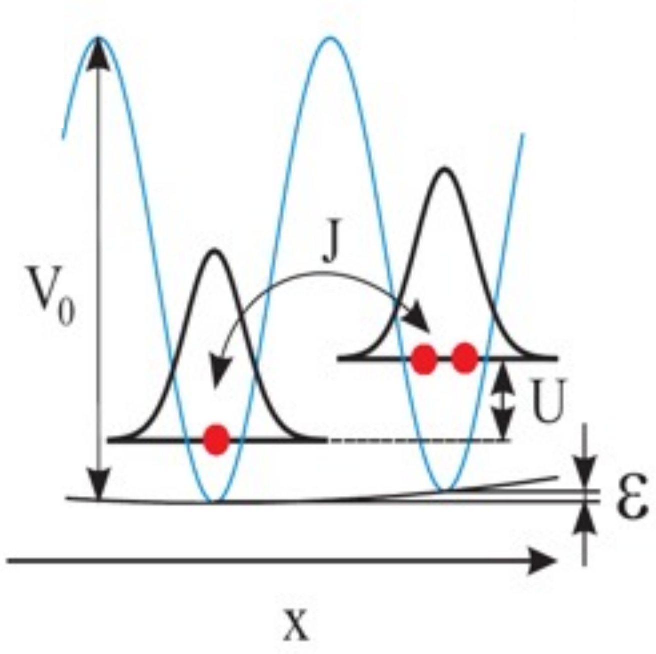
- This is always violated at low enough T: classical-quantum crossover

- Phase transitions in classical models are driven by statistical (thermal) fluctuations. They freeze to fluctuationless ground state at T=0
- Quantum models have fluctuations driven by Heisenberg uncertainty principle

➡ Quantum critical region features interplay of quantum (temporal) and statistical (spatial) fluctuations

Microscopic Physics of the Bose Hubbard Model

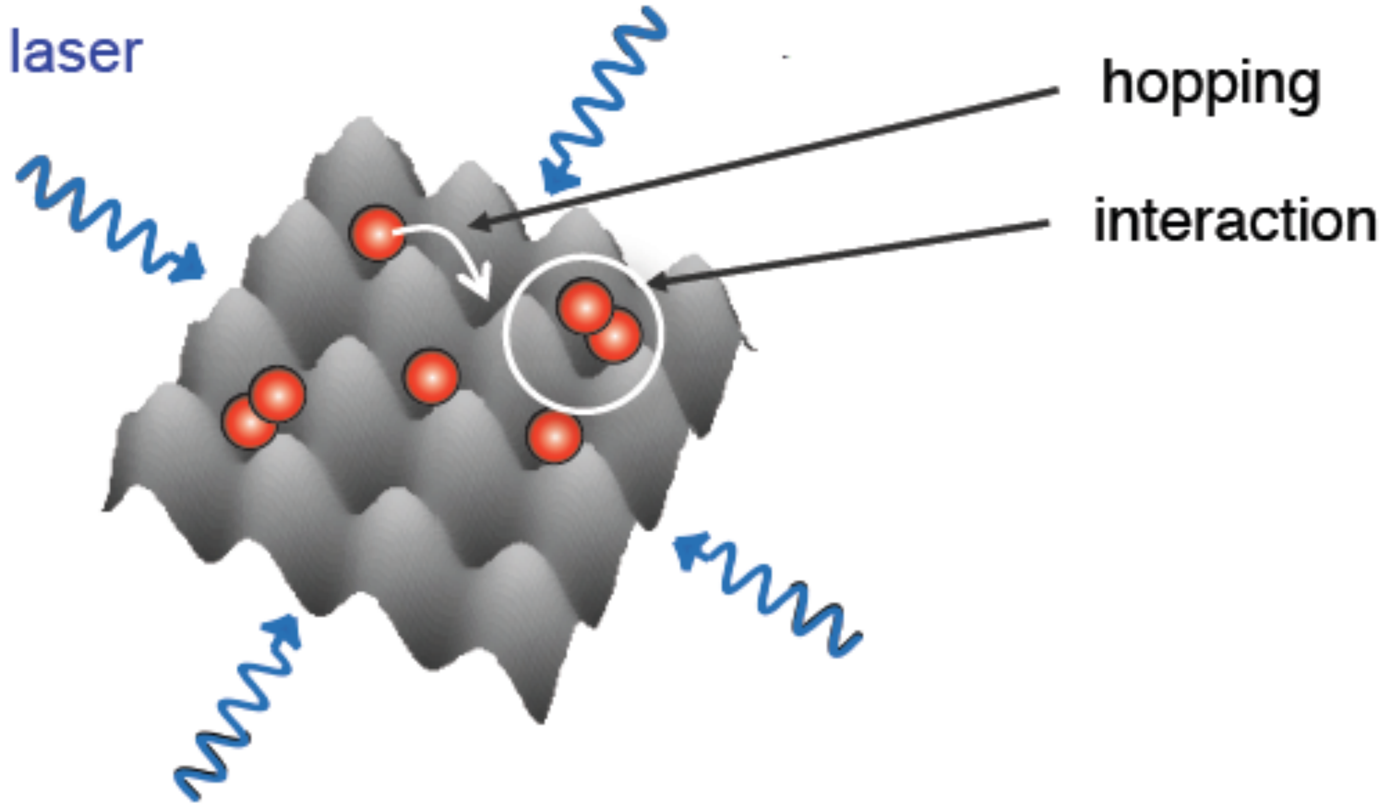
(see appendix for more details)



Bosons in the Optical Lattice

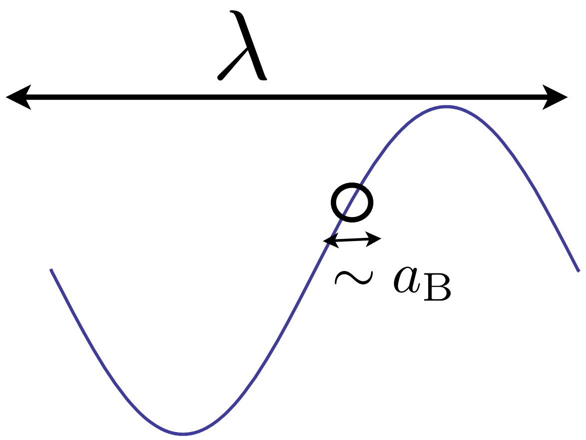
System: We consider N bosonic particles moving on a lattice ("lattice gas") consisting of M lattice sites. The essential ingredients of the dynamics are

- hopping of the bosonic particles between lattice sites (kinetic energy)
- repulsive / attractive interaction between the particles (interaction energy)
- Bose statistics



cold atoms in an optical lattice (see below)

Atoms in Optical Lattices



extent of atom much smaller than laser wavelength

$$a_{\mathrm{B}} \ll \lambda$$

- AC-Stark shift
  - Consider an atom in its electronic ground state exposed to laser light at fixed position $\vec{x}$.
  - The light be far detuned from excited state resonances: ground state experiences a second-oder *AC-Stark shift*

$$\delta E_g = \alpha(\omega) I$$

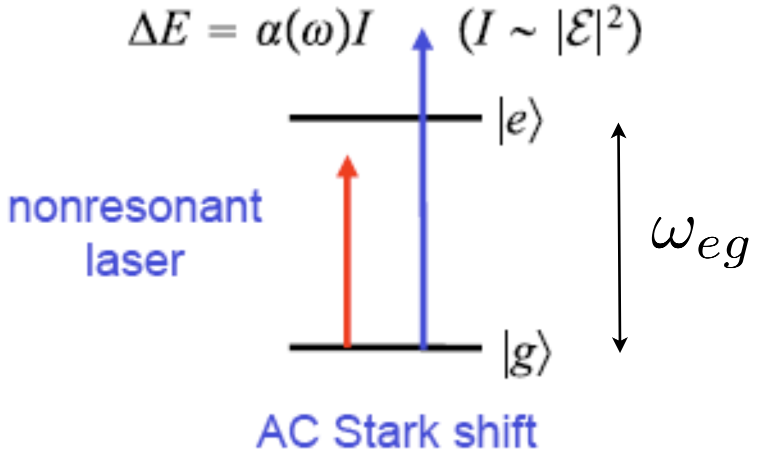
  with $\alpha(\omega)$ - dynamic polarizability of the atom for laser frequency ω, $I \propto \vec{E}^2$ - light intensity.
  - Example: two-level atom $\{|g\rangle, |e\rangle\}$.

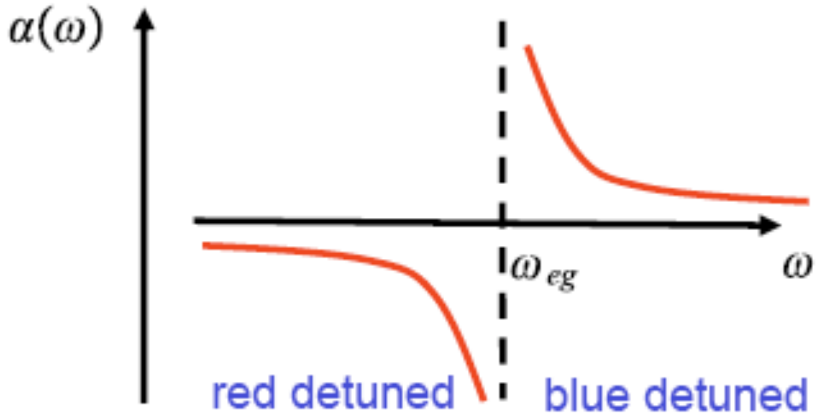
Rabi frequency

$$\delta E_g = \hbar \frac{\Omega^2}{4\Delta}$$

detuning from resonance $\Delta = \omega - \omega_{eg}$

$$\Omega \ll \Delta$$

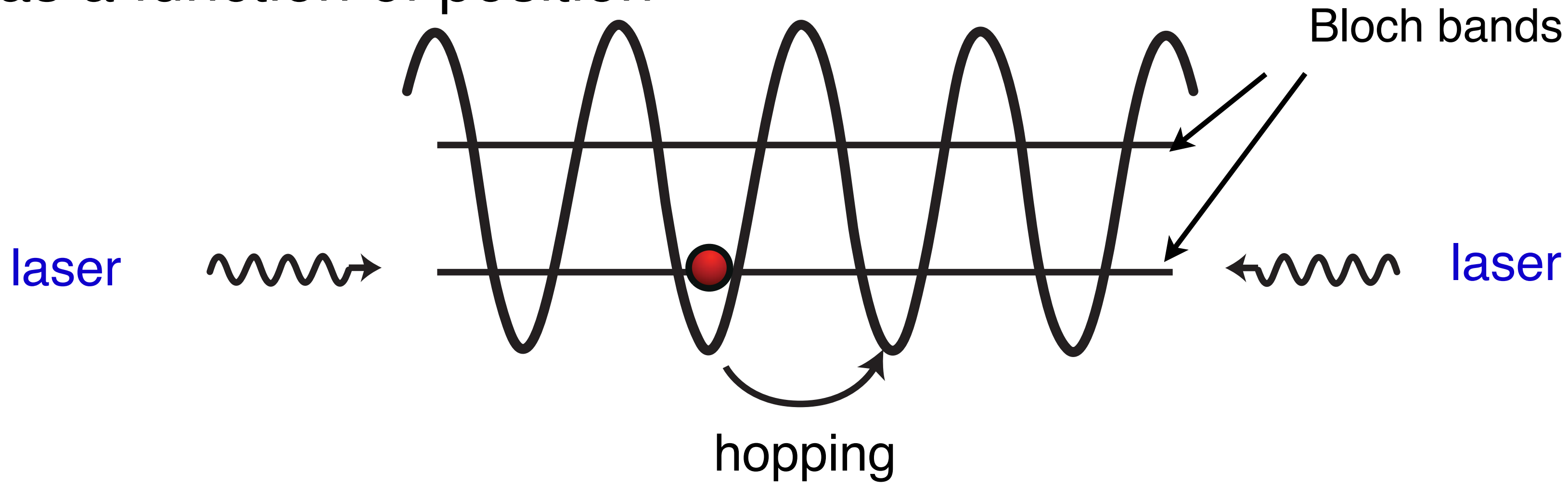




$\Delta < 0,\ \delta E_g < 0$ $\Delta > 0,\ \delta E_g > 0$

Atoms in Optical Lattices

- standing wave laser configuration: $\vec{E}(\vec{x},t) = \vec{e}\mathcal{E}\sin kx\, e^{-i\omega t} + \text{h.c.}$
- AC Starkshift as a function of position



- The AC Starkshift appears as a conservative potential for the center-of-mass motion of the atom

$$i\hbar\frac{\partial\psi(\vec{x},t)}{\partial t} = \left(-\frac{\hbar^2}{2m}\nabla^2 + V_{\text{opt}}(\vec{x})\right)\psi(\vec{x},t) \qquad (V_{\text{opt}}(\vec{x}) \equiv \delta E_g(\vec{x}) = \hbar\frac{\Omega^2(\vec{x})}{4\Delta})$$

where the *position dependent AC-Stark* shift appears as a (conservative) “optical potential”

$$V_{\text{opt}}(x) = V_0 \sin^2 kx \qquad (k = 2\pi/\lambda)$$

for the center-of-mass motion of the atom.

- The potential is periodic with lattice period $\lambda/2$, and thus supports a band structure (Bloch bands). The depth of the potential is proportional to the laser intensity

Boson Gas in Periodic Optical Potentials

- Starting point: workhorse Hamiltonian for weakly interacting ultracold bosons

$$H = \int_{\mathbf{x}} [\hat{\psi}^\dagger_{\mathbf{x}} (- \frac{\triangle}{2m} + \boxed{V(\mathbf{x})})\hat{\psi}_{\mathbf{x}} + g(\hat{\psi}^\dagger_{\mathbf{x}}\hat{\psi}_{\mathbf{x}})^2]$$

- see above: trapping potential can be treated classically due to scale separation
- instead, now we are interested in a periodic potential of wavelength comparable to the typical interparticle distance: light in with optical wavelength, as

$$\lambda \sim 500\mathrm{nm} = 5 \cdot 10^{-5}\mathrm{cm}$$

typical wavelength of light

$$d \lesssim 10^{-4}\mathrm{cm} \quad (n \gtrsim 10^{12}\mathrm{cm}^{-3})$$

typical interparticle separation

- create such conservative potential by weakly coupling the atoms in their ground state $(\leftrightarrow \hat{\psi}_{\mathbf{x}})$ to auxiliary internal level by above means: position dependent second order AC Stark shift

Rabi coupling to aux. level

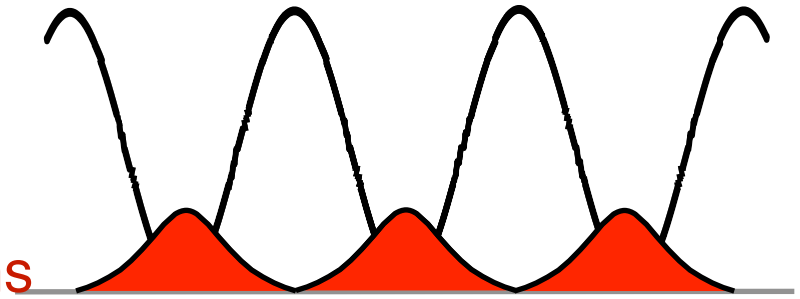
$$V(\mathbf{x}) = \hbar \frac{\Omega^2(\mathbf{x})}{4\Delta} \equiv V_0 \sum_i \sin^2(k_i x_i), \quad k_i = 2\pi/\lambda_i$$

laser detuning from aux. level

- atomic fermions can be treated analogously: Fermi Hubbard model

Bose Hubbard Hamiltonian (Jaksch et al. ’98)

spatially localized
Wannier functions

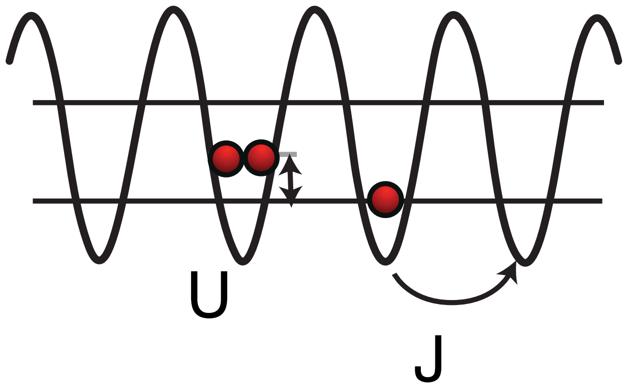


- For dominant optical potential $V_0 \gg$(other scales), we expect localized single particle wavefunctions to provide a useful description of the system.

- A suitable complete set of basis functions are the Wannier functions

- We expand the field operators in Wannier functions of the lowest band

$$\hat{\psi}(\vec{x}) = \sum_i w(\vec{x}-\vec{x}_i) b_i$$



to obtain the Bose Hubbard model

$$\boxed{\hat{H} \quad = \quad -\sum_{ij} J_{ij} b_i^\dagger b_j + \tfrac{1}{2}U \sum_i b_i^{\dagger 2} b_i^2}$$

with hopping $J_{ij} = \int d^3x w(\vec{x}-\vec{x}_i)\left[-\frac{\hbar^2}{2m}\nabla^2 + V_0(\vec{x})\right] w(\vec{x}-\vec{x}_j)$ and interaction $U = \frac{1}{2}g\int d^3x\, |w(\vec{x})|^4$ valid for $J, U, k_B T \ll \hbar\omega_{\text{Bloch}}$. (tight binding lowest band approximation)

---

additionally, we are bound to interactions (scattering lengths)

extent of Wannier function

$$g \ll a_0, a$$

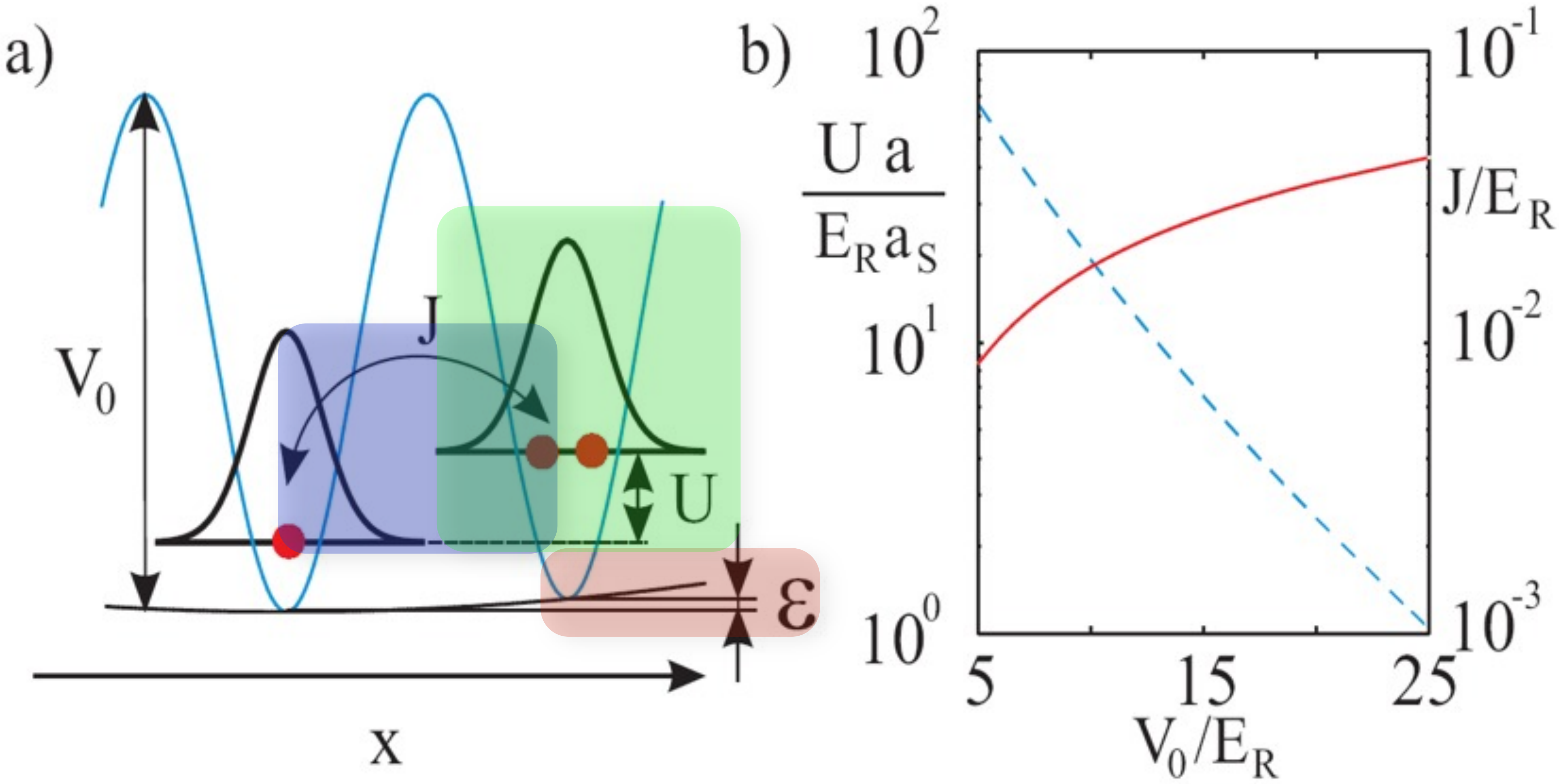
here, it means lattice spacing

This is not true close to Feshbach resonances!

Bose Hubbard Parameters

Parameters as function of laser intensity

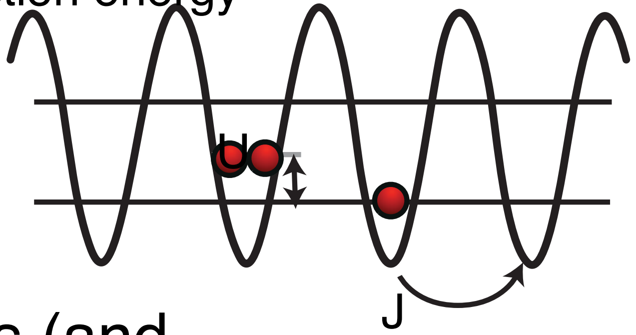
$$H = -J\sum_{\langle i,j\rangle} b_i^\dagger b_j + \sum_i \epsilon_i \hat{n}_i + \frac{1}{2}U\sum_i \hat{n}_i(\hat{n}_i - 1)$$



- J/U mainly controlled by extraction of kinetic energy via deepening the lattice

Summary: Bose-Hubbard Model

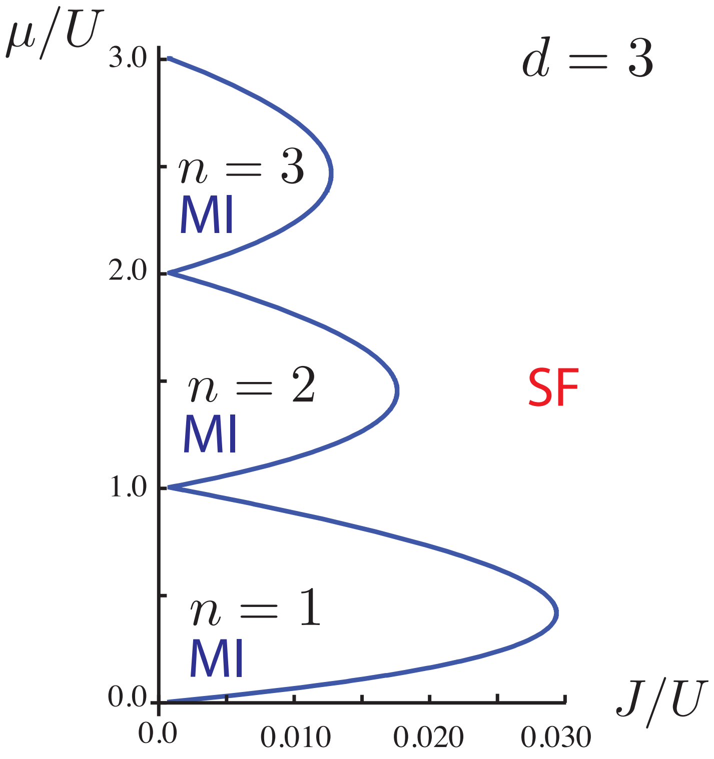
$$H = \underbrace{-J \sum_{\langle i,j \rangle} b_i^\dagger b_j}_{\text{kinetic energy}} - \mu \sum_i \hat{n}_i + \underbrace{\sum_i \epsilon_i \hat{n}_i}_{\text{trapping potential}} + \underbrace{\tfrac{1}{2} U \sum_i \hat{n}_i (\hat{n}_i - 1)}_{\text{interaction energy}}$$



- Achieved via coherent manipulation of ultracold atoms.
- Ratio of kinetic and interaction energy tunable via lattice parameters (and Feshbach resonances). In particular, reach interaction dominated regime.
- Possible to penetrate high density regime $\langle \hat{n}_i \rangle = \mathcal{O}(1)$. Not possible in the continuum.
- The Bose-Hubbard model is an exemplary model for strongly correlated bosons. It is not realized in condensed matter.

- Remark: strong interactions and high density not in contradiction to earlier scale considerations:
  - strong interactions: $J/U \ll 1$ mainly from reduction of kinetic energy via lattice depth.
  - High density due to strong localization of onsite wave function.
  - For validity of lowest band approximation, it is however important that $a \ll \lambda$

Phase Diagram
of the
Bose Hubbard Model



Kinetic vs. Interaction Domination - Limiting Cases

- Goal: Find the ground state (gs) phase diagram for Bose-Hubbard model (T=0)
- Strategy: (i) analyze limiting cases, (ii) find interpolation scheme
- Restrict to the homogeneous system $\epsilon_i = 0$

- Interaction dominated regime: set J = 0

$$H = -\mu \sum_i \hat{n}_i + \tfrac{1}{2} U \sum_i \hat{n}_i (\hat{n}_i - 1) = \sum_i h_i$$

number eigenstates n=1

- Purely local Hamiltonian: gs many-body wavefunction takes product form

$$|\psi\rangle = \prod_i |\psi\rangle_i$$

$$\hat{n}_i |n\rangle_i = n |n\rangle_i$$

➡ Remains to analyze onsite problem only.

- Only onsite density operators occur, with (real space) occupation number eigenstates

➡ Onsite Hamiltonian also diagonal in this basis: Thus, minimize onsite energy and find the optimal n for given mu:

$$\begin{array}{ll} \text{for } \mu/U < 0 & n = 0 \\ \text{for } 0 < \mu/U < 1 & n = 1| \\ \text{for } 1 < \mu/U < 2 & n = 2 \end{array}$$

and so on

particle number quantization: for ranges of the chemical potential (particle reservoir), the system draws an integer number out or it: "Mott states"

Kinetic vs. Interaction Domination - Limiting Cases

- Kinetically dominated regime: set U=0

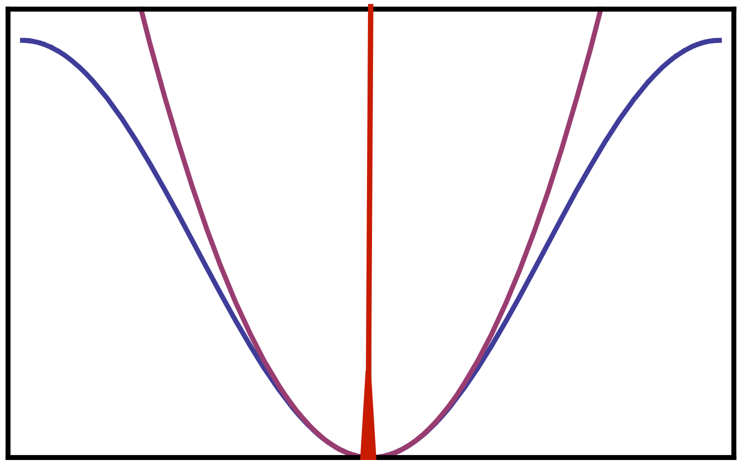
$$H = -J \sum_{\langle i,j \rangle} b_i^\dagger b_j - \mu \sum_i \hat{n}_i$$

  - Free bosons at T=0: Bose Einstein condensation!
  - See that: Diagonalize with Fourier transformation

$$H = \sum_{\mathbf{q}} (\epsilon_{\mathbf{q}} - \mu) b_{\mathbf{q}}^\dagger b_{\mathbf{q}}$$

lattice direction

lattice dispersion $\epsilon_{\mathbf{q}} = -2J \sum_\lambda \cos \mathbf{q}\mathbf{e}_\lambda$



momentum eigenstate q=0

- Ground state wave function: fixed particle number N (M - no. of lattice sites)

$$b_{\mathbf{q}=0}^{\dagger\, N} |vac\rangle = (M^{-1/2} \sum_i b_i^\dagger)^N |vac\rangle$$

  - product state in momentum space, not in position space

- Work in grand canonical ensemble: coherent state with av. density $\langle \hat{n}_i \rangle = N/M$

$$e^{N^{1/2} b_{\mathbf{q}=0}^\dagger} |vac\rangle = e^{(N/M)^{1/2} \sum_i b_i^\dagger} |vac\rangle = \prod_i \left(e^{((N/M)^{1/2} b_i^\dagger)} |vac\rangle_i \right)$$

ensures av. particle no.

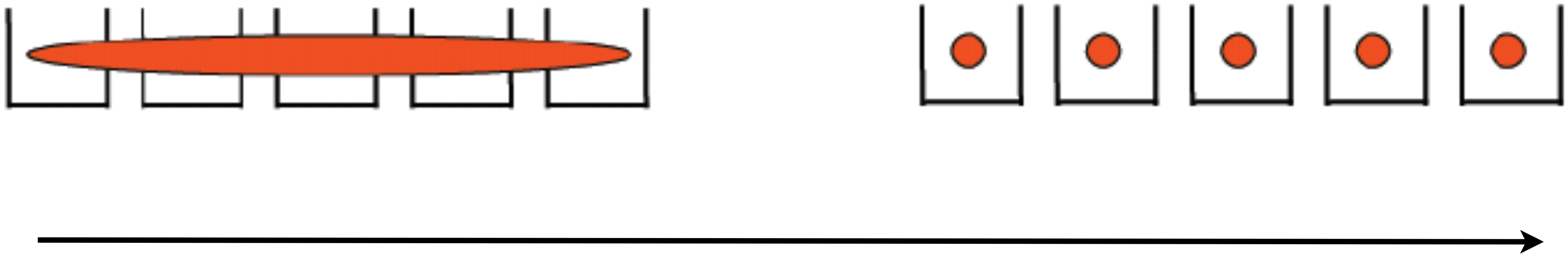
➡ grand canonical ground state can be written as a product of onsite coherent states

Intermediate Overview: Competition

- Hopping J favors delocalization in real space:
- Condensate (local in momentum space!)
- Fixed condensate phase: Breaking of phase rotation symmetry

$$\langle b_i \rangle \sim e^{\mathrm{i}\varphi}$$

- Interaction U favors localization in real space for integer particle numbers:
- Mott state with quantized particle no.
- no expectation value: phase symmetry intact (unbroken)



➡ Competition gives rise to a quantum phase transition as a function of

$$U/J$$

➡ Link between extremes: position space product ground states, respectively

Mean Field Theory

- Interpolation scheme encompassing the full range J/U
- Main ingredient: Based on above discussion, construct local mean field Hamiltonian

$$H^{(\mathrm{MF})} = \sum_i h_i$$

$$H = -J \sum_{\langle i,j \rangle} b_i^\dagger b_j - \mu \sum_i \hat{n}_i + \tfrac{1}{2} U \sum_i \hat{n}_i (\hat{n}_i - 1)$$

full Bose Hubbard Hamiltonian

$$h_i = -\mu \hat{n}_i + \frac{1}{2} U \hat{n}_i (\hat{n}_i - 1) - Jz(\psi^* b_i + \psi b_i^\dagger) + Jz\psi^*\psi$$

$$\hat{n}_i = b_i^\dagger b_i$$

coordination number

$z = 2d$ (cubic lattice)

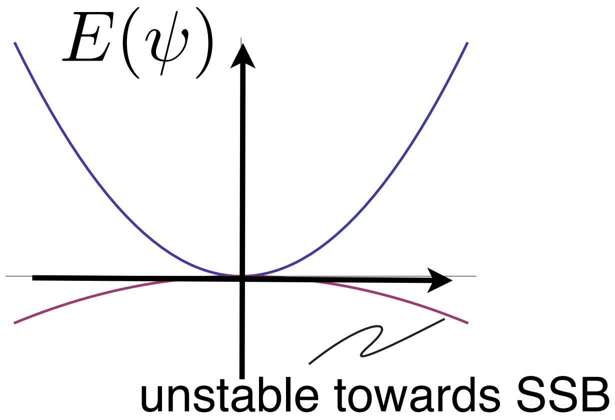
- Discussion:
  - Derivation: Decompose $b_i = \psi + \delta b_i$ neglect $\delta b_i^\dagger \delta b_j$ terms, rewrite in terms of b_i
  - The problem is reduced to an onsite problem
  - ψ is the “mean field”:
    - information on other other sites only via averages
    - if nonzero, assumes translation invariance but spontaneous phase symmetry breaking
  - Validity: approximation neglects spatial correlations via local form
    - becomes exact in infinite dimensions (Metzner and Vollhardt ’89)
    - reasonable in d=2,3 (T=0)

Phase Diagram: Derivation

- Assume second order phase transition and follow Landau procedure:
  - Study ground state energy

$$E(\psi) = \text{const.} + m^2|\psi|^2 + \mathcal{O}(|\psi|^4)$$

  - Determine zero crossing of mass term



- Calculate E in second order perturbation theory

$$h_i = h_i^{(0)} + \psi V_i$$

smallness parameter close to phase transition

$$h_i^{(0)} = -\mu \hat{n}_i + \tfrac{1}{2} U \hat{n}_i(\hat{n}_i - 1) + Jz\psi^*\psi$$

$$V_i = Jz(b_i + b_i^\dagger)$$

Phase Diagram: Derivation

- Zero order Hamiltonian $h_i^{(0)}$: diagonal in Fock basis $\{|n\rangle\}, n = 0, 1, 2, ...$
- The eigenvalues are $E_n^{(0)} = -\mu n + \frac{1}{2}Un(n-1) + Jz\psi^2$
- The ground state energies for given μ are

$$E_{\bar{n}}^{(0)} = \begin{cases} 0 & \text{for } \mu < 0 \\ -\mu\bar{n} + \frac{1}{2}U\bar{n}(\bar{n}-1) + Jz\psi^2 & \text{for } U(\bar{n}-1) < \mu < U\bar{n} \end{cases}$$

- The second order correction to the energy is

$$E_{\bar{n}}^{(2)} = \psi^2 \sum_{n\neq g} \frac{|\langle\bar{n}|V_i|n\rangle|^2}{E_{\bar{n}}^{(0)} - E_n^{(0)}} = (Jz\psi)^2 \left(\frac{\bar{n}}{U(\bar{n}-1)-\mu} + \frac{\bar{n}+1}{\mu - U\bar{n}} \right)$$

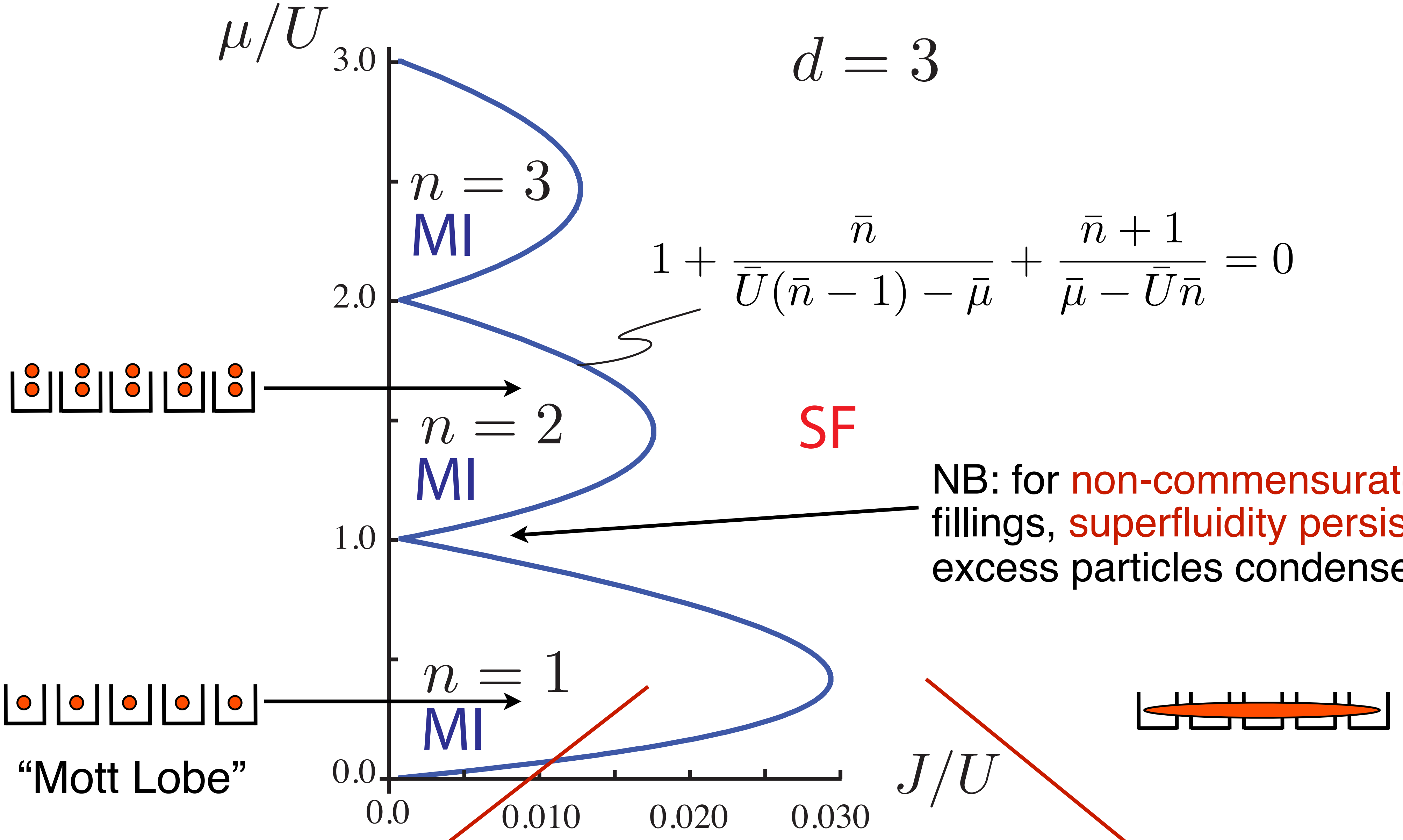
- For $E =$ const. $+ m^2\psi^2 +$ ... the phase transition happens at ($\bar{\mu} = \mu/Jz, \bar{U} = U/Jz$)

$$\frac{m^2}{Jz} = \boxed{1 + \frac{\bar{n}}{\bar{U}(\bar{n}-1)-\bar{\mu}} + \frac{\bar{n}+1}{\bar{\mu} - \bar{U}\bar{n}} = 0}$$

Bose-Hubbard phase border

Phase Diagram: Overall Shape

This gives the phase diagram as a function of μ/U and J/U.



$$1 + \frac{\bar{n}}{\bar{U}(\bar{n}-1) - \bar{\mu}} + \frac{\bar{n}+1}{\bar{\mu} - \bar{U}\bar{n}} = 0$$

NB: for non-commensurate (= integer) fillings, superfluidity persists for U -> 0: excess particles condense.

Simple picture:

MI: Quantization of particle number

SF: Quantization of phase

$$\text{"}[\hat{N}, \hat{\varphi}] = \mathrm{i}\text{"}$$ - conjugate variables

Limiting cases: Weak coupling, Superfluid

- Consider site dependent mean fields, $h_i = -\mu\hat{n}_i + \frac{1}{2}U\hat{n}_i(\hat{n}_i - 1) - J\sum_{\langle j|i\rangle}(\psi_j^* b_i + \psi_j b_i^\dagger) + \mathrm{const.}$
- Consider the equation of motion for the order parameter:
  - Heisenberg equation of motion for onsite Hamiltonian:

$$\partial_t\rho = -\mathrm{i}[h_i,\rho], \quad \rho = |\psi\rangle\langle\psi|, \quad |\psi\rangle = \prod_i |\psi\rangle_i$$

  - Equation of motion for the order parameter:

$$\mathrm{i}\partial_t\psi_i \equiv \mathrm{i}\partial_t \mathrm{tr}(b_i\rho) = -J\sum_{\langle j|i\rangle}\psi_i - \mu\langle\hat{b}_i\rangle + U\langle\hat{n}_i b_i\rangle$$

  - Weak coupling: assume coherent states $b_i|\psi\rangle_i = \psi_i|\psi\rangle_i \quad |\psi_i\rangle = e^{-|\psi_i|^2/2}\sum_{n=0}^{\infty}\frac{\psi_i^n}{\sqrt{n!}}|n\rangle$

$$\mathrm{i}\partial_t\psi_i = -J\sum_{\langle j|i\rangle}\psi_i - \mu\psi_i^*\psi_i + U\psi_i^*\psi_i^2 = -J\triangle\psi_i - \mu' \quad \psi_i + U\psi_i^*\psi_i^2$$

$$\triangle f_i = \sum_{\langle j|i\rangle} f_j - zf_i$$ lattice Laplacian

$$\mu' = \mu + Jz$$

shift: defines zero of kinetic energy

➡ At weak coupling, the (lattice) Gross-Pitaevski equation is reproduced

➡ certain spatial fluctuations are included: scattering off the condensate

➡ dispersion:

$$\omega_{\mathbf{q}} = \sqrt{\epsilon_{\mathbf{q}}(2U\psi^*\psi + \epsilon_{\mathbf{q}})} \qquad \epsilon_{\mathbf{q}} = 2J\sum_\lambda(1 - \cos aq_\lambda)$$

Limiting cases: Strong coupling, Mott Insulator

- Mean field Mott state : $|\bar{n}\rangle = \prod_i |\bar{n}_i\rangle = \bar{n}^{-M/2} \prod_i b_i^{\dagger \bar{n}} |\text{vac}\rangle$: Quantization of particle number
- Discussion:
  - Within mean field, Mott-ness follows as a consequence of purity:
    - $*$ assume mechanism that suppresses SF off-diagonal order: ρ diagonal, $1 = \mathrm{tr}\rho = \prod_i \mathrm{tr}_i \rho_i \overset{\text{hom.}}{=} (\sum p_m)^M$
    - $*$ Zero temperature: pure state, $1 = \mathrm{tr}\rho^2 = \prod_i \mathrm{tr}_i \rho_i^2 \overset{\text{hom.}}{=} (\sum p_m^2)^M$
    - $*$ only solution is $p_m = \delta_{n,\bar{n}}$
  - Quantization of particle number within MI is an exact result in the sense $\langle b_i^\dagger b_i \rangle = \bar{n}$
    - $*$ at $J = 0$, Mott state $|\bar{n}\rangle$ is (i) exact ground state, (ii) eigenstate to particle number $\hat{N} = \sum_i \hat{n}_i$, (iii) separated from other states by gap $\sim U$
    - $*$ kinetic perturbation $H_{\text{kin}} = -J \sum_{\langle i,j \rangle} b_i^\dagger b_j$
    - $*$ commutes with $\hat{N}$, $[H_{\text{kin}}, \hat{N}] = 0$

➡switching on J adiabatically, the ground state remains exact eigenstate to number operator. Assuming translation invariance gives exact result

$$\langle b_i^\dagger b_i \rangle = \bar{n}$$

- Implication: the Mott insulator is an incompressible state, $$\frac{\partial \langle \hat{N} \rangle}{\partial \mu} = 0$$

Excitation spectrum in the Mott phase

- We are looking for the single particle dispersion relation $\omega_{\mathbf{q}}$
- This is a dynamical quantity: hard to get within Hamiltonian framework above
- Path integral formulation of the Bose-Hubbard model

$$Z = \mathrm{tr} e^{-\beta \hat{H}} = \int \mathcal{D}a \exp - S_{\mathrm{BH}}[a]$$

$$S_{\mathrm{BH}}[a] = S_{\mathrm{loc}}[a] + S_{\mathrm{kin}}[a]$$

$$S_{\mathrm{loc}}[a] = \int_{-\beta/2}^{\beta/2} d\tau \sum_i \left[a_i^*(\partial_\tau - \mu)a_i + \tfrac{1}{2} U a_i^{*\,2} a_i^2\right]$$

local contribution

$$S_{\mathrm{kin}}[a] = \int_{-\beta/2}^{\beta/2} d\tau \sum_{i,j} t_{ij} a_i^* a_j$$

bi-local contribution; for nearest-neighbour hopping

$$t_{ij} = -J \sum_{\sigma\lambda} \delta_{i,j+\sigma \mathbf{e}_\lambda}$$

$$\sigma = \pm 1$$
$$\lambda = x, y, z$$

spatial directions

- Discussion:
  - Nonrelativistic action (on the lattice)
  - Note symmetry (T=0): temporally local gauge invariance $a_i \to a_i e^{\mathrm{i}\phi(\tau)}, \ \mu \to \mu + \mathrm{i}\partial_\tau \phi(\tau)$
  - so far: weak coupling problems J>>U, decoupling in the interaction U
  - now: Mott physics, i.e. strong coupling problem U>>J: decoupling in J

Decoupling in J: Hopping Expansion

$$S_{\mathrm{BH}}[a] = S_{\mathrm{loc}}[a] + S_{\mathrm{kin}}[a]$$

$$\sim U \qquad\qquad \sim J$$

- Goal: treat the strong coupling problem U>>J via decoupling in J

- Hubbard-Stratonovich transformation:

$$\begin{aligned} Z &= \int \mathcal{D}a \exp - S_{\mathsf{BH}}[a] = \mathcal{N} \int \mathcal{D}a\mathcal{D}\psi \exp - S_{\mathsf{BH}}[a] + \int d\tau \textstyle\sum_{ij} t_{ij}(\psi_i^* - a_i^*)(\psi_j - a_j) \\ &= \mathcal{N} \int \mathcal{D}a\mathcal{D}\psi \exp - S_{\mathsf{loc}}[a] + \int d\tau \textstyle\sum_{ij} t_{ij}(\psi_i^*\psi_j - \psi_i^* a_j - \psi_j a_i^*) = \mathcal{N} \int \mathcal{D}\psi \exp - S_{\mathsf{eff}}[\psi] \\ S_{\mathsf{eff}}[\psi] &= \int d\tau \textstyle\sum_{ij} t_{ij}\psi_i^*\psi_j - \log\langle \exp - \int d\tau \textstyle\sum_{ij} (\psi_i^* a_j + \psi_j a_i^* \rangle_{S_{\mathsf{loc}}} \\ \langle \mathcal{O} \rangle_{S_{loc}} &= \int \mathcal{D}a\mathcal{O} \exp - S_{\mathsf{loc}}[a] \end{aligned}$$

- Discussion
  - Form of intermediate action identical to mean field decoupling above (for site dependent mean fields)
  - The effective action $S_{\mathsf{eff}}[\psi]$ can now be calculated perturbatively

Decoupling in J: Hopping Expansion

- expansion in powers of the hopping

$$\langle \exp - \int d\tau \sum_{ij} t_{ij} (\psi_i^* a_j + \psi_j a_i^*) \rangle_{S_{\text{loc}}} = 1 + \sum_{m=1}^{\infty} \langle [\int d\tau \sum_{ij} t_{ij} (\psi_i^* a_j + \psi_j a_i^*)]^{2m} \rangle_{S_{\text{loc}}}$$

$\rightarrow$ note: averages of odd powers of a_i or a_i^* vanish in the Mott state

- To lowest order, the effective action thus reads

$$S_{\text{eff}}[\psi] = \int d\tau \sum_{ij} t_{ij} \psi_i^*(\tau) \psi_j(\tau) + \int d\tau d\tau' \sum_{iji'j'} t_{ij} t_{i'j'} \psi_j^*(\tau) \psi_{j'}(\tau') \langle a_i(\tau) a_i^*(\tau') \rangle_{S_{\text{loc}}}$$

- Discussion
  - the approach is inherently perturbative: no known closed form expression for above average
  - the hopping expansion does not lead to an exact solution of the problem: $Z = \int \mathcal{D}\psi \exp - S_{\text{eff}}[\psi]$ would need to be calculated for this purpose
  - the hopping expansion is closely related to the mean field approximation (see below)

Quadratic Effective Action

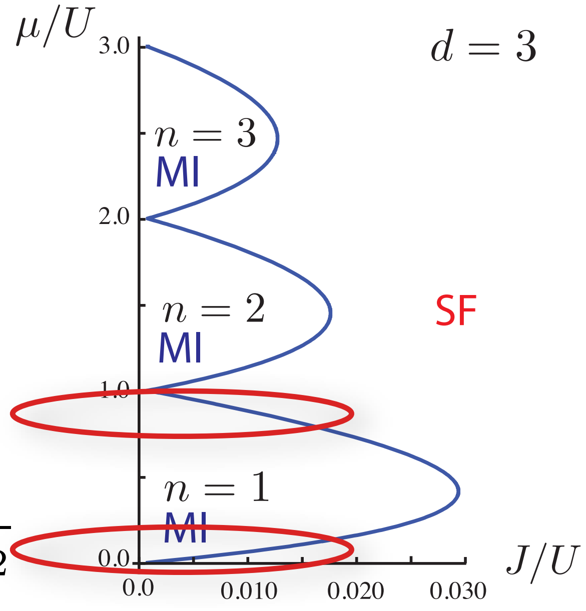
- The correlation functions $\langle a_i(\tau) a^*_{i'}(\tau') \rangle_{S_{\text{loc}}}$ can be evaluated explicitly since the local onsite problem is solved exactly
- The effective action is then, in frequency and momentum space and for nearest neighbour hopping

$$\begin{aligned} S^{(2)}_{\text{eff}}[\psi] &= \int \tfrac{d\omega}{2\pi} \tfrac{d^dq}{(2\pi)^d} \psi^*_{\mathbf{q}}(\omega) G^{-1}(\omega, \mathbf{q}) \psi_{\mathbf{q}}(\omega) \\ G^{-1}(\omega, \mathbf{q}) &= \epsilon_{\mathbf{q}} - \epsilon^2_{\mathbf{q}} \left(\tfrac{\bar{n}+1}{-\mathrm{i}\omega - \mu + \bar{n}U} + \tfrac{\bar{n}}{\mathrm{i}\omega + \mu - (\bar{n}-1)U} \right), \quad \epsilon_{\mathbf{q}} = 2J \textstyle\sum_\lambda \cos \mathbf{q}\mathbf{e}_\lambda \end{aligned}$$

- Evaluating $G^{-1}(\omega = 0, \mathbf{q} = 0)$ reproduces the above mean field result ($\epsilon_{\mathbf{q}} = Jz$): The fluctuations included here are the same, but their spatial and temporal dependence is resolved within the functional integral formulation
- The frequency dependence is dictated by the temporally local gauge invariance to $-\mathrm{i}\omega - \mu$
- The quasiparticle spectrum obtains from the poles of the Green's function analytically continued to real frequencies,

$$G^{-1}(\omega \to \mathrm{i}\omega, \mathbf{q}) \overset{!}{=} 0$$

Excitation Spectrum: Particles and Holes



- Solving $G^{-1}(\omega \to \mathrm{i}\omega, \mathbf{q}) \overset{!}{=} 0$ yields the quasiparticle dispersion

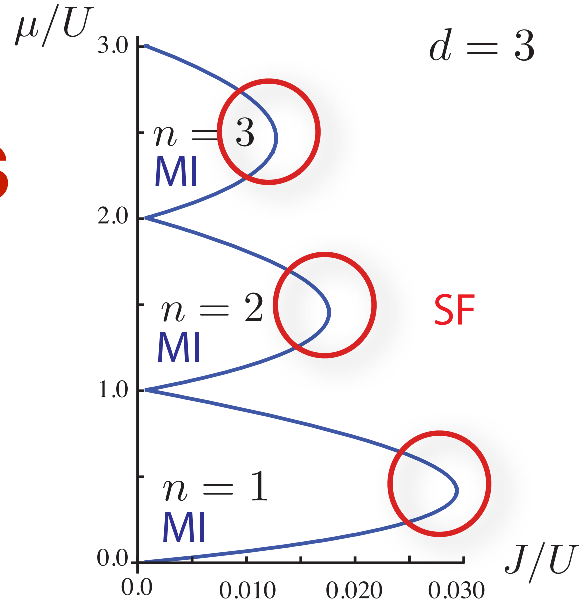
$$\omega^{\pm}_{\mathbf{q}} = -\mu + \tfrac{U}{2}(2\bar{n}-1) - \tfrac{\epsilon_{\mathbf{q}}}{2} \pm \tfrac{1}{2}\sqrt{\epsilon^2_{\mathbf{q}} - 2(2\bar{n}+1)U\epsilon_{\mathbf{q}} + U^2}$$

- For μ within the Mott phase, $\omega^{+}_{\mathbf{q}} \geq 0$ and $\omega^{-}_{\mathbf{q}} \leq 0$. They correspond to quasiparticle and quasihole excitations.
- If we are interested in the true excitation spectrum, we need to consider that the quasiholes are propagating backward in time. The true particle and hole excitation energies are therefore

$$E^{\pm}_{\mathbf{q}} = \pm\omega^{\pm}_{\mathbf{q}} = \pm\big(-\mu + \tfrac{U}{2}(2\bar{n}-1) - \tfrac{\epsilon_{\mathbf{q}}}{2}\big) + \tfrac{1}{2}\sqrt{\epsilon^2_{\mathbf{q}} - 2(2\bar{n}+1)U\epsilon_{\mathbf{q}} + U^2}$$

- Generically, both branches of the spectrum are gapped: $E^{\pm}_{\mathbf{q=0}} = \mathcal{O}(U) > 0$
- Study the phase border for $Jz \ll U$, defined with $G^{-1}(\omega = 0, \mathbf{q} = 0) \overset{!}{=} 0 \longrightarrow \mu_{\mathrm{crit}}(U)$ in the upper branch of the lobe:
  - there is a gapless particle with quadratic dispersion for $\mathbf{q} \to 0$, $E^{+}_{\mathbf{q}} \approx (1 + \frac{(\bar{n}+1)U+Jz}{\Delta})\delta\epsilon_{\mathbf{q}}$, $\delta\epsilon_{\mathbf{q}} = 2J\sum_{\lambda}(1-\cos\mathbf{q}\mathbf{e}_{\lambda}) \approx J\mathbf{q^2}$
  - there is a gapped hole with gap $\Delta = E_{\mathbf{q=0}} = \sqrt{Jz^2 - 2(2\bar{n}+1)UJz + U^2}$
- For the lower branch of the lobe and $Jz \ll U$, the holes disperse $E^{-}_{\mathbf{q}} \approx J\mathbf{q^2}$ and the particles are gapped with $\Delta \approx U$

Bicritical point: Change of Universality Class



- The interpretation in terms of particle and hole excitation only holds for $Jz \ll U$
- In general, at the phase transition there is one gapless mode. Choosing it to set the zero of energy, the gap of the other mode is given by

$$\Delta = E^{+}_{\mathbf{q=0}} - E^{-}_{\mathbf{q=0}} = \sqrt{Jz^2 - 2(2\bar{n}+1)UJz + U^2}$$

- At the tip of the lobe, $U/Jz = 2\bar{n} + 1 + \sqrt{(2\bar{n}+1)^2 - 1}$ and thus $\Delta = 0$: there are two gapless modes (particle-hole symmetry)
- The excitation spectrum at this point is dominanted by the square root for $\mathbf{q} \to 0$ and reads

$$E^{\pm}_{\mathbf{q}} = \frac{1}{2}\sqrt{(2(2\bar{n}+1)U + Jz)\delta\epsilon_{\mathbf{q}}} \sim |\mathbf{q}|$$

- The spectrum changes form a nonrelativistic spectrum $E \sim \mathbf{q^2}$ (dynamic exponent $z_d = 2$) to a relativistic spectrum $E \sim |\mathbf{q}|$ (dynamic exponent $z_d = 1$)

➡At a generic point on the phase border, the system is in the z_d = 2 O(2) universality class
➡At the tip of the lobe, the system is in the z_d = 1 O(2) universality class

Bicritical point: Symmetry Argument

- We show that the change in universality class at the tip of the lobe is not an artifact of mean field theory
- The full effective action (including fluctuations) at low energies has a derivative expansion

$$\Gamma[\psi] = \int \psi^*[Z\partial_\tau + Y\partial_\tau^2 + m^2 + ...]\psi + \lambda(\psi^*\psi)^2 + ...$$

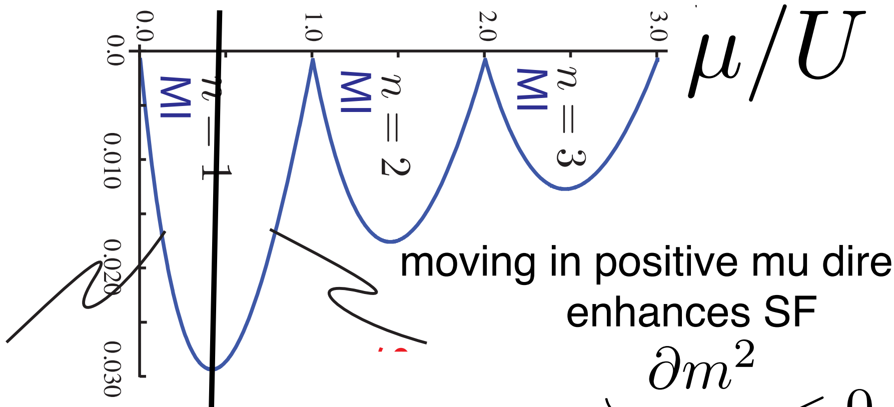
- At the phase transition, we have $m^2 = 0$. At the tip of the lobe, we have additionally(vertical tangent)

$$\frac{\partial m^2}{\partial \mu} = 0$$

- Using the invariance under temporally the local symmetry$\psi \to \psi e^{\mathrm{i}\theta(\tau)}, \mu \to \mu + \mathrm{i}\partial_\tau\theta(\tau)$, we find the Ward identity ($q = (\omega, \mathbf{q})$)

$$-\frac{\partial m^2}{\partial \mu} = -\frac{\partial}{\partial \mu}\frac{\delta^2\Gamma}{\delta\psi^*(q)\delta\psi(q)}\Big|_{\psi=0;q=0} = \frac{\partial}{\partial(\mathrm{i}\omega)}\frac{\delta^2\Gamma}{\delta\psi^*(q)\delta\psi(q)}\Big|_{\psi=0;q=0} = Z$$

- Thus, there cannot be a linear time derivative ath the tip of the lobe, $Z = 0$. The leading frequency dependence is quadratic



moving in positive mu direction suppresses SF

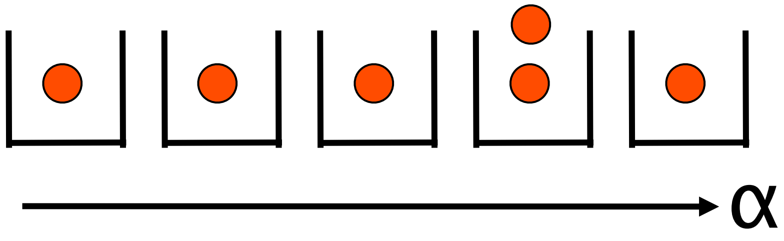
$$\to \frac{\partial m^2}{\partial \mu} > 0$$

moving in positive mu direction enhances SF

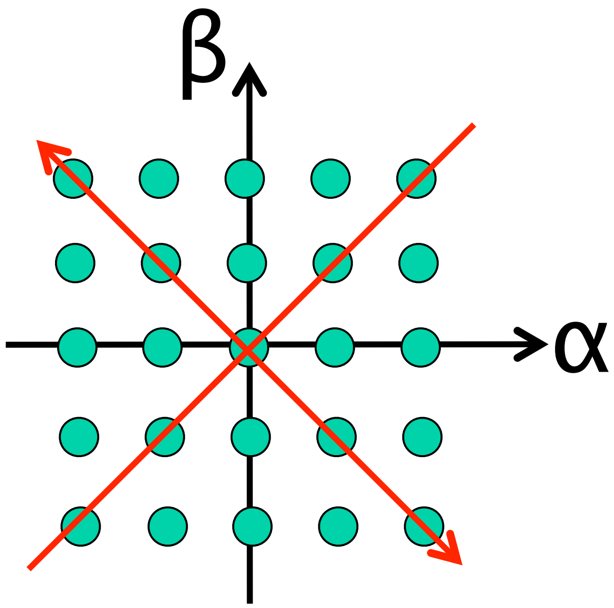
$$\to \frac{\partial m^2}{\partial \mu} < 0$$

Experimental signatures 1: Interference

- spatial correlation function $\langle b_\alpha^\dagger b_\beta \rangle$



superfluid

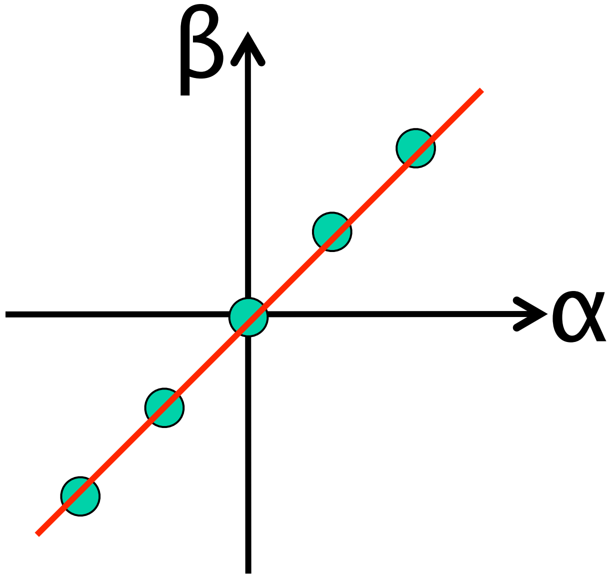


off-diagonal long range order:

interference

$$\langle b_\alpha^\dagger b_\beta \rangle \approx \psi_\alpha^* \psi_\beta$$

Mott

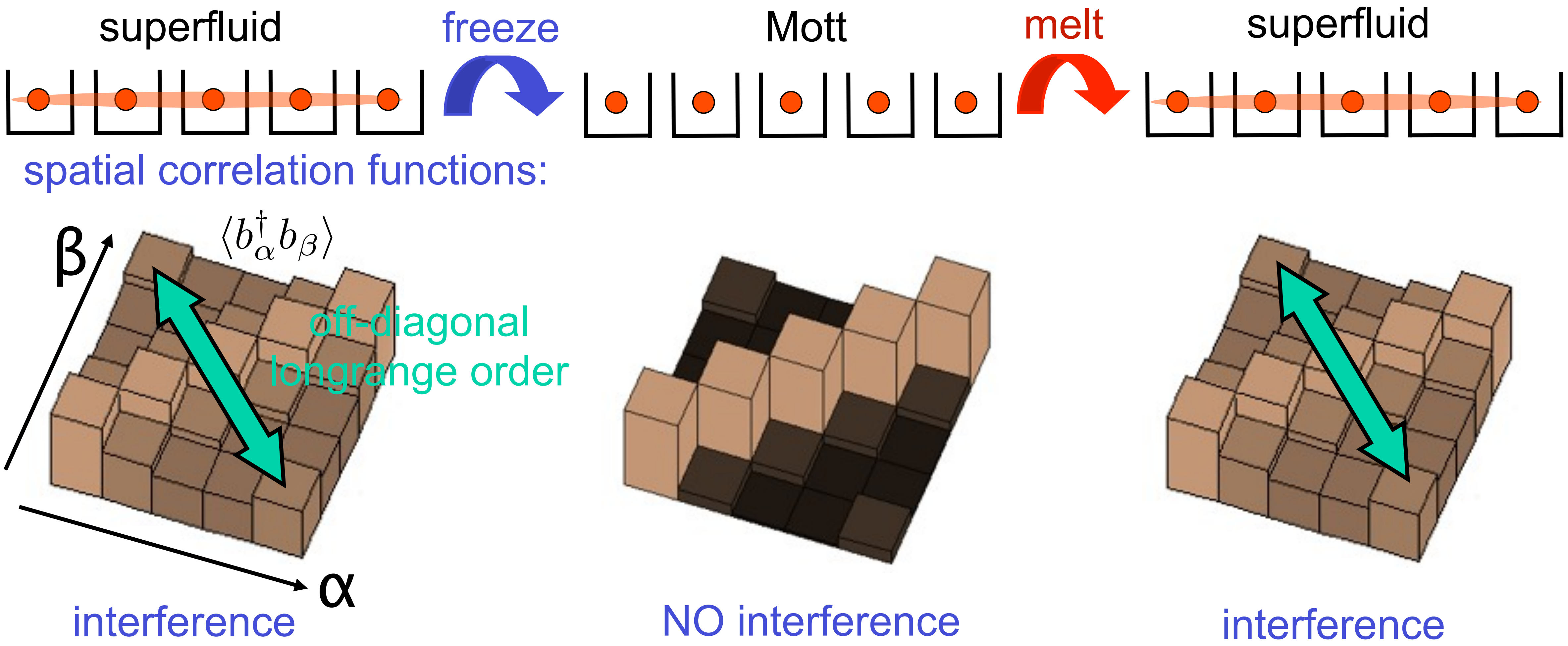


no interference

exp signature

$$\langle b_\alpha^\dagger b_\beta \rangle \approx n_\alpha \delta_{\alpha\beta}$$

Interference Patterns



superfluid freeze Mott melt superfluid

spatial correlation functions:

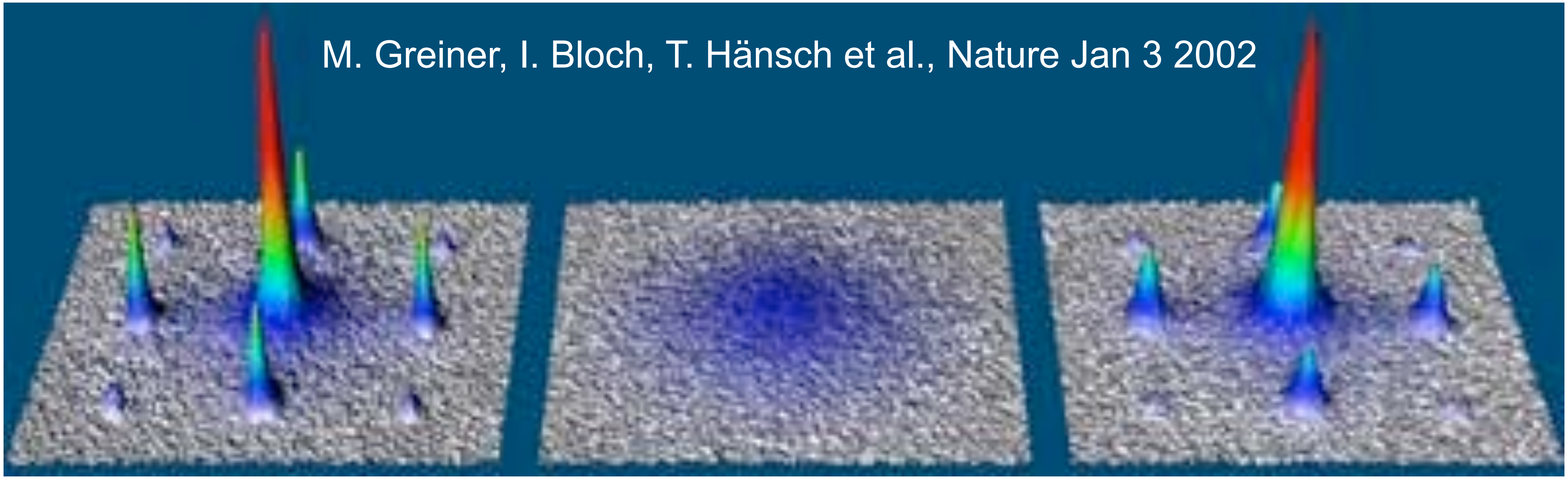
$\langle b_\alpha^\dagger b_\beta \rangle$

off-diagonal longrange order

interference

NO interference

interference

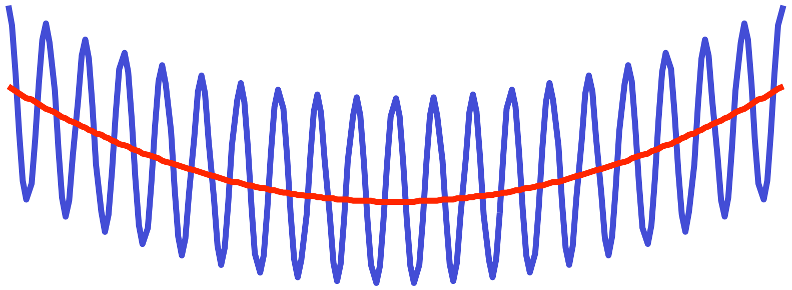


M. Greiner, I. Bloch, T. Hänsch et al., Nature Jan 3 2002

Experimental Signatures 2: Mott Gap

- The gap in the Mott phase causes staggered structure in density profile

(1)Consider situation



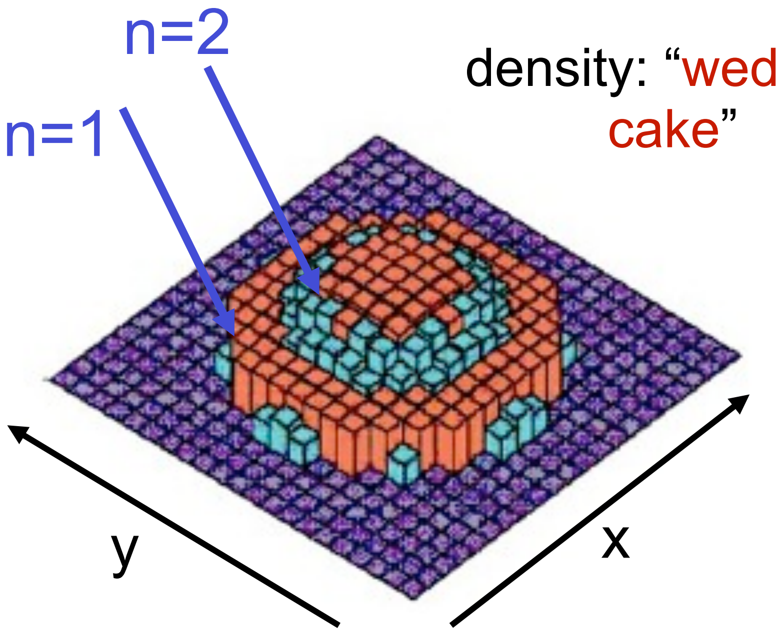
lattice + trapping energy

(2)Assume local density approximation: local applicability of mean field theory

$$\mu(x_i) = \mu - V(x_i),\ V(x_i) = \frac{k}{2}x_i^2$$

(3)The incompressibility within Mott state leads to (2d)

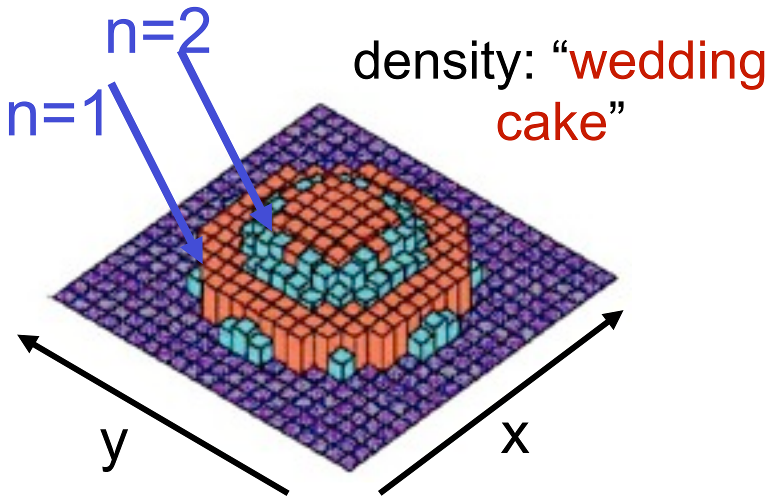
$$\frac{\partial\langle\hat{N}\rangle}{\partial\mu} = 0$$

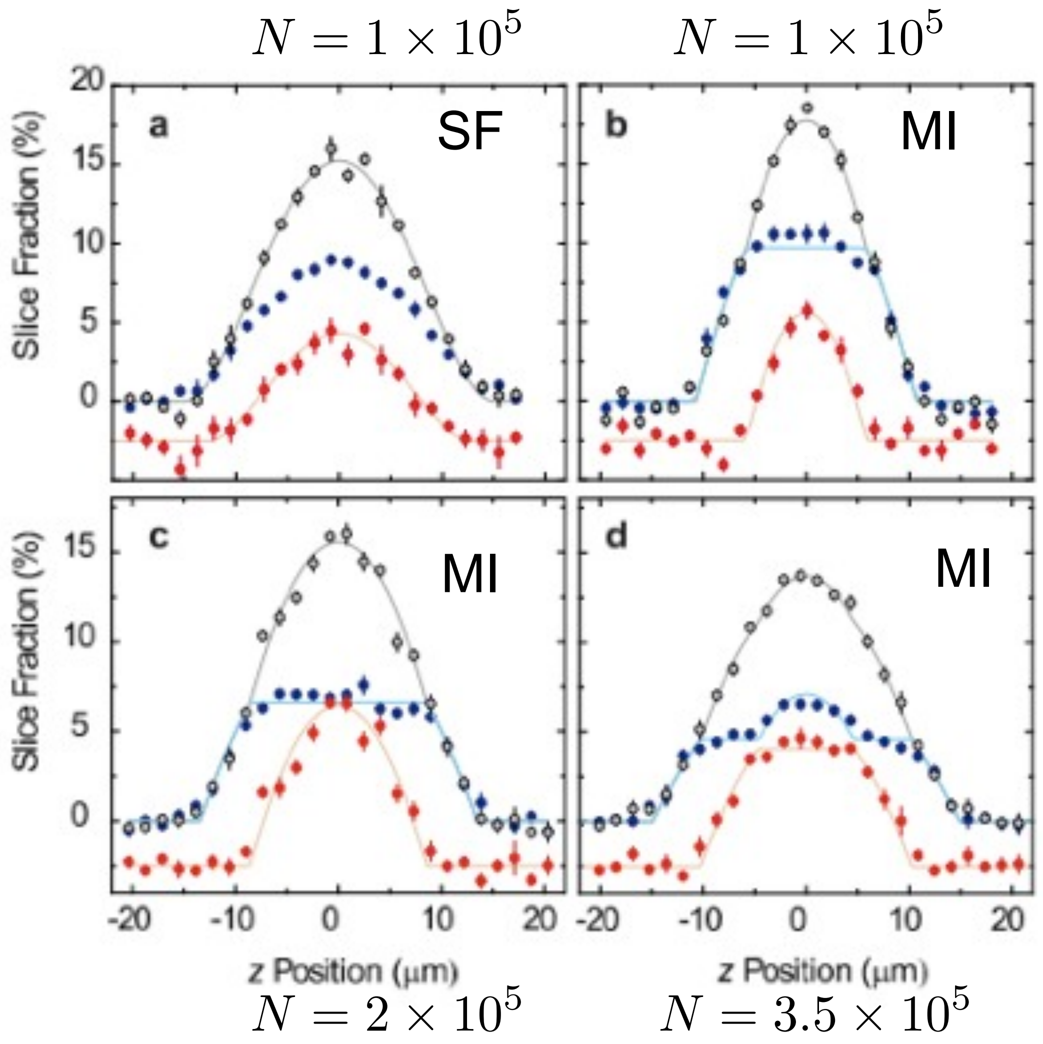


density: “wedding cake”

Experimental Signatures 2: Mott Gap

- Experiment:
  - 3D isotropic trap
  - resolve x-y-integrated density profile in z-direction
    - total density (grey)
    - singly occupied sites (red)
    - doubly occupied sites (blue)





Bloch group, 2006

- Superfluid region:
  - Thomas-Fermi quadratic shape
  - resolution of singly and doubly sites from Poissonian number statistics for SF state
- Mott insulator region
  - e.g. for spherical Mott shells of Radius R at the core of the trap, integrated profile:

$$\nu(R;z) = \text{const.} \times \max(0, R^2 - z^2)$$

  - profile for inner shell of radius R_2, n=2:

$$\nu(R_1;z)$$ -- red line

  - profile of outer shell of radius R_1, n=1

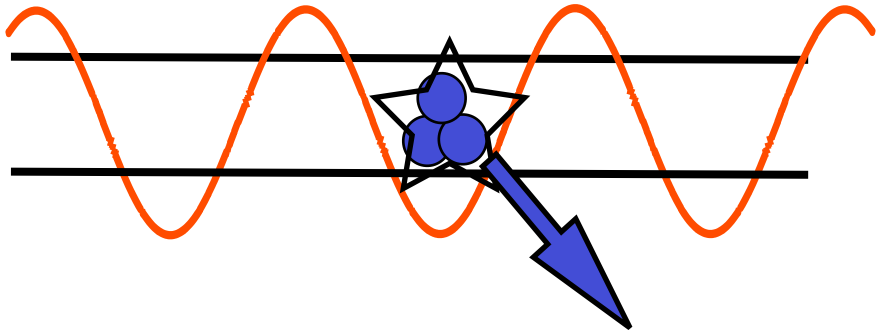
$$\nu(R_1;z) - \nu(R_2;z)$$ -- blue line

$$\int dxdy\theta(R^2-(x^2+y^2+z^2)) = 2\pi \int drr\theta((R^2-z^2)-r^2) = \pi\max(0, R^2-z^2)$$

Summary

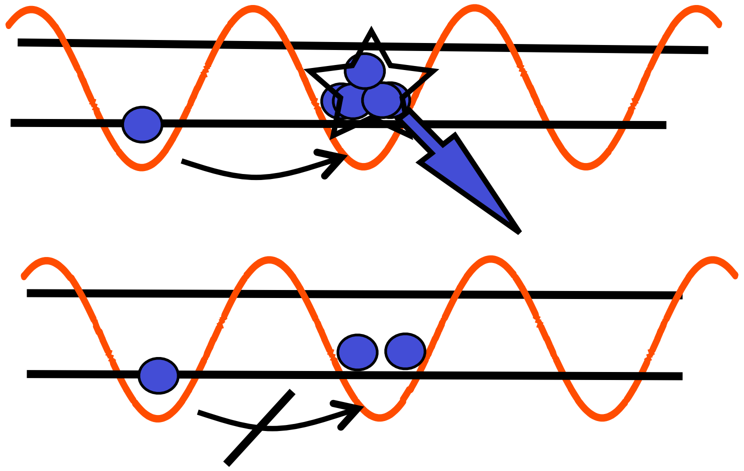
- Cold bosonic atoms loaded into optical lattices allow to implement an interacting many-body system with quantum phase transition with no counterpart in condensed matter physics
  - Optical lattices are standing wave laser configurations which couple to atoms via a position dependent AC Stark shift
  - In an accessible parameter regime the microscopic model for bosonic atoms reduces to a single band Bose-Hubbard model with parameters J (kinetic energy) and onsite interaction U
  - In such systems, it is possible to realize high densities (O(1)) and strong interactions U>J
  - The competition of kinetic and interaction energy g = J/U gives rise to a quantum phase transition for commensurate fillings n=1,2,...
  - The strong coupling "Mott phase" is an ordered phase (quantized particle number) without symmetry breaking
  - One characteristic property is incompressibility, which has been observed in experiments

Excursion:
3-Body Interactions from 3-Body Loss:
2 Applications



Outline

(1) Dissipative generation of a 3-body hardcore interaction



- Mechanism and experimental perspectives

A. J. Daley, J. Taylor, SD, M. Baranov, P. Zoller, Phys. Rev. Lett. **102**, 040402 (2009)

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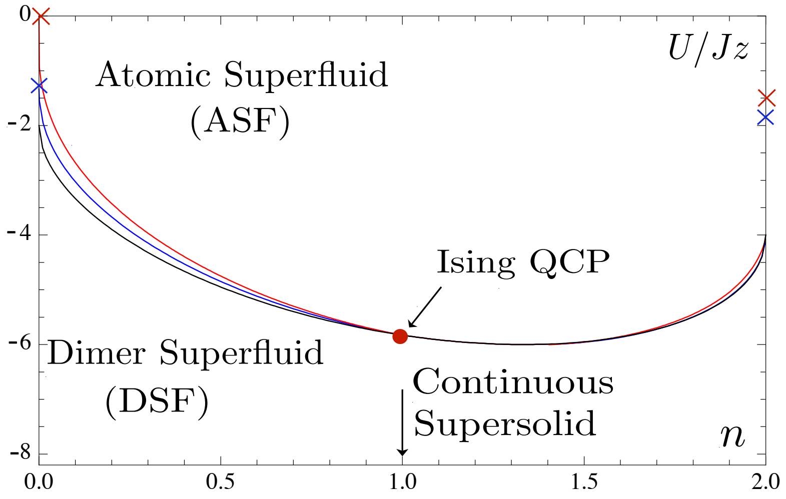
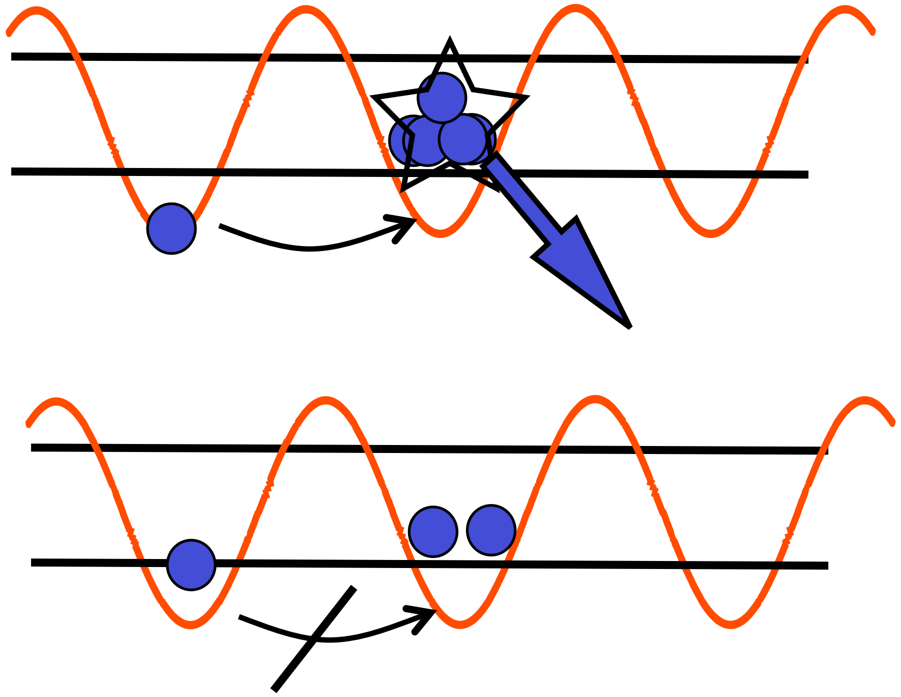
(2) Phase diagram for 3-body hardcore bosons

- Unique effects of interactions and the constraint

SD, M. Baranov, A. J. Daley, P. Zoller, Phys. Rev. Lett, **104**, 165301(2010);
SD, M. Baranov, A. J. Daley, P. Zoller , Phys. Rev. B **82**, 064509 (2010);
Phys. Rev. B **82**, 064510 (2010)



Motivation

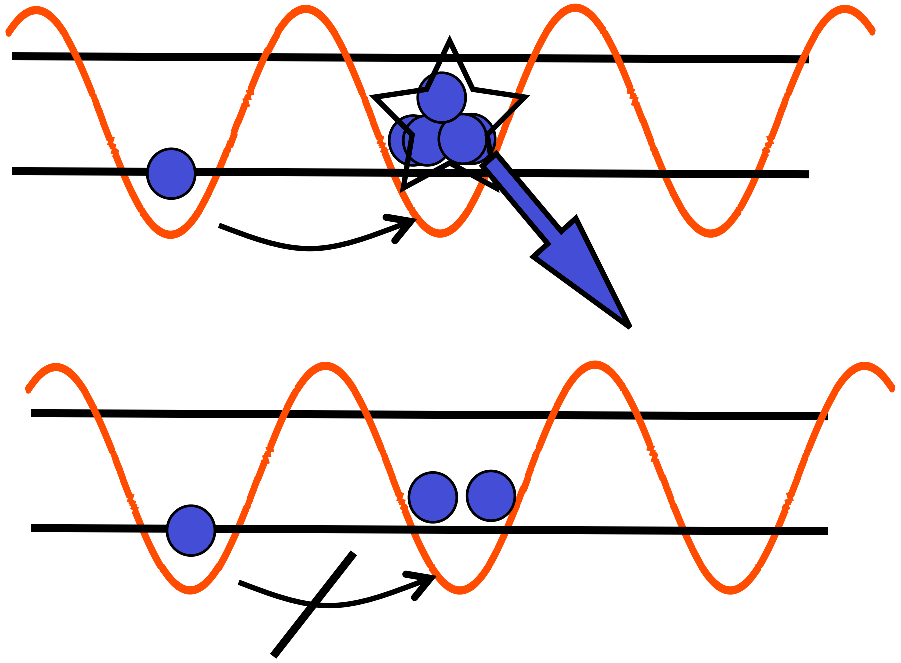


- 3-body loss processes (-)
    - ubiquitous, but typically undesirable
    - inelastic 3 atom collision
    - molecule + atom ejected from lattice
- 3-body interactions (+)
    - Stabilize bosonic system with attractive interactions
    - interesting many-body consequences
    - 3-component fermion system: stabilize atomic color superfluidity

➡ We make use of strong 3-body loss to generate a 3-body hard-core constraint

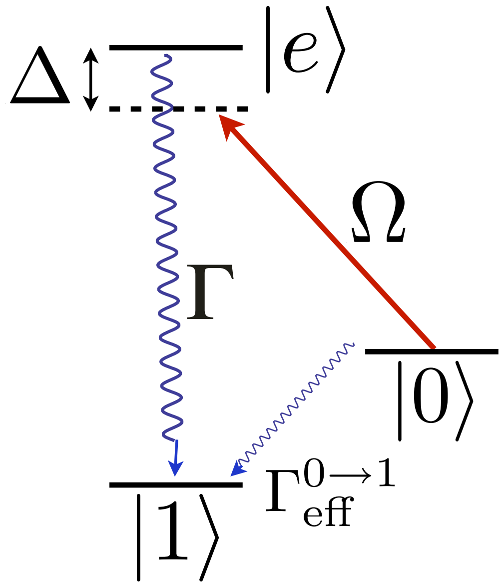
$$i\gamma_3 \rightarrow \gamma_3$$

3-body interactions via 3-body loss



A. J. Daley, J. Taylor, SD, M. Baranov, P. Zoller, Phys. Rev. Lett. **102**, 040402 (2009)

An analogy: optical pumping



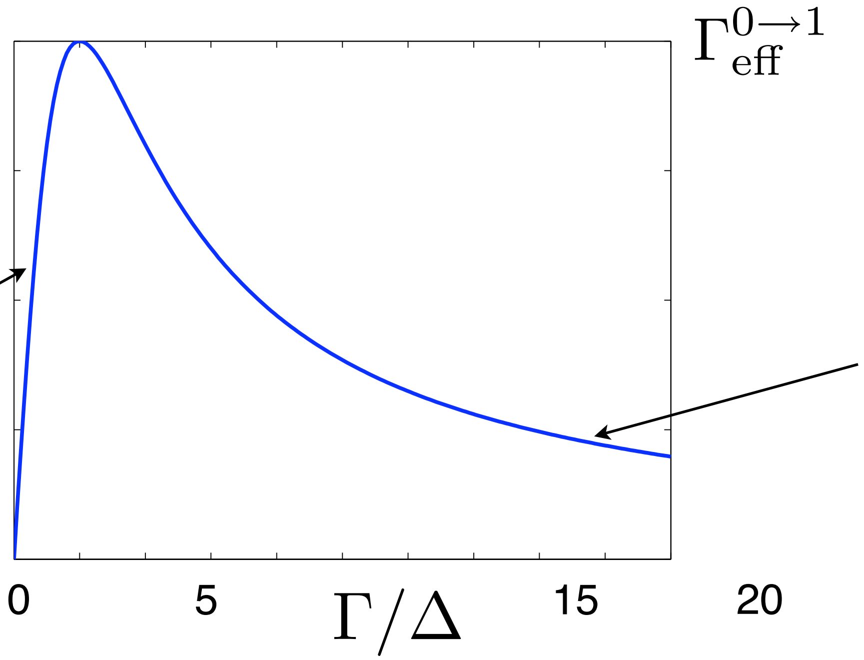
master equation in Lindblad form

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho = -i[H,\rho] + \mathcal{L}[\rho]$$

with $$H = \frac{\Omega}{2}(|0\rangle\langle e| + |e\rangle\langle 0|) - \Delta |e\rangle\langle e|$$

$$\mathcal{L}[\rho] = \Gamma\left(J\rho J^\dagger - \frac{1}{2}(J^\dagger J\rho + \rho J^\dagger J)\right) \qquad J = |1\rangle\langle e|$$

pumping rate $$\Gamma_{\rm eff}^{0\to 1} = \frac{\Omega^2}{4\Delta^2 + \Gamma^2}\Gamma$$ (for $\Omega \ll \Gamma, \Delta$)



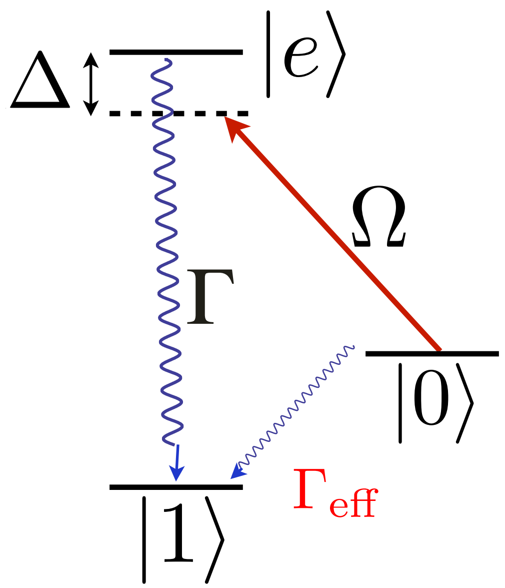
$$\Gamma_{\rm eff}^{0\to 1} \approx \frac{\Omega^2}{4\Delta^2}\Gamma$$

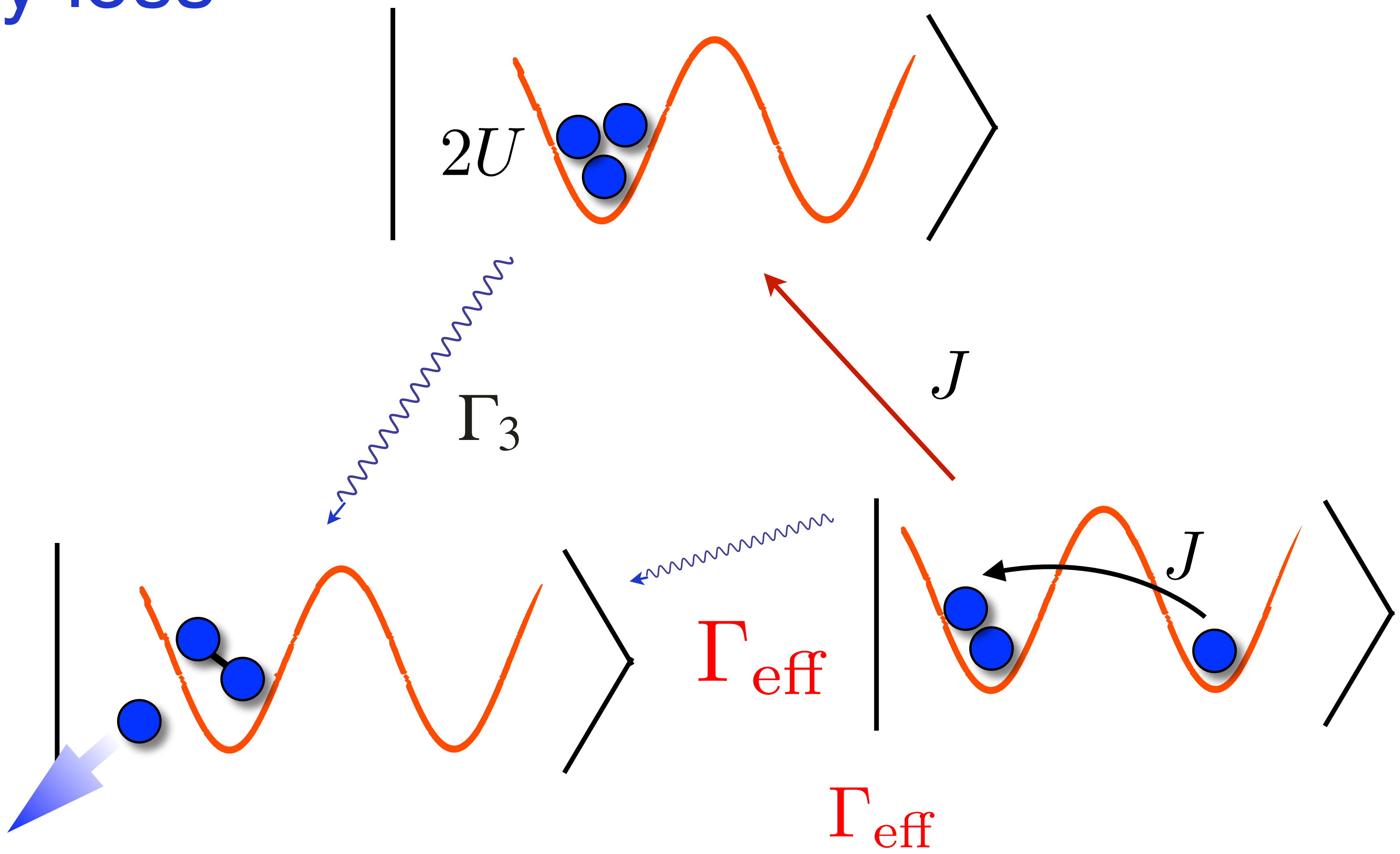
$$\Gamma_{\rm eff}^{0\to 1} \approx \frac{\Omega^2}{\Gamma}$$

Zeno regime: system frozen in $|0\rangle$

large Γ:
- system “freezes” in I0>
- leading correction is effective small loss rate 0 -> 1 $\Gamma_{\rm eff}^{0\to 1} \approx \Omega^2/\Gamma$

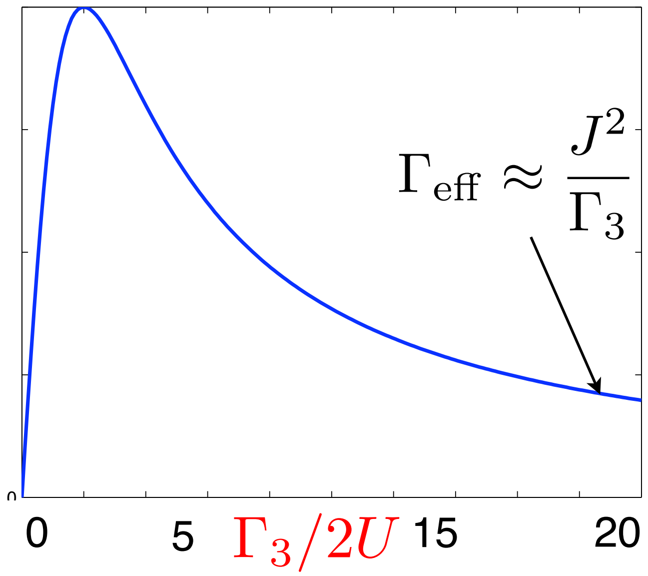
Analogy to three-body loss





detuning	Δ	$\longleftrightarrow$	$2U$	onsite interaction energy
Rabi frequency	Ω	$\longleftrightarrow$	J	tunnel coupling
decay rate	Γ	$\longleftrightarrow$	Γ_3	three-body recombination rate

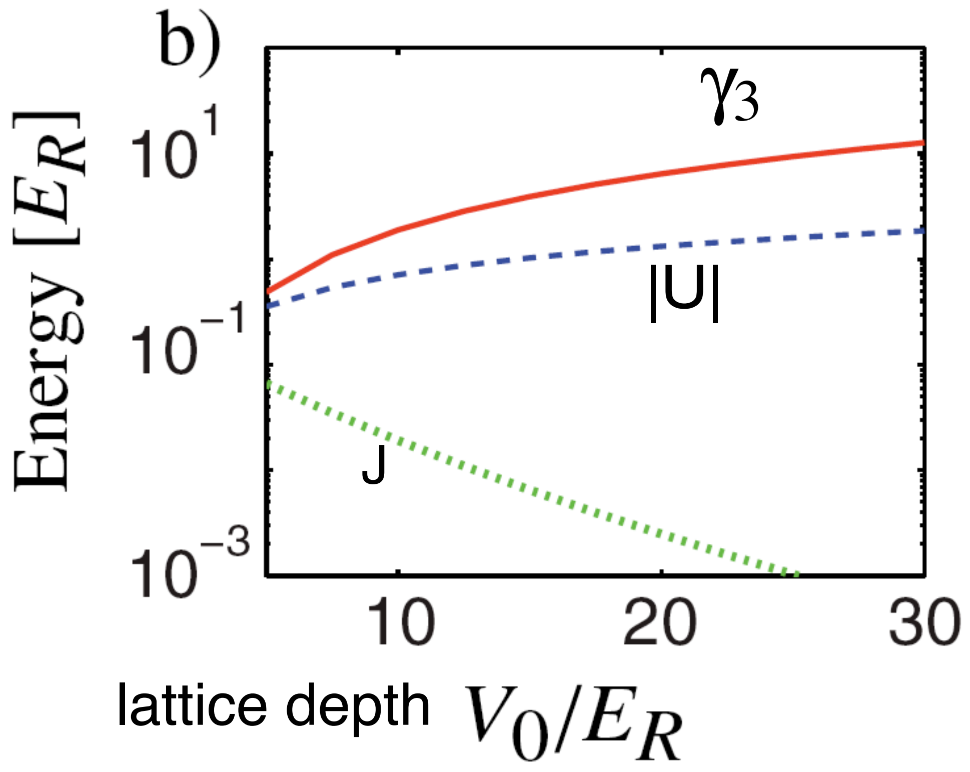
- system “freezes” in subspace with fewer 3 particles per site: 3-body constraint
- stabilizes against particle loss: effective loss rate $\Gamma_{\rm eff} \approx J^2/\Gamma_3$



➡ For $\Gamma_3 \gg U, J$ realization of a Bose-Hubbard-Hamiltonian with three-body hard-core constraint on time scales $t < 1/\Gamma_{\rm eff}$

Physical Realization in Cold Atomic Gases

- Estimate loss rate for Cesium close to a zero crossing of the scattering length (e.g. Naegerl et al.)

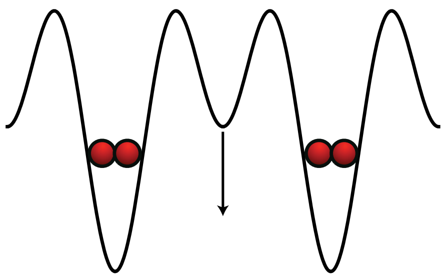


➡ 3-body loss can be made the dominant energy scale

- Preparation of the ground state of constrained Hamiltonian:
  - role of heating effects due to residual particle loss
  - Approach: Exact numerical time evolution of full Master Equation in 1D; combine DMRG method with stochastic simulation of ME
  - Find optimal experimental sequence to avoid heating

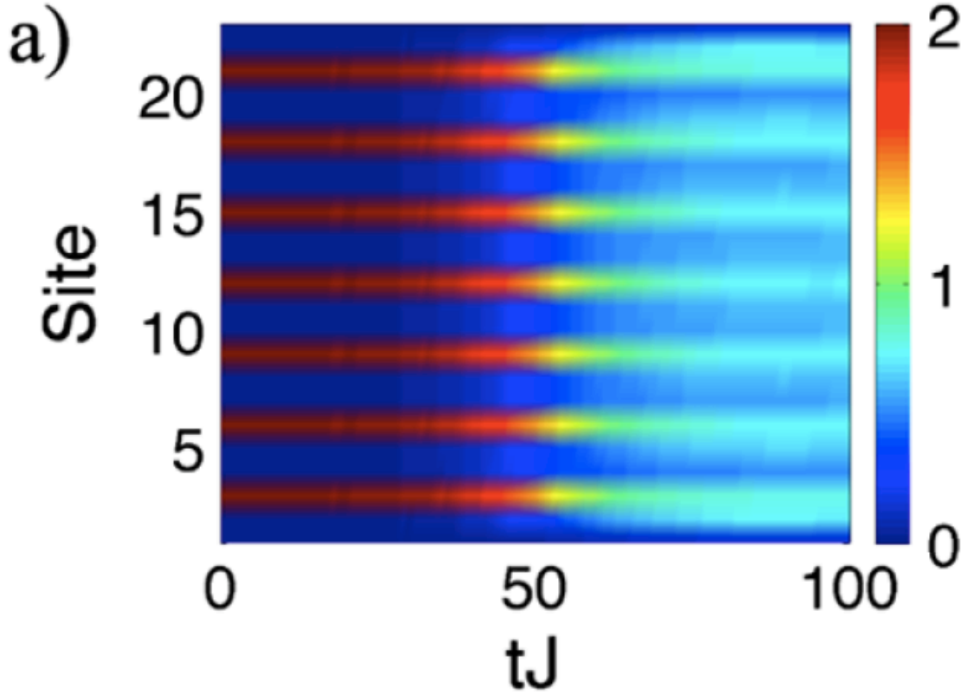
Ground State Preparation

Ramp: Superlattice, V/J=30 to V/J=0,
N=M=20
$\Gamma = 250J$

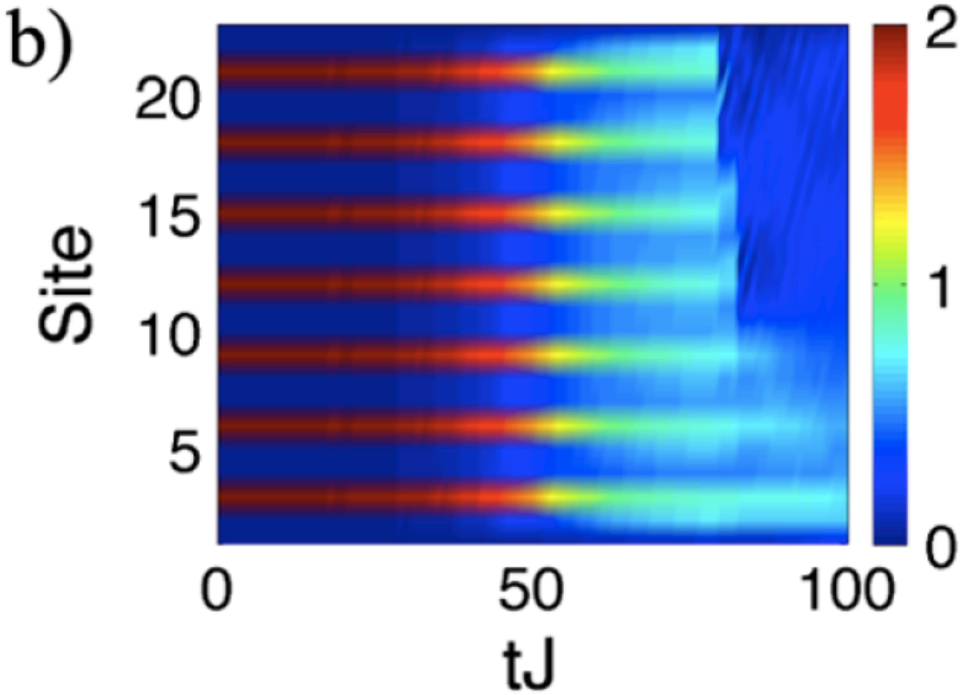


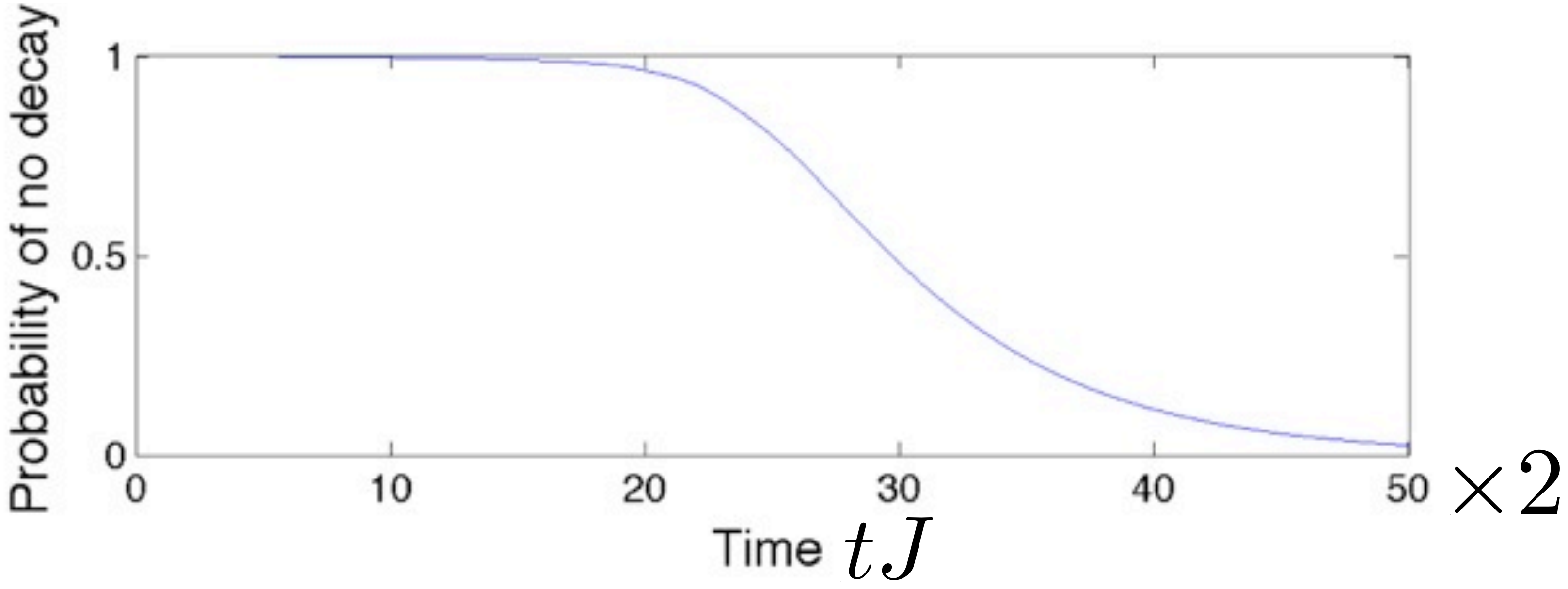
- Start from Mott ground state in superlattice
- Loss causes heating, inhibits reaching ground state

“lucky” trajectory



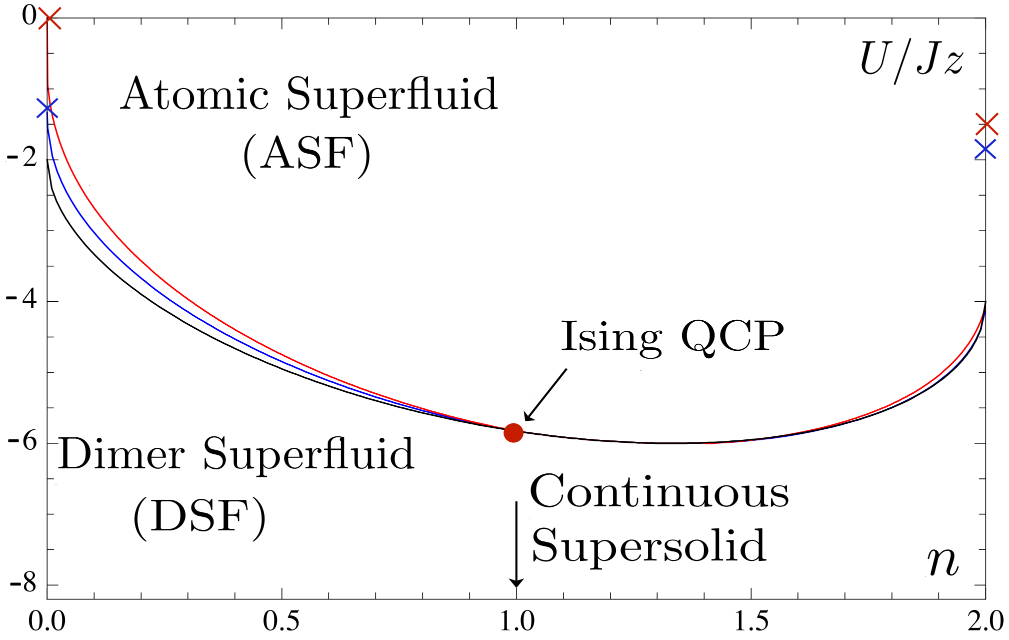
“unlucky” trajectory





➡ “Probabilistic” ground state preparation

Phase Diagram for Three-Body Hardcore Bosons



microscopic

interactions

thermodynamic

interactions
condensation

long distance

interactions
condensation
spin waves

SD, M. Baranov, A. J. Daley, P. Zoller, Phys. Rev. Lett, **104**, 165301(2010);
SD, M. Baranov, A. J. Daley, P. Zoller , Phys. Rev. B **82**, 064509 (2010);
Phys. Rev. B **82**, 064510 (2010)

Physics of the constrained Hamiltonian

- The constrained Bose-Hubbard Hamiltonian stabilizes attractive two-body interactions

$$PHP = -J \sum_{\langle i,j \rangle} \hat{b}_i^\dagger \hat{b}_j + \frac{U}{2} \sum_i \hat{n}_i (\hat{n}_i - 1) \ \ \& \ \boxed{b_i^{\dagger 3} \equiv 0}$$

$$\boxed{U < 0}$$

- Qualitative picture for ground state: Mean Field Theory
  - homogenous Gutzwiller Ansatz for projected on-site Hilbert space

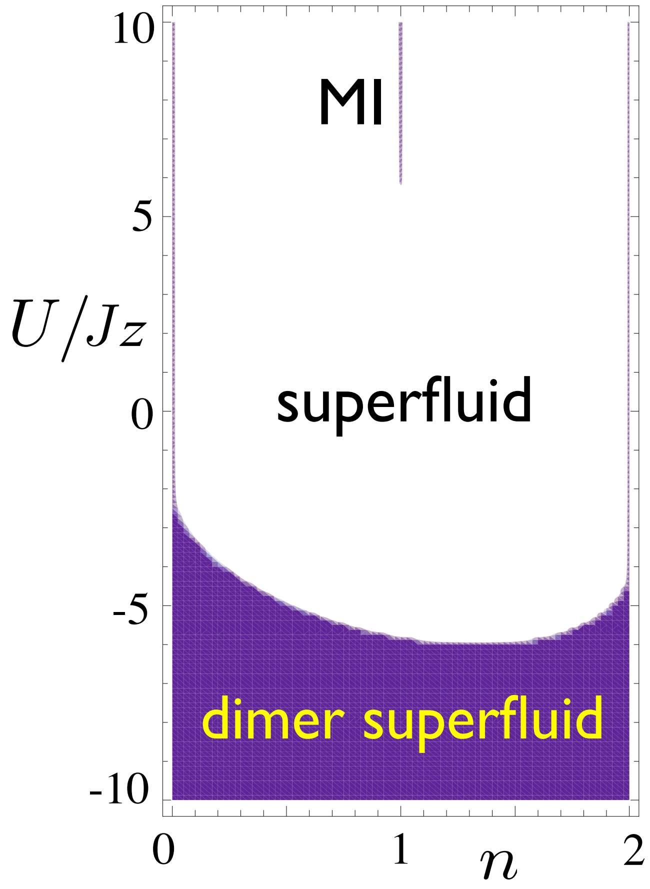
$$|\Psi\rangle = \prod_i |\Psi\rangle_i \qquad |\Psi\rangle_i = f_0|0\rangle + f_1|1\rangle + f_2|2\rangle \qquad f_\alpha = r_\alpha e^{i\phi_\alpha}$$

  - Gutzwiller energy

$$\Phi = \phi_2 + \phi_0 - 2\phi_1$$

$$E(r_\alpha, \phi_\alpha) = U r_2^2 - JZ r_1^2 \left[r_0^2 + 2\sqrt{2} r_2 r_0 \cos\Phi + 2 r_2^2 \right]$$

Mean Field Phase Diagram



critical interaction strength:

$$\frac{U_c}{Jz} = -2\left(1+n/2+2\sqrt{n(1-n/2)}\right)$$

- Two symmetry breaking patterns occur:

$\langle\hat{b}\rangle \neq 0, \quad \langle\hat{b}^2\rangle \neq 0$ - Conventional SF

$\langle\hat{b}\rangle = 0, \quad \langle\hat{b}^2\rangle \neq 0$ - "Dimer SF"

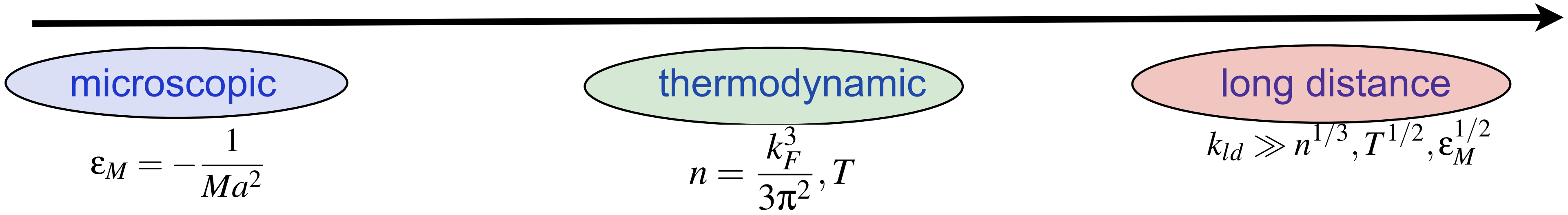
- Phase transition reminiscent of Ising (cf Radzihovsky& '03; Stoof, Sachdev& '03):

$$\langle\hat{b}\rangle \sim \exp i\theta \qquad \langle\hat{b}^2\rangle \sim \exp 2i\theta$$

➡ Spontaneous breaking of Z_2 symmetry $\theta \rightarrow \theta + \pi$ of the DSF order parameter

Beyond Mean Field Phase Diagram

- Why?
  - Mean Field Theory (MFT) misses out physics at various length scales



microscopic

$\varepsilon_M = -\frac{1}{Ma^2}$

thermodynamic

$n = \frac{k_F^3}{3\pi^2}, T$

long distance

$k_{ld} \gg n^{1/3}, T^{1/2}, \varepsilon_M^{1/2}$

- How?
  - MFT is a classical field theory
  - Find a means to requantize this MFT: classical field theory -> quantum field theory
    - exact mapping of the constrained Hamiltonian to a coupled boson theory with polynomial interactions
    - the bosonic operators find natural interpretation in terms of “atoms” and “dimers”

$$PHP \rightarrow$$

$$X_i = 1 - \hat{n}_{1,i} - \hat{n}_{2,i} \qquad \text{“atoms”} \qquad \text{“dimers”}$$

$$H = (U - 2\mu)\sum_i \hat{n}_{2,i} - \mu \sum_i \hat{n}_{1,i} - J \sum_{\langle i,j \rangle} \left[t^\dagger_{1,i} X_i X_j t_{1,j} + \sqrt{2}(t^\dagger_{2,i} t_{1,i} X_j t_{1,j} + t^\dagger_{1,i} X_i t^\dagger_{1,j} t_{2,j}) + 2 t^\dagger_{2,i} t_{2,j} t^\dagger_{1,j} t_{1,i} \right]$$

➡ We have identified several quantitative and qualitative effects:

✓Tied to interactions

✓Tied to the constraint

Implementation of the Hard-Core Constraint

- Introduce operators to parameterize on-site Hilbert space (Auerbach, Altman ‘98)

$$t^{\dagger}_{\alpha,i}|\text{vac}\rangle = |\alpha\rangle, \quad \alpha = 0, 1, 2$$

- They are not independent:

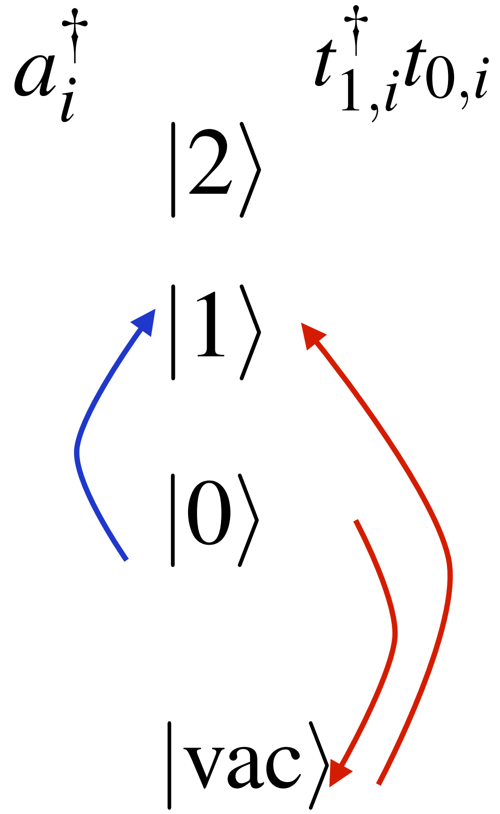
$$\sum_{\alpha} t^{\dagger}_{\alpha,i} t_{\alpha,i} = \mathbf{1}$$

- Representation of Hubbard operators:

$$a^{\dagger}_{i} = \sqrt{2} t^{\dagger}_{2,i} t_{1,i} + t^{\dagger}_{1,i} t_{0,i}$$

$$\hat{n}_i = 2 t^{\dagger}_{2,i} t_{2,i} + t^{\dagger}_{1,i} t_{1,i}$$

Action of operators



Implementation of the Hard-Core Constraint

- Hamiltonian:

$$H_{\text{pot}} = -\mu \sum_i 2 t^\dagger_{2,i} t_{2,i} + t^\dagger_{1,i} t_{1,i} + U \sum_i t^\dagger_{2,i} t_{2,i}$$

$$H_{\text{kin}} = -J \sum_{\langle i,j \rangle} \left[t^\dagger_{1,i} t_{0,i} t^\dagger_{0,j} t_{1,j} + \sqrt{2} (t^\dagger_{2,i} t_{1,i} t^\dagger_{0,j} t_{1,j} + t^\dagger_{1,i} t_{0,i} t^\dagger_{1,j} t_{2,j}) + 2 t^\dagger_{2,i} t^\dagger_{1,j} t_{1,i} t_{2,j} \right]$$

- Properties:
  - Mean field: Gutzwiller energy (classical theory)
  - interaction: quadratic
  - hopping: higher order
    - Role of interaction and hopping reversed
    - Strong coupling approach facilitated
  - One phase is redundant: absorb via *local* gauge transformation

$$t_{1,i} = \exp \mathrm{i}\varphi_{0,i} \, |t_{0,i}| \qquad\qquad t_{1,i} \longrightarrow \exp -\mathrm{i}\varphi_{0,i} \, t_{1,i}, \quad t_{2,i} \longrightarrow \exp -\mathrm{i}\varphi_{0,i} \, t_{2,i}$$

➡ e.g. t_0 can be chosen real

Implementation of the Hard-Core Constraint

- Resolve the relation between t-operators (zero density)

$$t^\dagger_{1,i} t_{0,i} = t^\dagger_{1,i}\sqrt{1 - t^\dagger_{1,i}t_{1,i} - t^\dagger_{2,i}t_{2,i}} \to t^\dagger_{1,i}(1 - t^\dagger_{1,i}t_{1,i} - t^\dagger_{2,i}t_{2,i})$$

  - justification: for projective operators one has from Taylor representation

$$X^2 = X \to f(X) = f(0)(1-X) + Xf(1) \qquad X = 1 - t^\dagger_{1,i}t_{1,i} - t^\dagger_{2,i}t_{2,i}$$

- Now we can interpret the remaining operators as standard bosons:
  - on-site bosonic space $\mathcal{H}_i = \{|n\rangle_i^1 |m\rangle_i^2\}, \quad n,m = 0,1,2,\ldots$
  - decompose into physical/unphysical space: $\mathcal{H}_i = \mathcal{P}_i \oplus U_i$

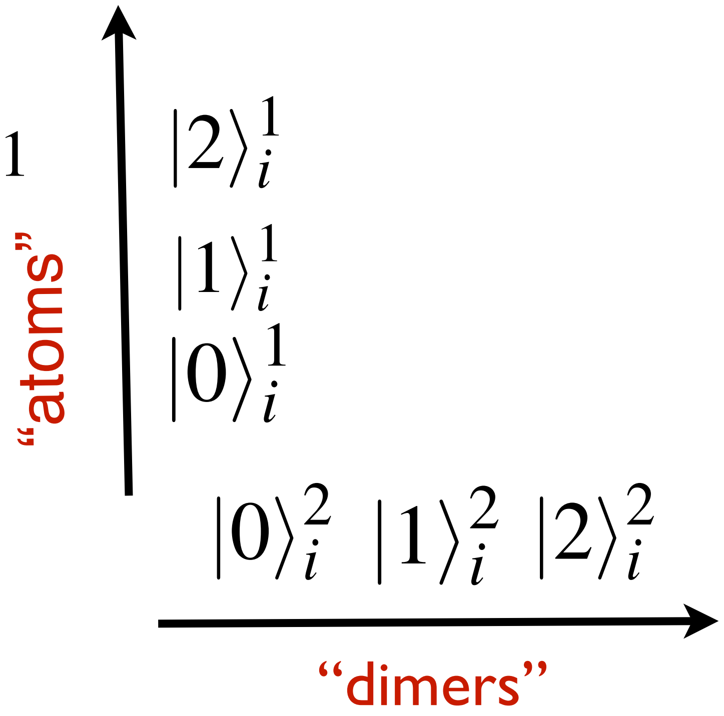
$$\mathcal{P}_i = \{|0\rangle_i^1|0\rangle_i^2, |1\rangle_i^1|0\rangle_i^2, |0\rangle_i^1|1\rangle_i^2\}$$

  - correct bosonic enhancement factors on physical subspace $\sqrt{n} = 0,1$
  - the Hamiltonian is an involution on P and U:

$$H = H_{PP} + H_{UU}$$

  - remaining degrees of freedom: "atoms" and "dimers"

➡ similarity to Hubbard-Stratonovich transformation



Implementation of the Hard-Core Constraint

- The partition sum does not mix U and P too:

$$Z = Tr \exp - \beta H = Tr_{PP} \exp - \beta H_{PP} + Tr_{UU} \exp - \beta H_{UU}$$

- Need to discriminate contributions from U and P: Work with Effective Action

  - Legendre transform of the Free energy $W[J] = \log Z[J]$

$$\Gamma[\chi] = -W[J] + \int J^T \chi, \quad \chi \equiv \frac{\delta W[J]}{\delta J}$$

Quantum Equation of Motion for J=0

  - Has functional integral representation:

$$\exp - \Gamma[\chi] = \int \mathcal{D}\delta\chi \exp - S[\chi + \delta\chi] + \int J^T \delta\chi, \quad J = \frac{\delta\Gamma[\chi]}{\chi}$$

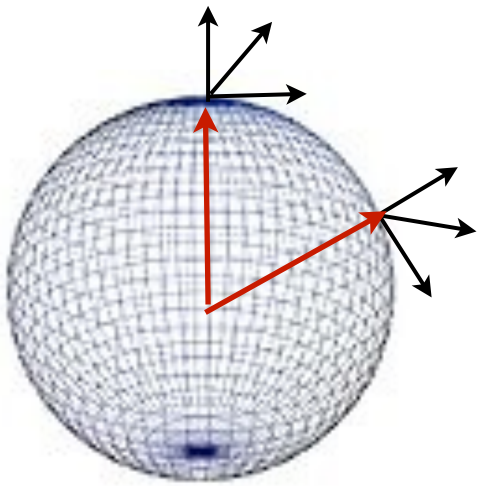
$$S[\chi = (t_1, t_2)] = \int d\tau \Big(\sum_i t^\dagger_{1,i} \partial_\tau t_{1,i} + t^\dagger_{2,i} \partial_\tau t_{2,i} + H[t_1, t_2] \Big)$$

- Usually: Effective Action shares all symmetries of S
- Here: symmetry principles are supplemented with a constraint principle

Condensation and Thermodynamics

- Physical vacuum is continuously connected to the finite density case:

Introduce new, expectationless operators by (complex) Euler rotation



$$\vec{t} = (t_0, t_1, t_2)^T$$

$$\vec{b} = R_\theta \, R_\varphi \, \vec{t}$$

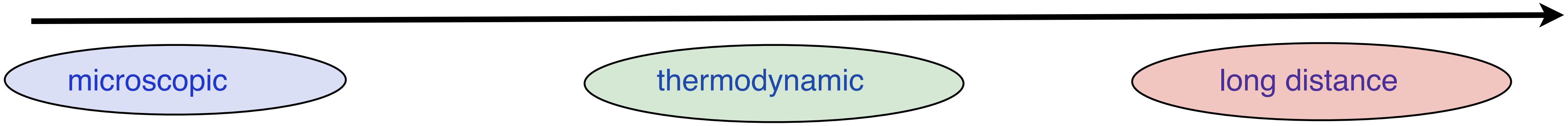
- Hamiltonian in new coordinates takes form:

Quadratic part: Spin waves (Goldstone for n > 0)

$$H = E_{\mathrm{GW}} + H_{\mathrm{SW}} + H_{\mathrm{int}}$$

Mean field: Gutzwiller Energy

higher order: interactions



interactions

interactions
condensation

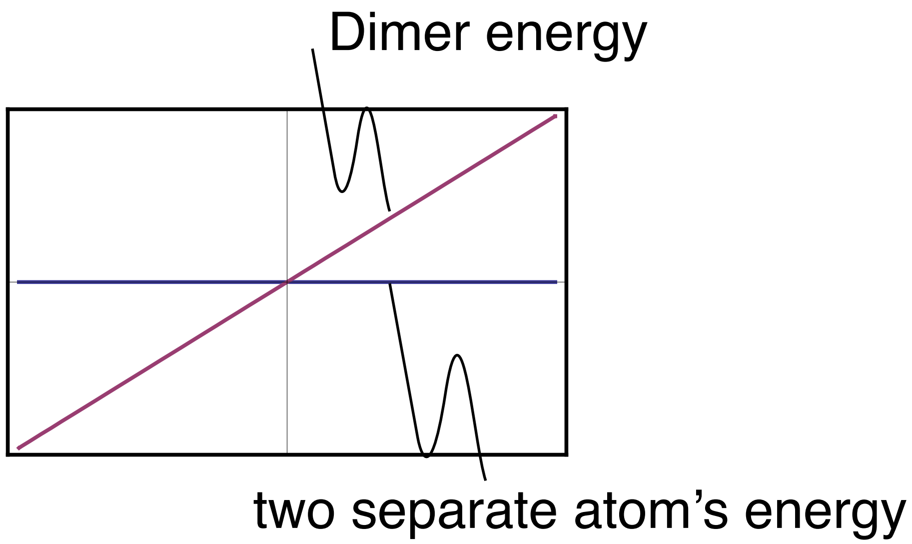
interactions
condensation
spin waves

The requantized Gutzwiller model

- Hamiltonian to cubic order is of Feshbach type:
  - quadratic part:

$$H_{\text{pot}} = \sum_i (U - 2\mu) n_{2,i} - \mu n_{1,i}$$

detuning from atom level



  - leading interaction:

$$H_{\text{kin}} = -J \sum_{\langle i,j \rangle} \left[t^\dagger_{1,i} t_{1,j} + \sqrt{2} (t^\dagger_{2,i} t_{1,i} t_{1,j} + t^\dagger_{1,i} t^\dagger_{1,j} t_{2,j}) \right]$$

(bilocal) dimer splitting into atoms

- Compare to standard Feshbach models:

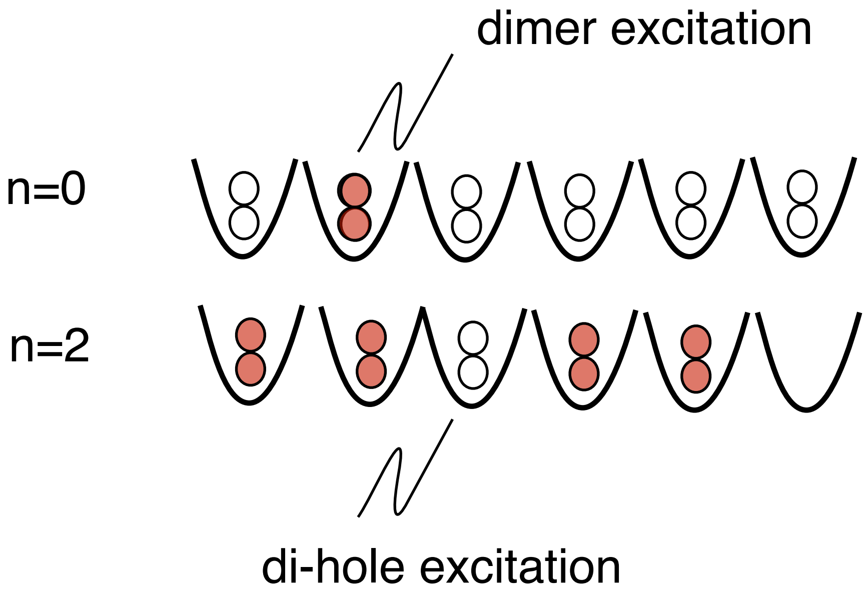
detuning $\sim 1/U$

here: detuning $\sim U$

➡ we can expect resonant (strong coupling) phenomenology at weak coupling

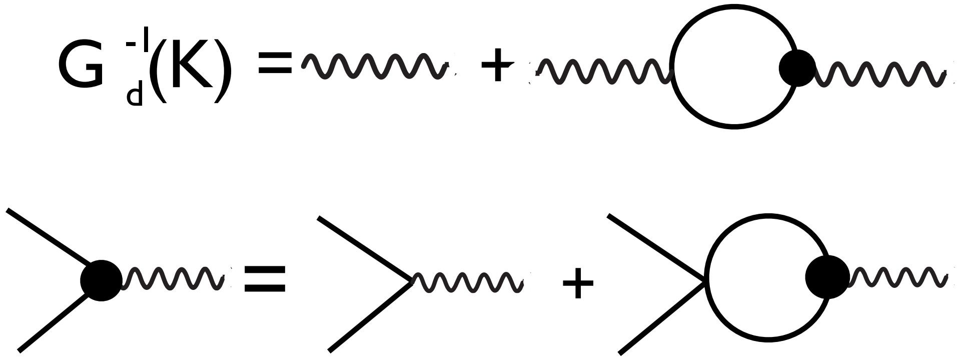
$$H_{\text{kin}} = -J \sum_{\langle i,j \rangle} \left[t^\dagger_{1,i} (1 - n_{1,i} - n_{2,i})(1 - n_{1,j} - n_{2,j}) t_{1,j} + \sqrt{2} (t^\dagger_{2,i} t_{1,i} (1 - n_{1,j} - n_{2,j}) t_{1,j} + t^\dagger_{1,i} (1 - n_{1,i} - n_{2,i}) t^\dagger_{1,j} t_{2,j}) + 2 t^\dagger_{2,i} t_{2,j} t^\dagger_{1,j} t_{1,i} \right]$$

Vacuum Problems



- The physics at n=0 and n=2 are closely connected:
  - “vacuum”: no spontaneous symmetry breaking
  - low lying excitations:
    - n=0: atoms and dimers on the physical vacuum
    - n=2: holes and di-holes on the fully packed lattice

- Two-body problems can be solved exactly
  - Bound state formation: $G_d^{-1}(\omega=\mathbf{q}=0)=0$



$$\frac{1}{a_n|\tilde{U}|+b_n}=\int\frac{d^dq}{(2\pi)^d}\frac{1}{-\tilde{E}_b+c_n/d\sum_\lambda(1-\cos\mathbf{q}\mathbf{e}_\lambda)}$$

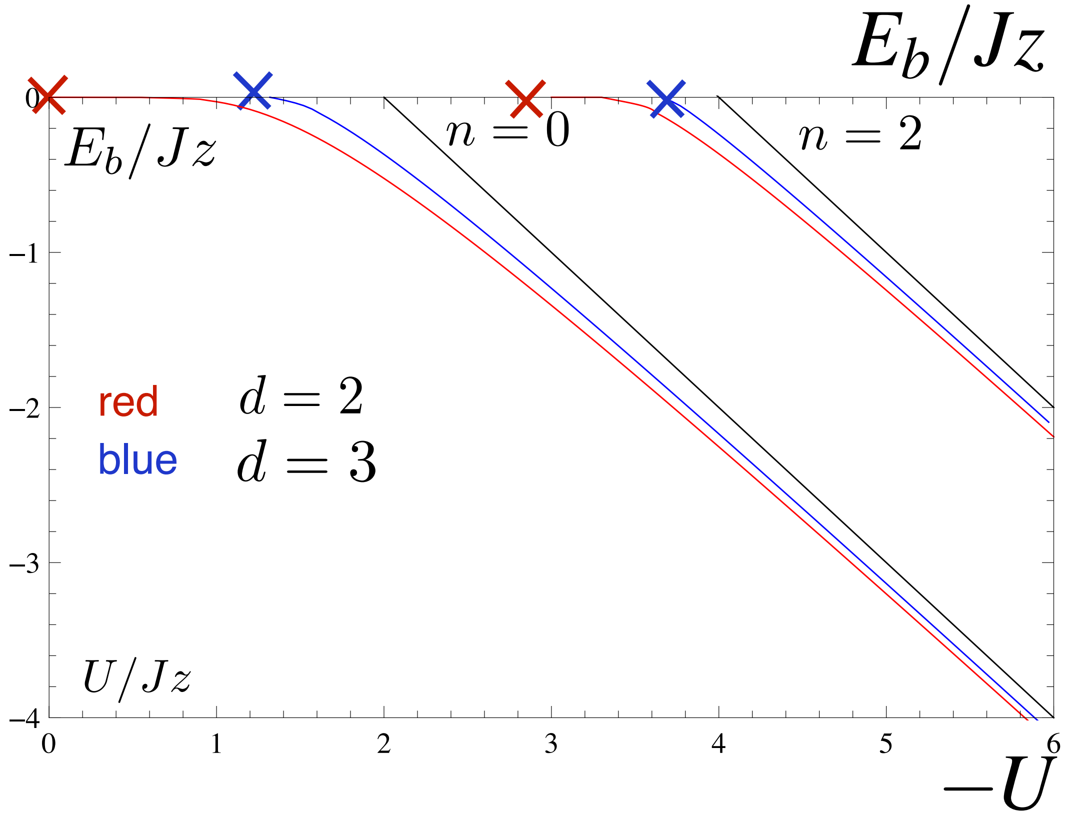
$$n=0:\quad a_0=1,\ b_0=0,\ c_0=2$$

➡ reproduces Schrödinger Equation: benchmark

➡ Square root expansion of constraint fails

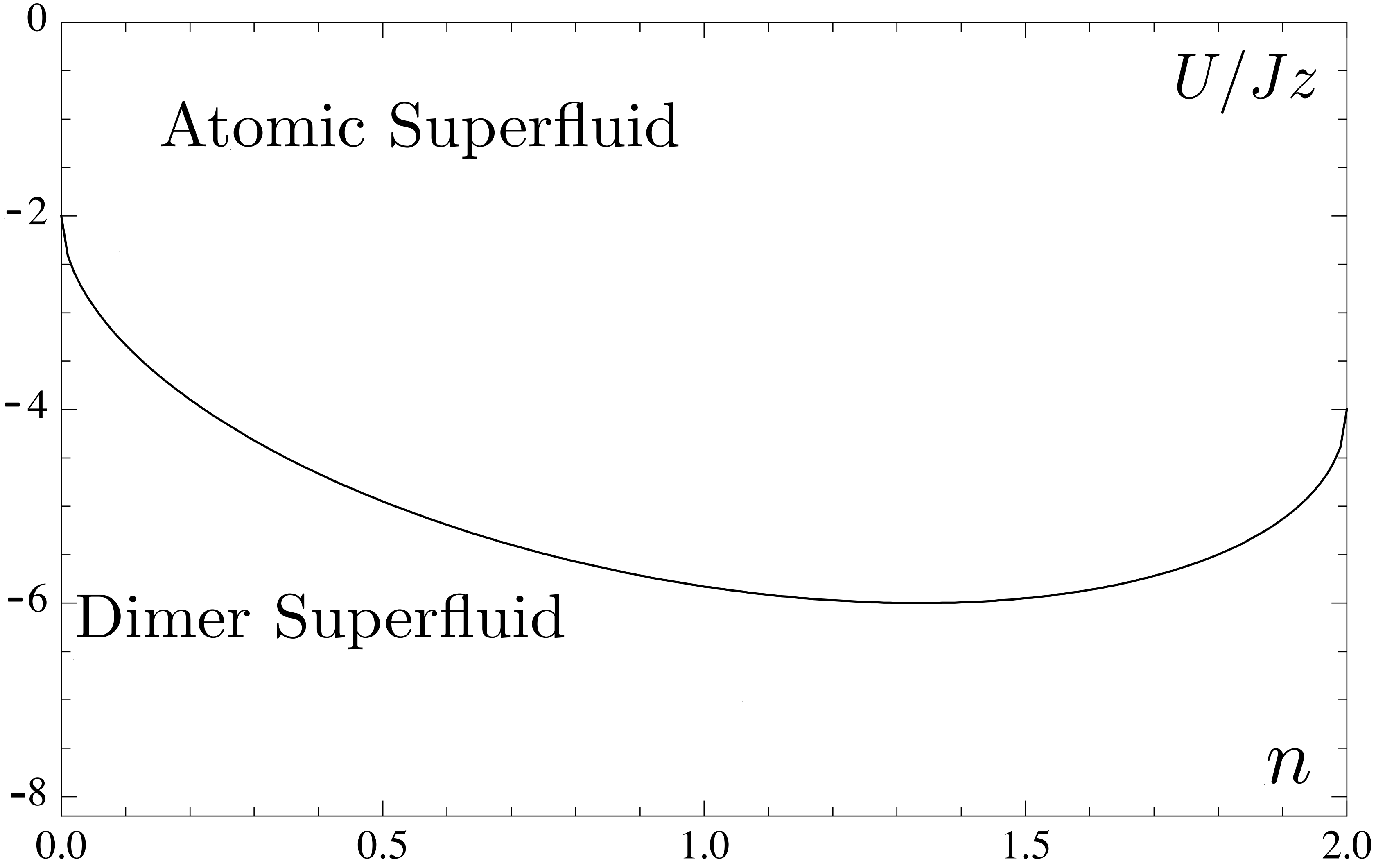
$$n=2:\quad a_2=4,\ b_2=-6+3\tilde{E}_b\ c_2=4$$

➡ di-hole-bound state formation at finite U in 2D



Beyond Mean Field Phase Diagram

- Start here!



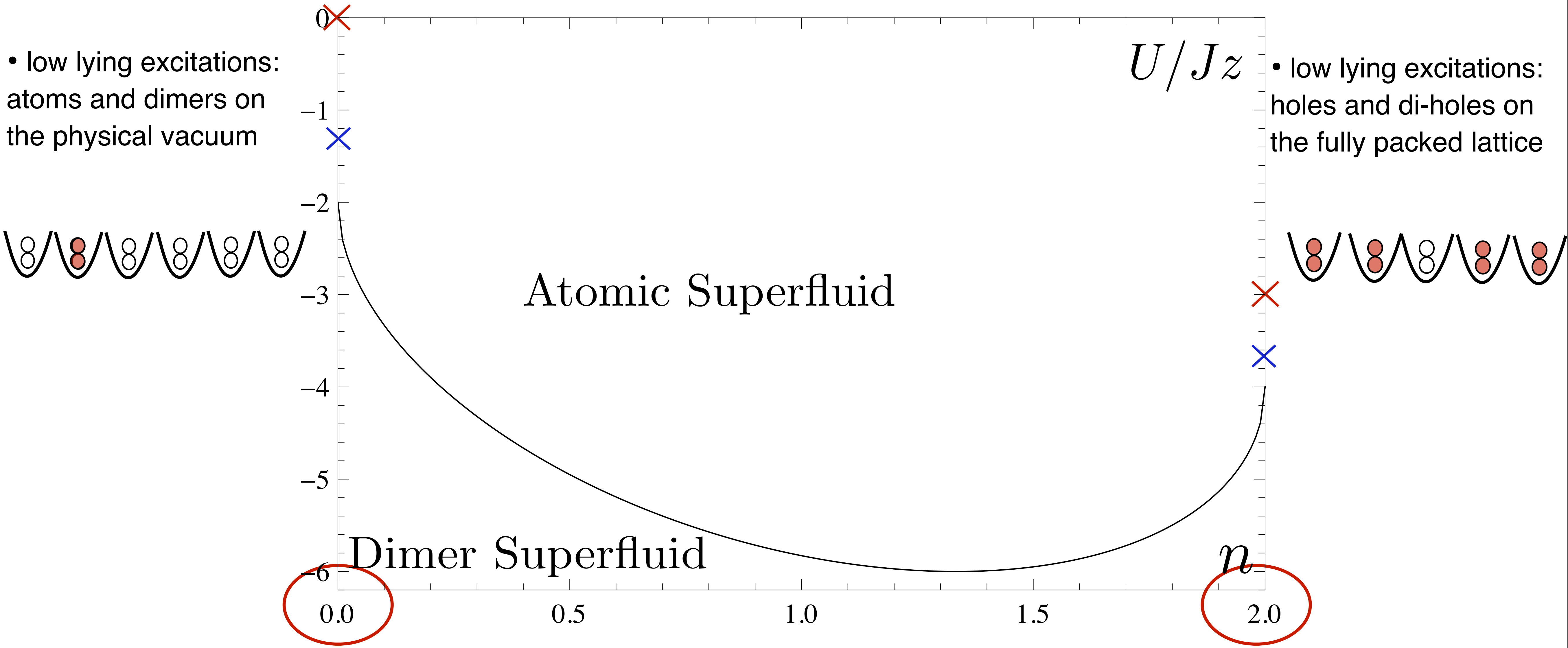
microscopic $\varepsilon_M = -\frac{1}{Ma^2}$

thermodynamic $n = \frac{k_F^3}{3\pi^2}, T$

long distance $k_{ld} \gg n^{1/3}, T^{1/2}, \varepsilon_M^{1/2}$

Beyond Mean Field Phase Diagram

- Vacuum limit:
  - Scattering of a few particles
  - Requantized Hamiltonian is of Feshbach type

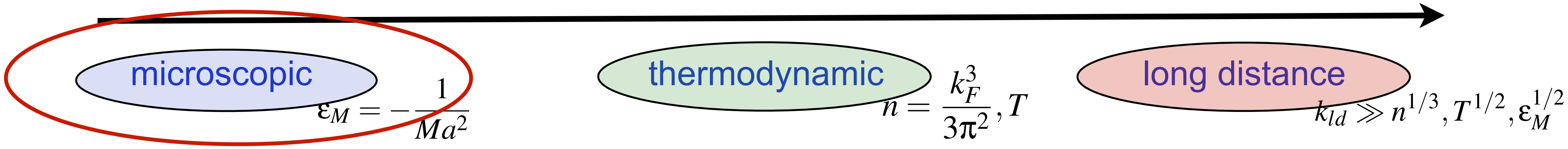


- low lying excitations: atoms and dimers on the physical vacuum

- low lying excitations: holes and di-holes on the fully packed lattice

➡ n = 0: Schrödinger Equation reproduced: Benchmark

➡ n = 2: finite critical interaction for di-hole bound state in 2D



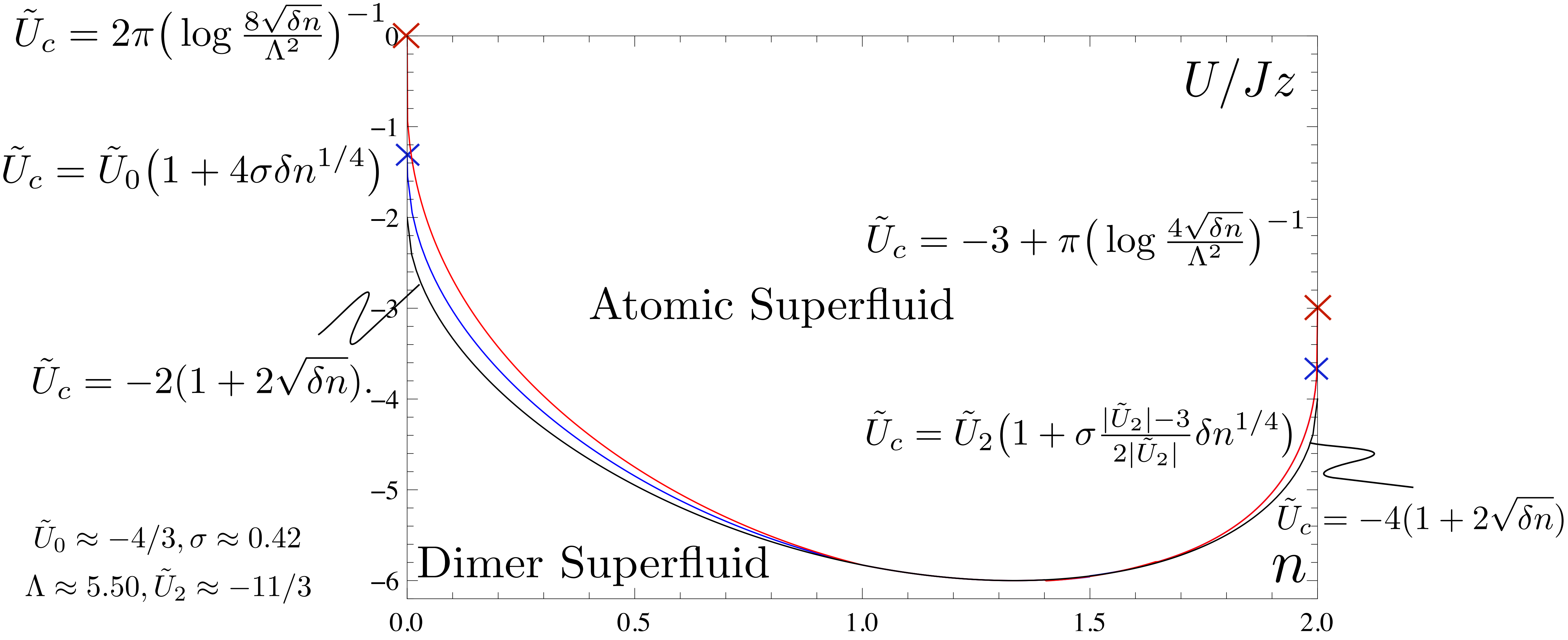
microscopic $\varepsilon_M = -\frac{1}{Ma^2}$

thermodynamic $n = \frac{k_F^3}{3\pi^2}, T$

long distance $k_{ld} \gg n^{1/3}, T^{1/2}, \varepsilon_M^{1/2}$

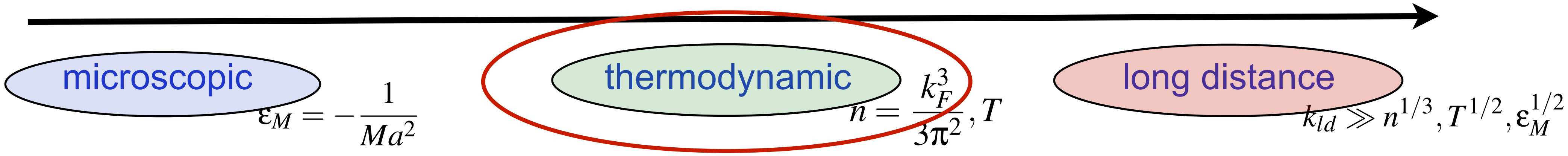
Beyond Mean Field Phase Diagram

- Thermodynamic scales: Nonuniversal shifts on the phase border



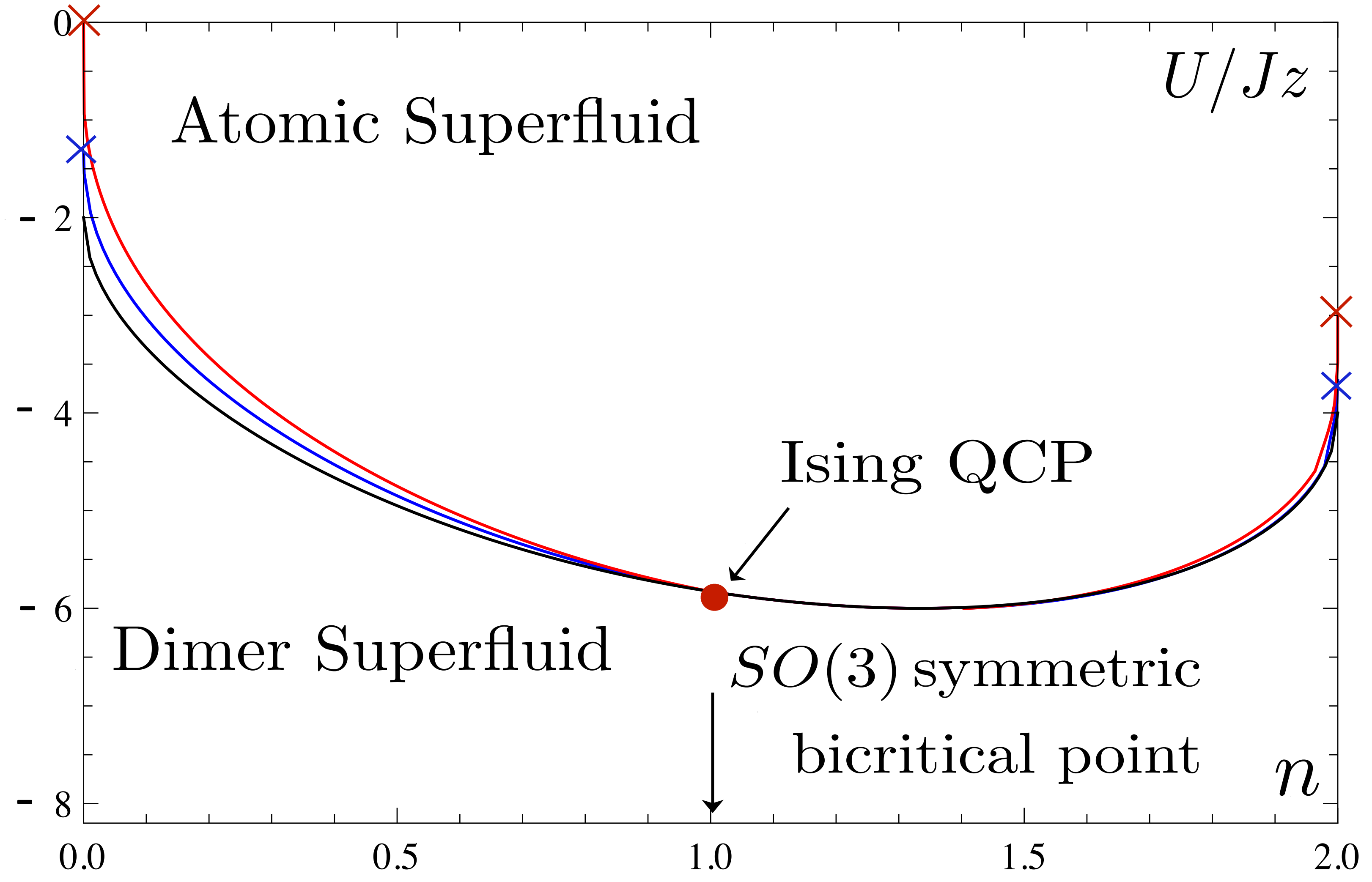
➡ Quantum fluctuations lead to quantitative deviation from MFT

➡ Stronger shifts for small densities: weaker vacuum fluctuations



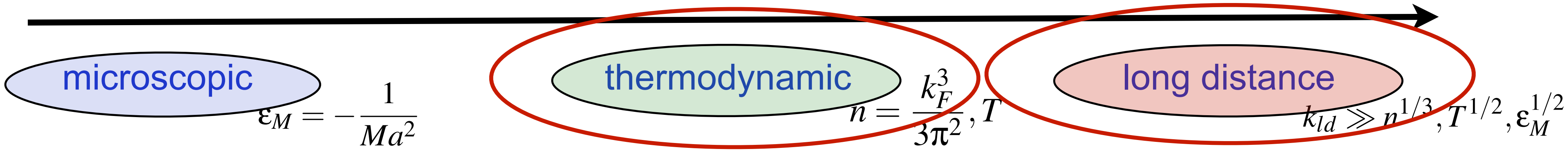
Beyond Mean Field Phase Diagram

- Qualitative effects of the constraint and interactions:



➡ Enhancement of symmetry from $SO(2) \sim U(1) \to SO(3)$

➡ Ising quantum critical point near half filling



microscopic $\varepsilon_M = -\frac{1}{Ma^2}$

thermodynamic $n = \frac{k_F^3}{3\pi^2}, T$

long distance $k_{ld} \gg n^{1/3}, T^{1/2}, \varepsilon_M^{1/2}$

Symmetry Enhancement in Strong Coupling

- Perturbative limit U >> J: expect dimer hardcore model
- Interpret EFT as a spin 1/2 model in external field:

$$H_{\text{eff}} = -2t \sum_{\langle i,j \rangle} \left(s_i^x s_j^x + s_i^y s_j^y + \lambda s_i^z s_j^z \right) \qquad t = \frac{2J^2}{|U|}$$

- Leading (second) order perturbation theory:

$$\lambda = \frac{v}{2t} = 1$$

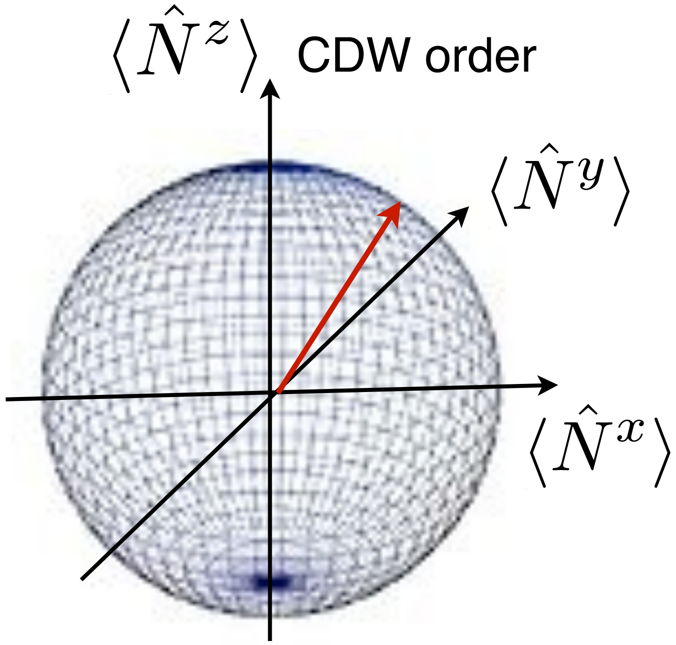
➡ Isotropic Heisenberg model (half filling n=1):

  - Emergent symmetry: SO(3) rotations vs. SO(2) sim U(1)
  - Bicritical point with Neel vector order parameter

$$\hat{N}^\alpha = \sum_j (-)^j s_i^\alpha$$

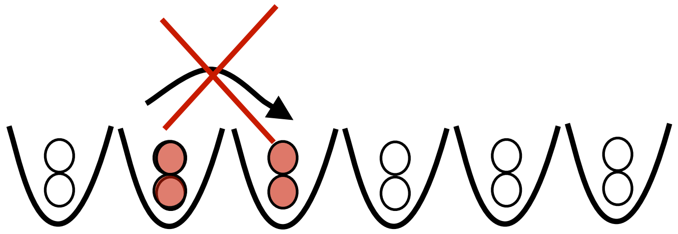
    - charge density wave and superfluid exactly degenerate
      - CDW: Translation symmetry breaking
      - DSF: Phase symmetry breaking
    - physically distinct orders can be freely rotated into each other:

"continuous supersolid"

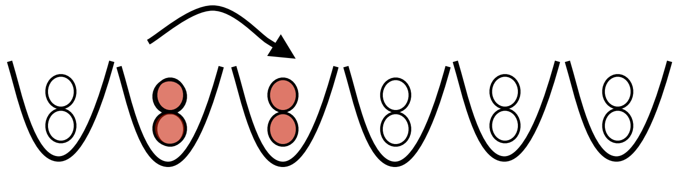


xy plane: superfluid order

with constraint $\lambda = 1$



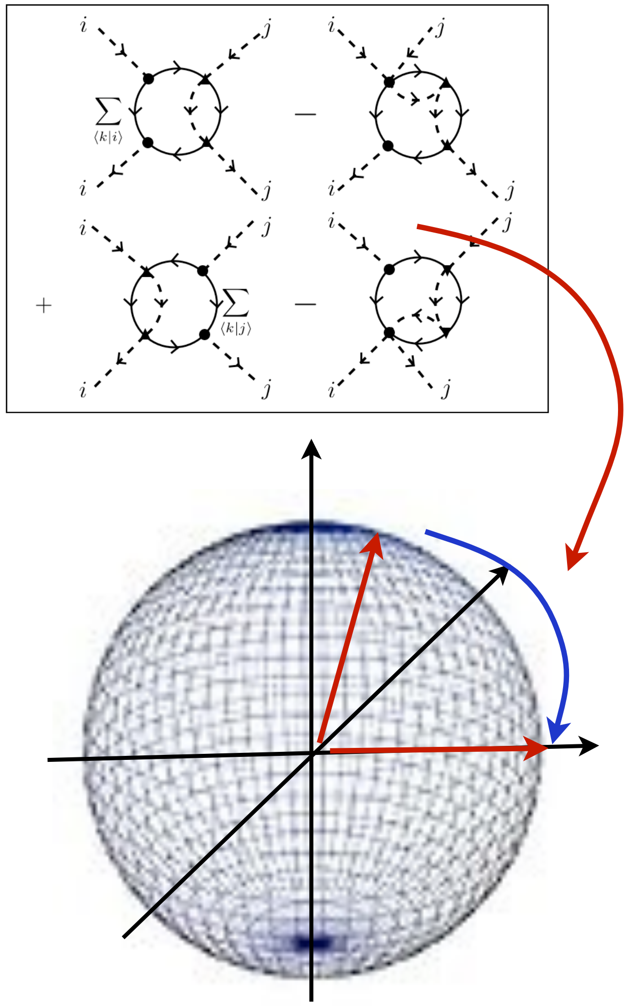
without constraint $\lambda = 4$



(similar to fermions: S.C. Zhang '93)

➡ The symmetry enhancement is unique to the 3-body hardcore constraint

Signatures of “continuous supersolid”



- Next (fourth) order perturbation theory: Superfluid preferred

$$\lambda = 1 - 8(z-1)(J/|U|)^2 < 1$$

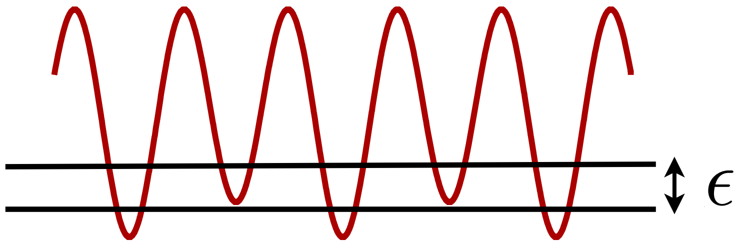
- Proximity to bicritical point governs physics in strong coupling

(1) Second collective (pseudo) Goldstone mode

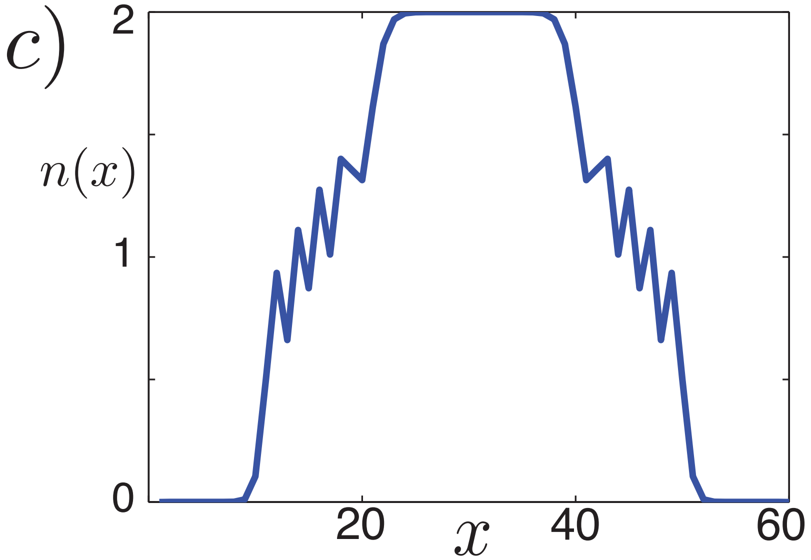
$$\omega(\mathbf{q}) = tz\big((\lambda\varepsilon_{\mathbf{q}}+1)(1-\varepsilon_{\mathbf{q}})\big)^{1/2}$$

(2) Use weak superlattice to rotate Neel order parameter

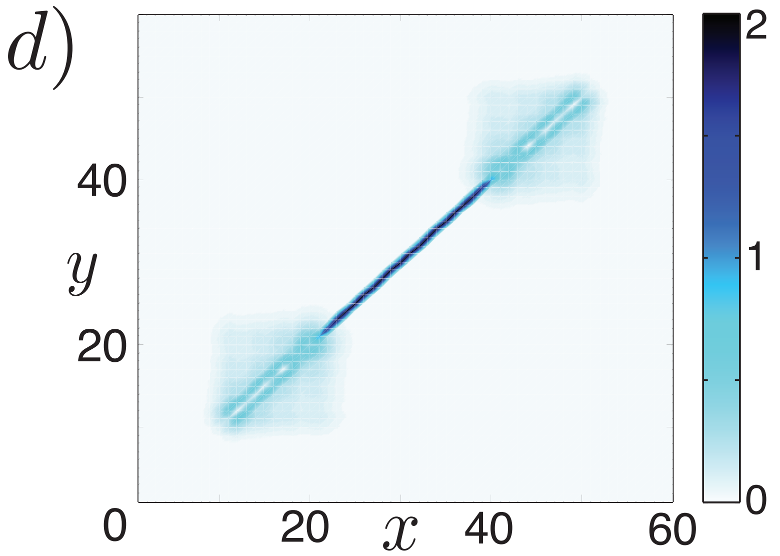
$$\epsilon/tz = \Delta/tz = 1-\lambda \approx 8(z-1)(J/U)^2$$



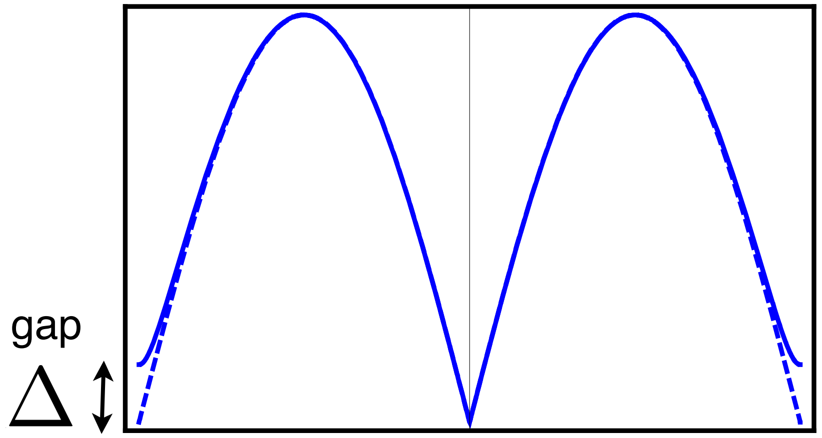
(3) Simulation of 1D experiment in a trap (t-DMRG)



density profile: Onset of CDW



DSF order in textured regions



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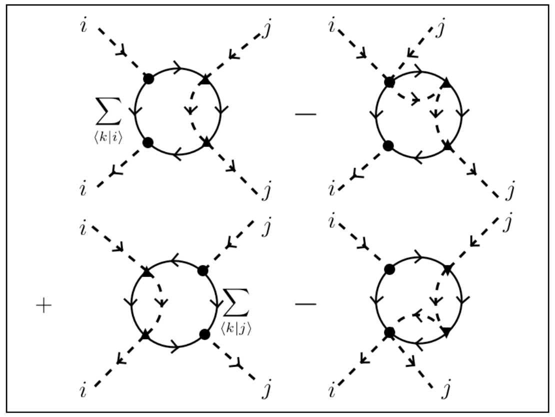

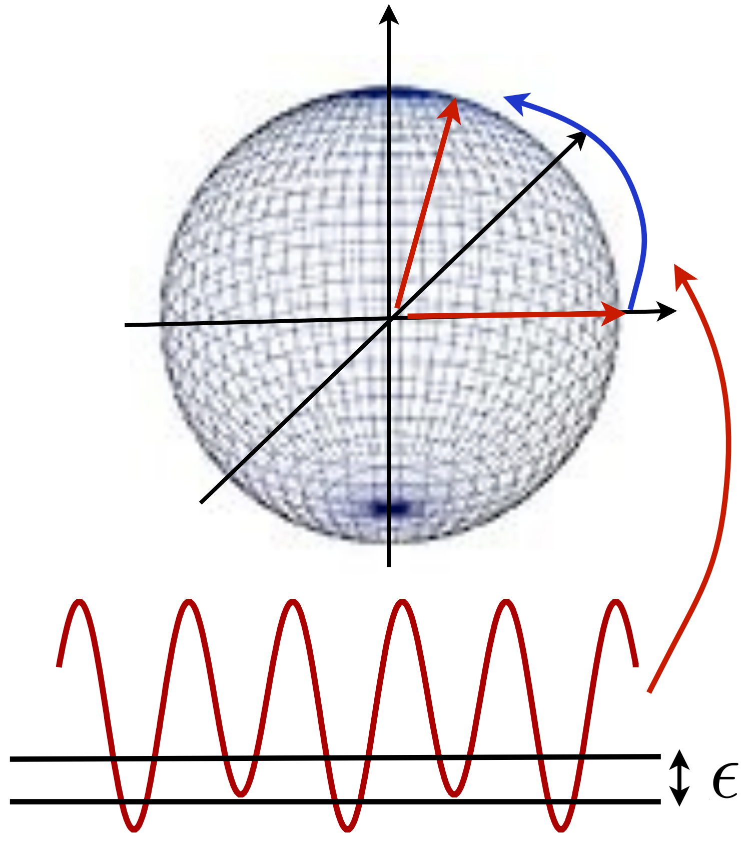

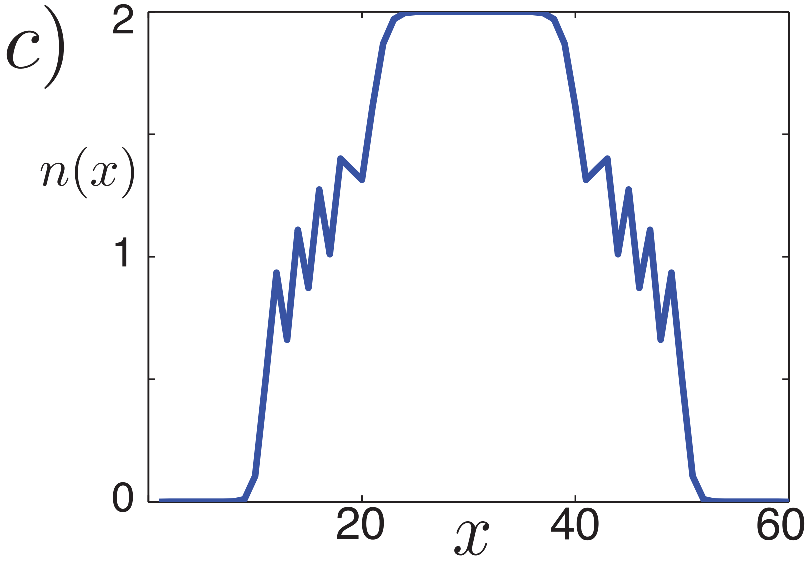

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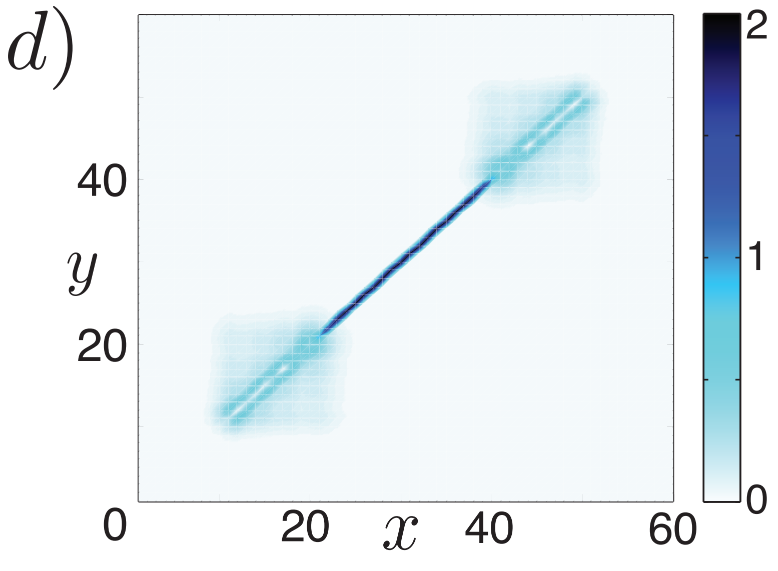
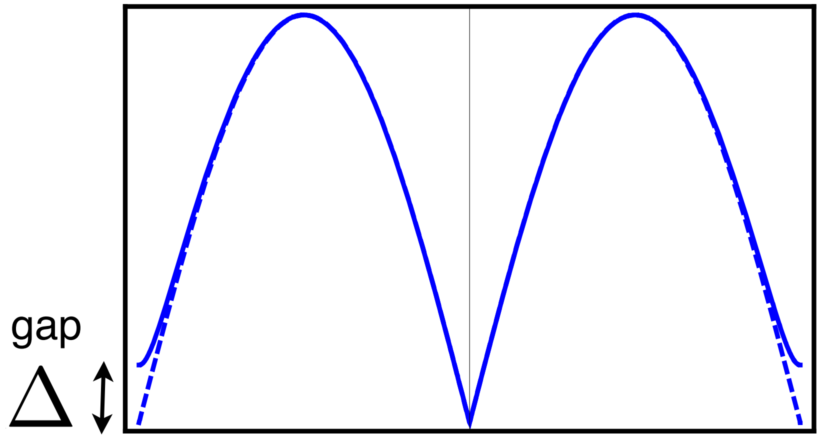


DSF order in textured regions



Second (pseudo) Goldstone mode

Infrared Limit: Nature of the Phase Transition

- Two near massless modes: Critical atomic field, dimer Goldstone mode
- Coleman-Weinberg phenomenon for coupled real fields: Radiatively induced first order PT
- Perform the continuum limit and integrate out massive modes:

pure Goldstone action

$$S[\vartheta,\phi] = S_{\mathrm{I}}[\phi] + S_{\mathrm{G}}[\vartheta] + S_{\mathrm{int}}[\vartheta,\phi]$$

pure Ising action

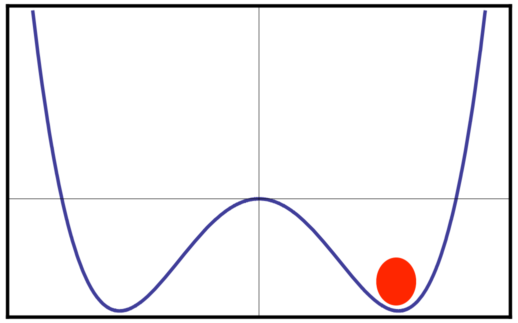
coupling term

$$S_{\mathrm{I}}[\phi] = \int \partial_\mu\phi\partial^\mu\phi + m^2\phi^2 + \lambda\phi^4$$

$$\boxed{S_{\mathrm{int}}[\vartheta,\phi] = \mathrm{i}\kappa\int \partial_\tau\vartheta\,\phi^2}$$

Frey, Balents; Radzihovsky&

Ising field: Real part of atomic field



Ising potential landscape:
Z_2 symmetry breaking

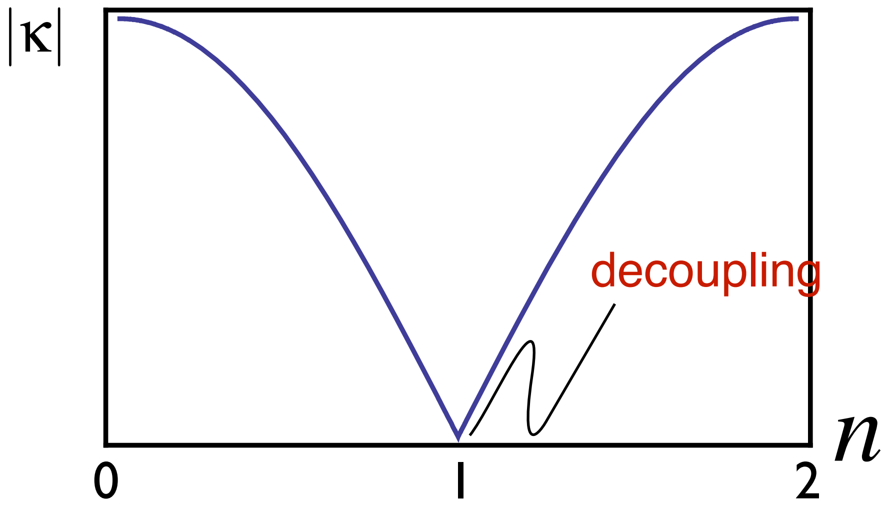
➡ Interactions persist to arbitrary long wavelength (cf. decoupling SW)

➡ $\kappa \neq 0$ Phase transition is driven first order by coupling of Ising and Goldstone mode

Ising Quantum Critical Point around n=1

- Plot the Ising-Goldstone coupling:

$$S_{\text{int}}[\vartheta, \phi] = i\kappa \int \partial_\tau \vartheta \, \phi^2$$



$$\Gamma \ni \int_{\vec{x},\tau} b^\dagger_{2,i}(-g_2\mu)b_{2,i}$$

- Symmetry argument:
  - dimer compressibility must have zero crossing
  - Ward identies for time-local gauge invariance and atom-dimer phase locking

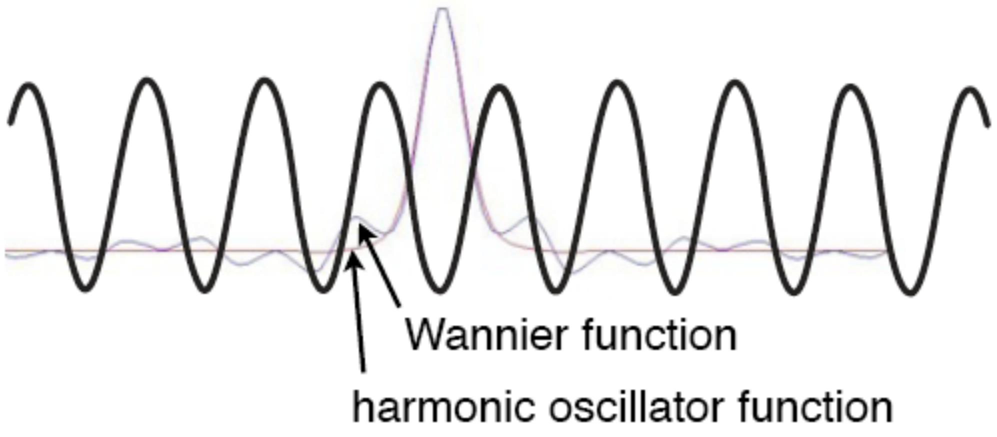
➡κ must have zero crossing: true quantum critical Ising transition

- Estimate correlation length: $\xi/a \sim \kappa^{-6} \sim |1-n|^{-6}$

➡weakly first order, broad near critical domain

➡ Second order quantum critical behavior is a lattice + constraint effect

Effective Lattice Hamiltonian



- Start from our model Hamiltonian, add optical potential:

$$H = \int_{\mathbf{x}} [a^\dagger_{\mathbf{x}}(- \frac{\triangle}{2m} - \mu + V(\mathbf{x}) + V_{\text{opt}}(\mathbf{x}) \ )a_{\mathbf{x}} + g\hat{n}^2_{\mathbf{x}}]$$

- Periodicity of the optical potential suggests expansion of field operators into localized lattice periodic Wannier functions (complete set of orthogonal functions)

$$a_{\mathbf{x}} = \sum_{i,n} w_n(\mathbf{x} - \mathbf{x}_i)b_{i,n}$$

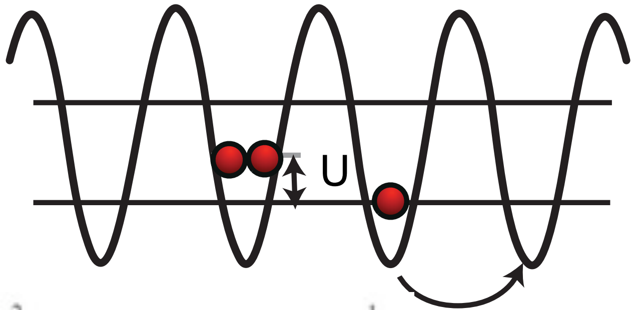
band index

minimum position

- For low enough energies (temperature), we can restrict to lowest band:

$$T, U, J \ll \sqrt{4V_0E_R}, E_R = k^2/(2m) \rightarrow n = 0$$

- Then we obtain the single band (Bose-) Hubbard model

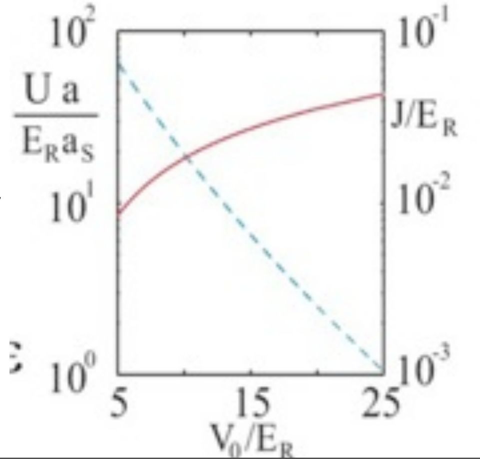


$$H = -J\sum_{\langle i,j \rangle} b^\dagger_i b_j - \mu \sum_i \hat{n}_i + \sum_i \epsilon_i \hat{n}_i + \tfrac{1}{2}U \sum_i \hat{n}_i(\hat{n}_i - 1)$$

$$\hat{n}_i = b^\dagger_i b_i$$

$$J = -\int dx w^*_0(x)(-\hbar^2/2m\triangle - V_{\text{opt}}(x))w_0(x - \lambda/2)$$

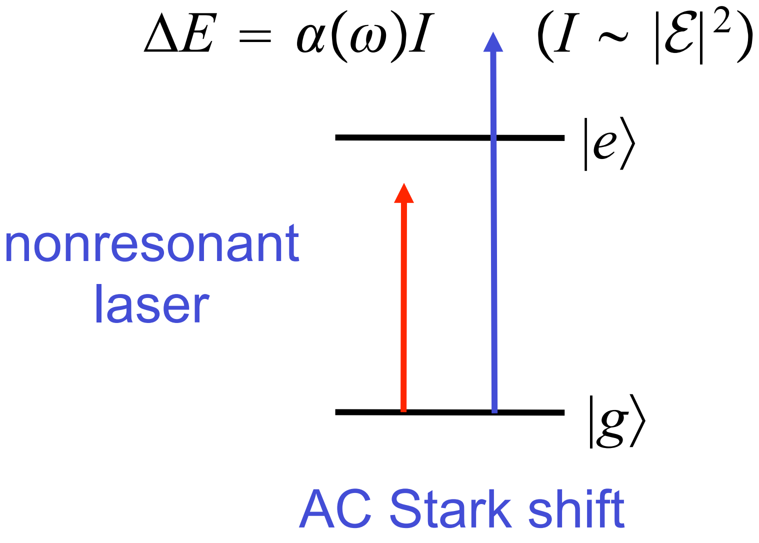
$$U = g\int dx|w_0(x)|^4$$

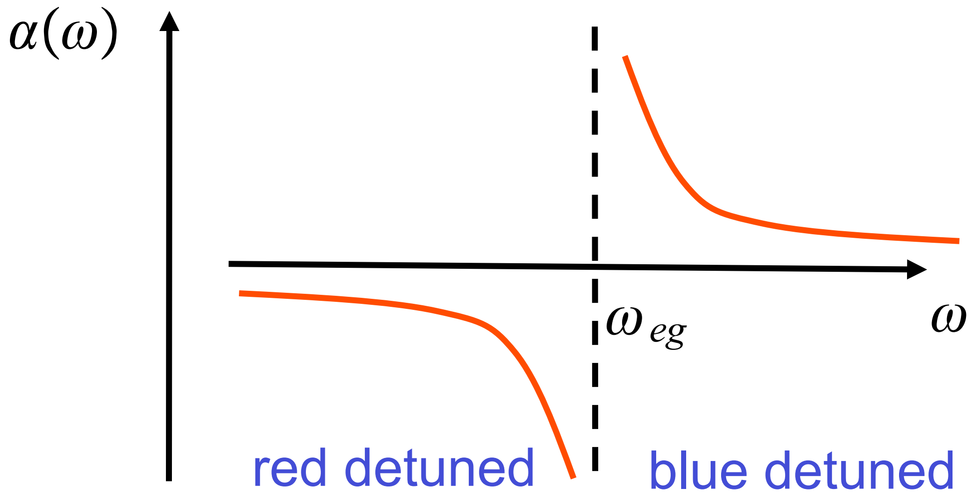


Cold Atoms in Optical Lattices

Optical Lattices

AC-Stark shift: We consider an atom in its electronic ground state exposed to laser light at fixed position $\vec{x}$. If the light is far detuned from excited state resonances, the ground state will experience a second-oder *AC-Stark shift* $\delta E_g(\vec{x}) = \alpha(\omega) I(\vec{x})$ with $\alpha(\omega)$ the dynamic polarizability of the atom for frequency ω, and $I(\vec{x})$ the light intensity.





Example: for a two-level atom $\{|g\rangle, |e\rangle\}$ in the RWA the AC-Starkshift is given by $\delta E_g(\vec{x}) = \hbar \frac{\Omega^2(\vec{x})}{4\Delta}$ with Rabi frequeny Ω and detuning $\Delta = \omega - \omega_{eg}$ ($\Omega \ll \Delta$). Note that for red detuning ($\Delta < 0$) the ground state shifts down $\delta E_g < 0$, while for blue detuning ($\Delta > 0$) we have $\delta E_g > 0$.

Bloch Theorem for Periodic Potentials

- Consider a Hamiltonian (in 1D) $\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x})$ with periodic potential $V(x) = V(x+a)$. We are interested in the eigenfunctions $H\psi(x) = E\psi(x)$. (We set $\hbar = 1$).
- We define a translation operator $T = e^{-i\hat{p}a}$ so that $T\psi(x) = \psi(x+a)$.
  - T is unitary, and thus has eigenfunctions $T\phi_\alpha(x) = e^{i\alpha}\phi_\alpha(x)$ with $\alpha = (-\pi, \pi]$ real.
  - Because $\phi_\alpha(x+a) = e^{i\alpha}\phi_\alpha(x)$ we can write $\phi_\alpha(x) = e^{i\alpha}u_\alpha(x)$ with periodic Bloch functions $u_\alpha(x) = u_\alpha(x+a)$.
- We have $[H, T] = 0$, and we can find simultaneous eigenfunctions of $\{H, T\}$

$$\begin{aligned} H\varphi_q(x) &= E\varphi_q(x) \\ T\varphi_q(x) &= e^{iqa}\varphi_q(x) \end{aligned}$$

with $q \in [-\pi/a, \pi/a]$. We call $\hbar q$ quasimomentum.

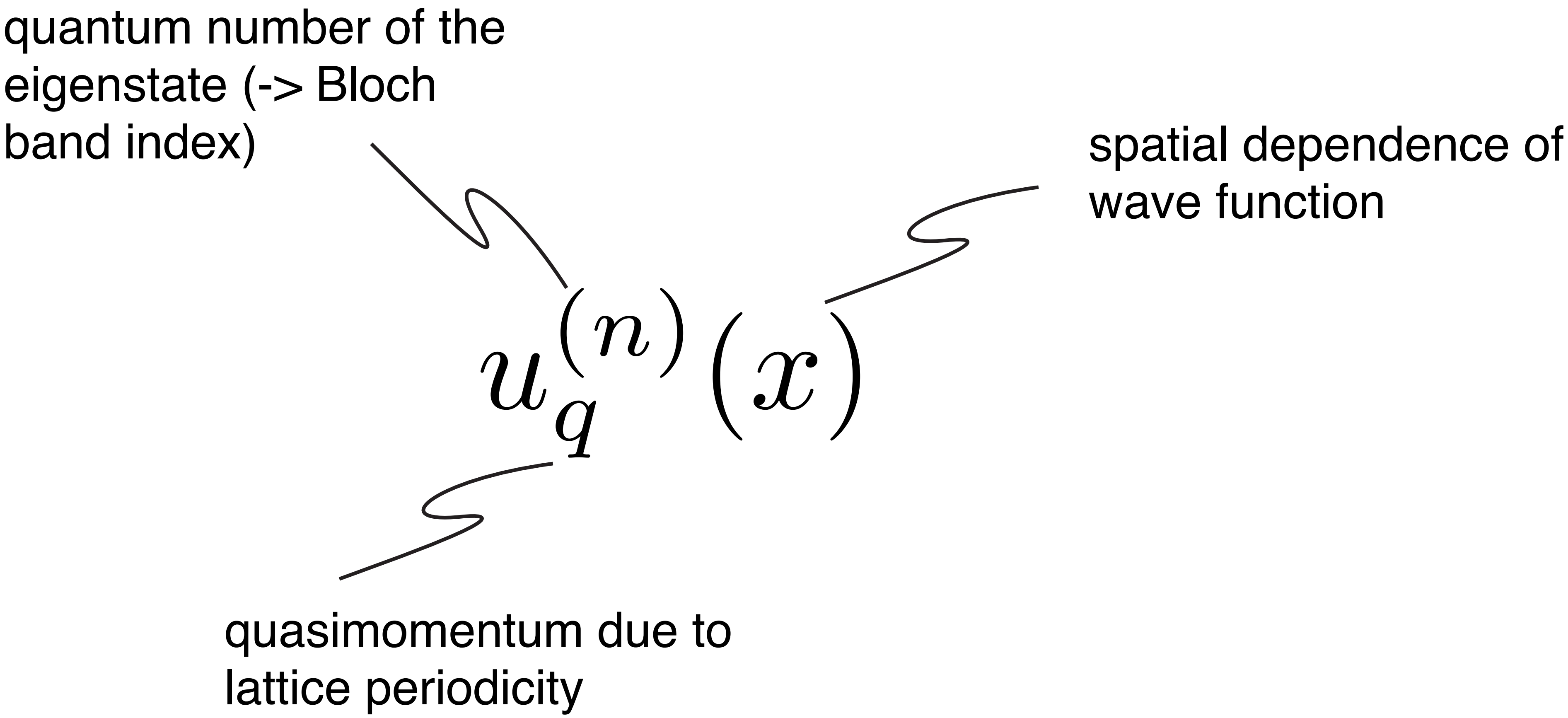
Bloch Theorem for Periodic Potentials

- Eigenstates of the Hamiltonian thus have the form

$$\boxed{\phi_q^{(n)}(x) = e^{iqx} u_q^{(n)}(x) \quad q \in [-\pi/a, \pi/a]}$$

and the Bloch functions $u_q^{(n)}(x)$ are eigenstates of

$$\boxed{\hat{h}_q u_q^{(n)}(x) \equiv \left(\frac{(\hat{p}+q)^2}{2m} + V(\hat{x}) \right) u_q^{(n)}(x) = \epsilon_q^{(n)} u_q^{(n)}(x)}$$



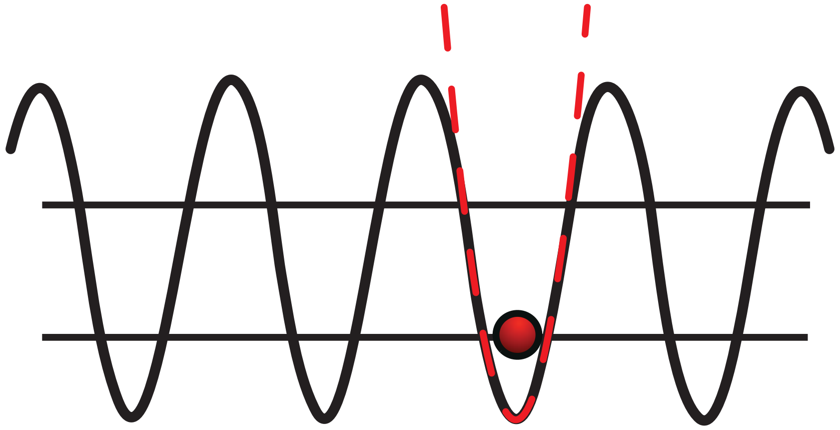
quantum number of the eigenstate (-> Bloch band index)

spatial dependence of wave function

$$u_q^{(n)}(x)$$

quasimomentum due to lattice periodicity

Solution of Schroedinger Equation for 1D optical lattice



Harmonic approximation (1D): For deep lattices we can ignore tunneling. Assuming $V_0 > 0$ we have for the lowest states a *harmonic oscillator potential*

$$V(x) = V_0 \sin^2(kx) \approx V_0 \, (kx)^2 \approx \frac{1}{2} m \nu^2 x^2$$

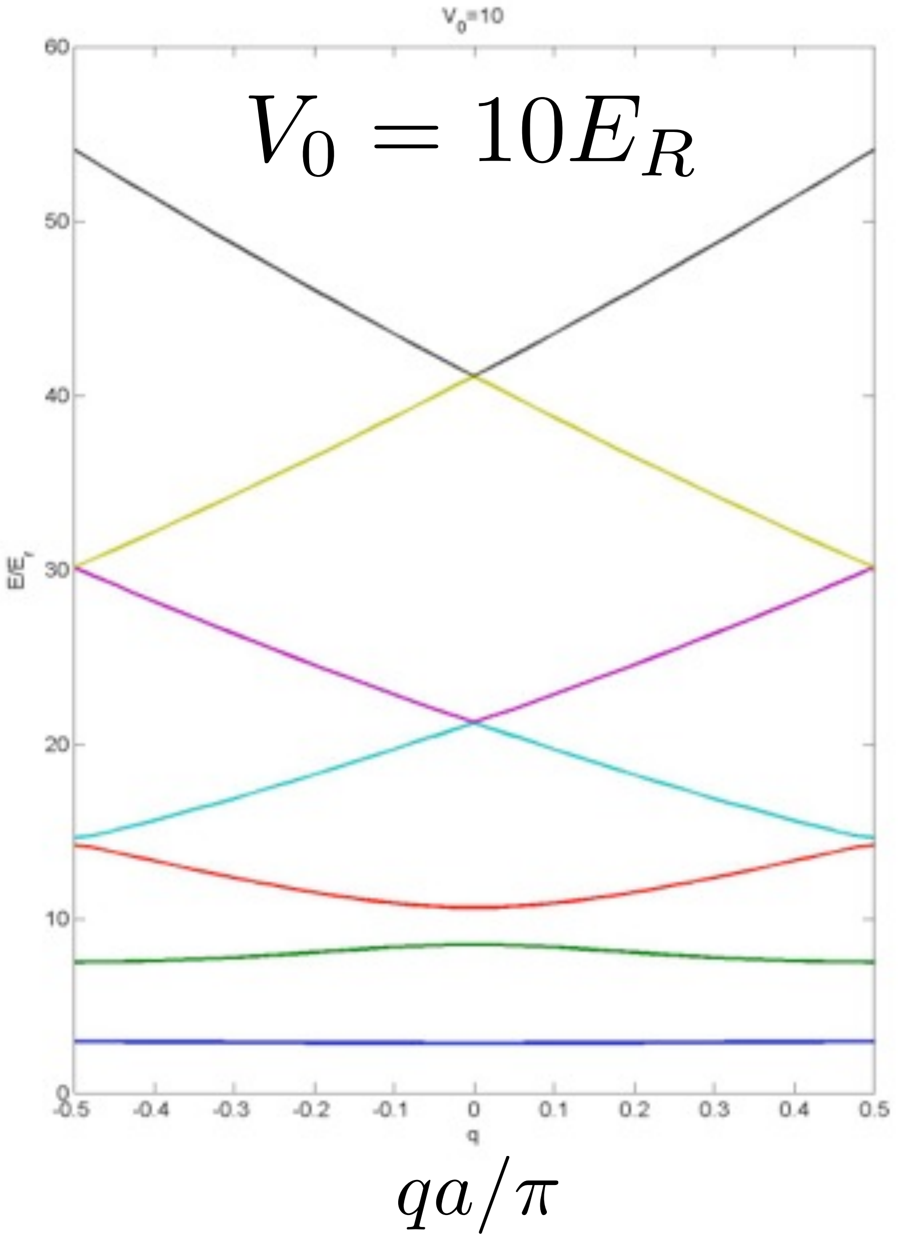
with *trapping frequency* $\nu = \sqrt{4 V_0 E_R}/\hbar$ and with *recoil frequency / energy* $E_R \equiv \hbar^2 k^2/2m$. (Typcially$E_R \sim$ kHz, and $V_0 \sim$ few tens of kHz.)

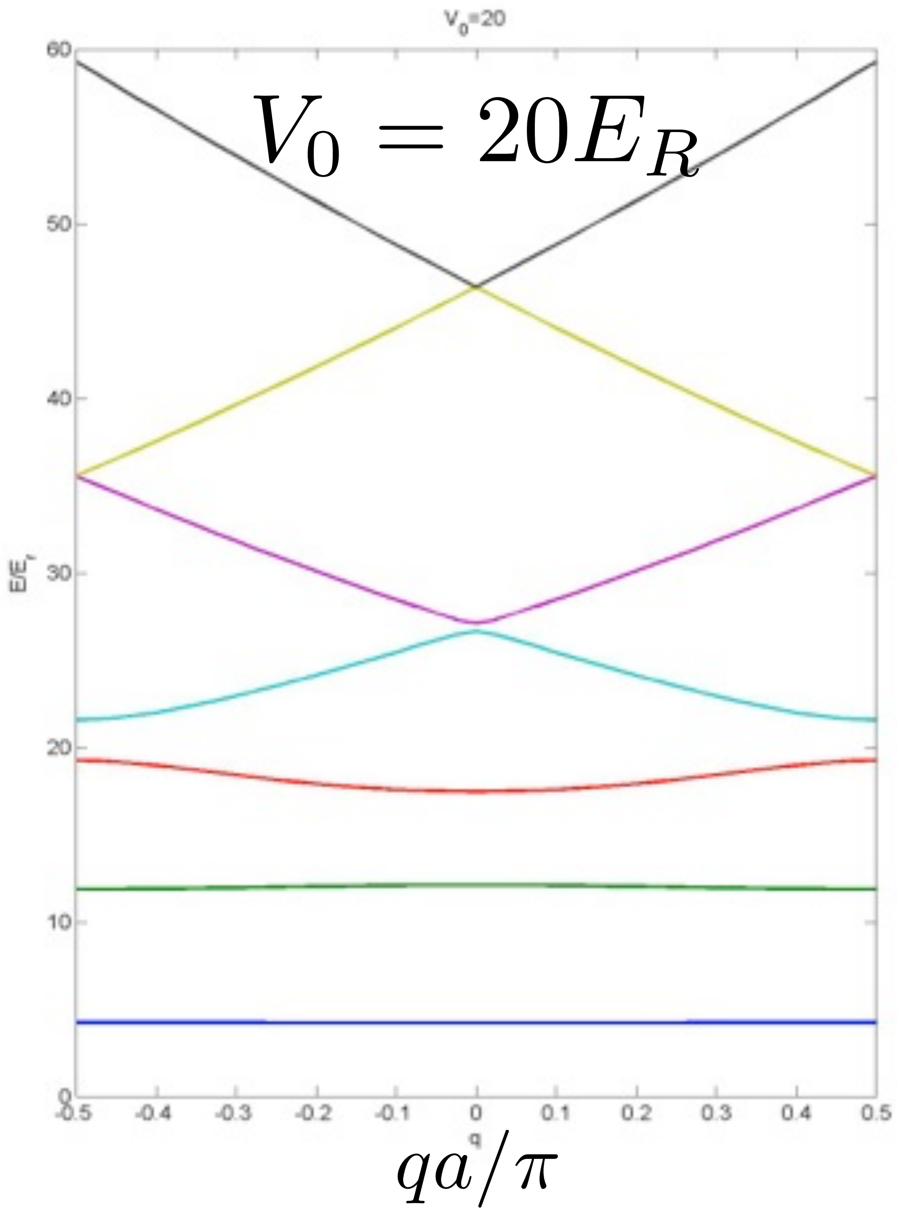
The ground state wave function

$$\psi_{n=0}(x) = \sqrt{\frac{1}{\pi^{1/2} a_0} \mathrm{e}^{-x^2/(2a_0^2)}}$$

has size $a_0 = \sqrt{\hbar/m\nu} \ll \lambda/2$, and we are in the Lamb-Dicke limit $\eta = 2\pi a_0/\lambda \ll 1$.

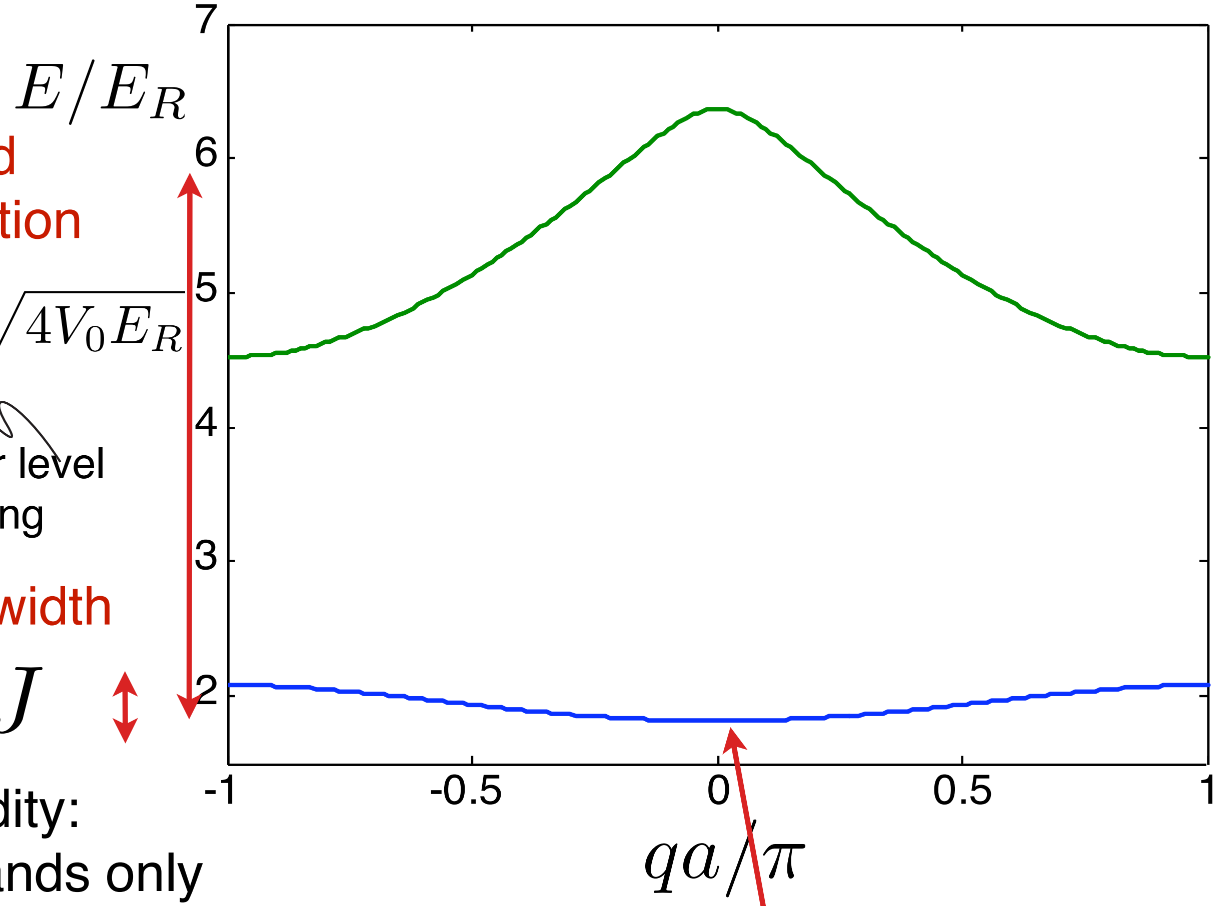
Band Structure





Bloch wave functions and bands (1D): In general the eigen-solutions of the time-independent Schrödinger equation with periodic potential, $H\psi_{nq}(x) = \epsilon_{nq}\psi_{nq}(x$ has the form $\psi_{nq}(x) = e^{iqx}u_{nq}(x)$ with (periodic) Bloch wave functions $u_{nq}(x) = u_{nq}(x+a)$, q the quasimomentum in the first Brillouin zone $-\pi/a < q \leq +\pi/a$, and $n = 0, 1, \ldots$ labelling the Bloch bands.

Lowest Two Bloch Bands for V_0=5 E_R



band separation

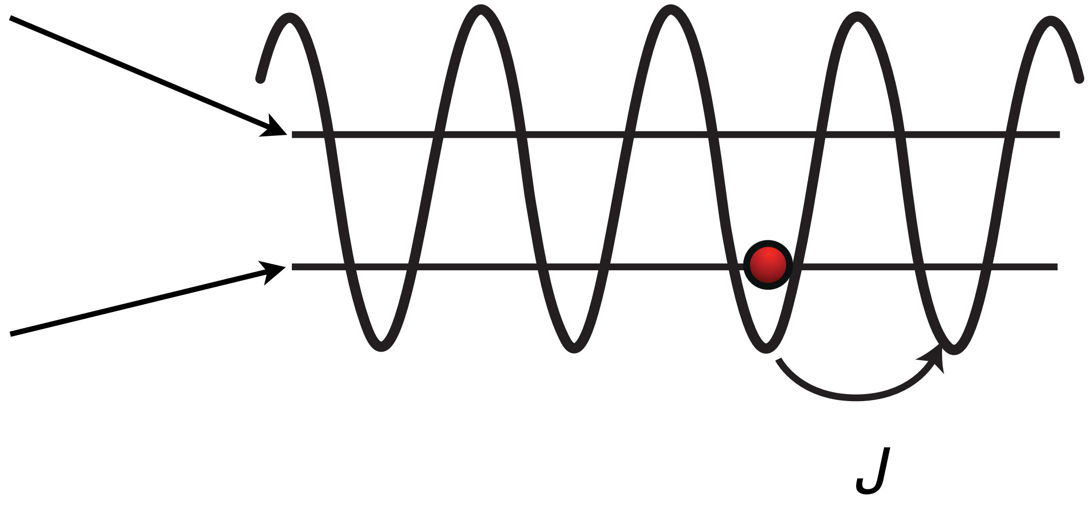
$\omega_{\text{Bloch}} \approx \sqrt{4V_0 E_R}$

oscillator level spacing

bandwidth

$4J$

validity:
lowest bands only



Compare: Bloch bands in tight binding approximation. Above we introduced the Hamiltonian

$$\hat{H} = -J \sum_i \left(b_i^\dagger b_{i+1} + b_{i+1}^\dagger b_i \right) = \sum_q \epsilon_q b_q^\dagger b_q$$

with the tight-binding dispersion relation

$$\epsilon_q = -2J \cos qa \quad (-\pi/a < q \leq \pi/a).$$

For well separated bands the Bloch band calculation fits this relation well. This is typically fulfilled for the lowest bands.

Wannier functions

Wannier functions (1D): Instead of Bloch wave functions we can also work with *Wannier wave functions*

$$u_{\boxed{q}}^{(n)}(x) = \sqrt{\frac{a}{2\pi}} \sum_{x_i = ia} w_n(x - x_i) \mathrm{e}^{\mathrm{i} x_i q},$$

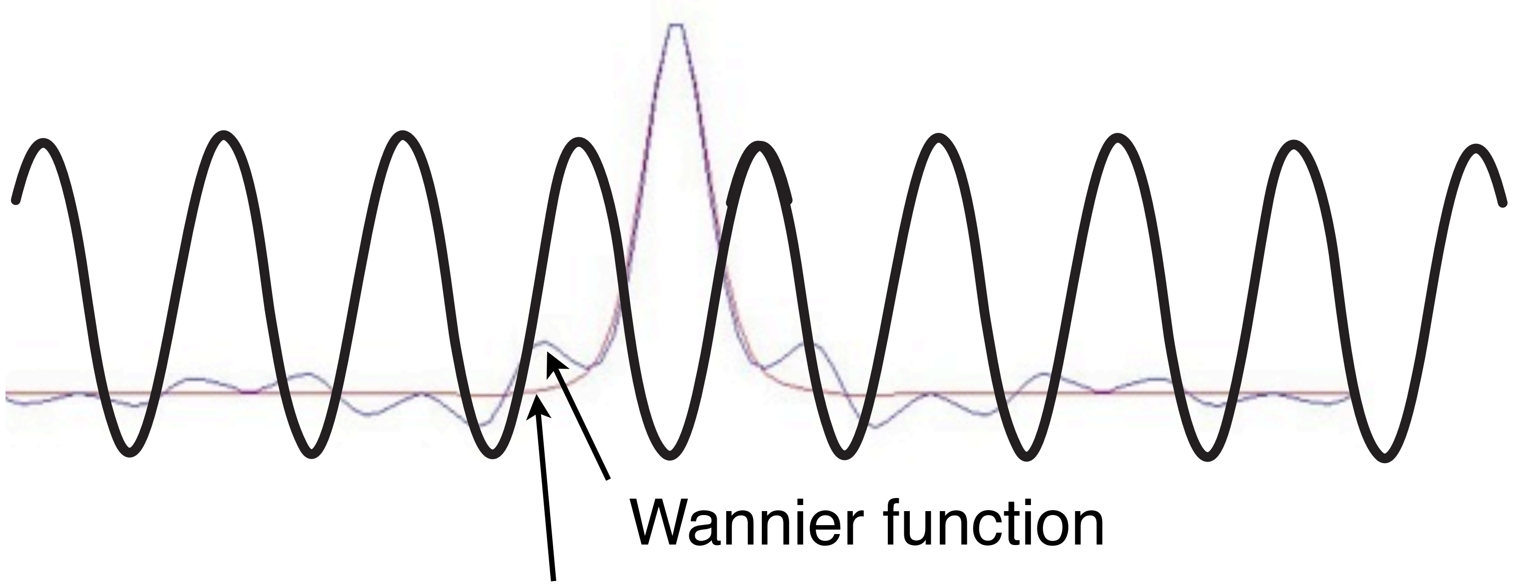
discrete Fourier transform

$$w_n(x - \boxed{x_i}) = \sqrt{\frac{a}{2\pi}} \int_{-\pi/a}^{\pi/a} \mathrm{d}q \, u_{nq}(x) \, \mathrm{e}^{-iqx_i}$$

trade quasimomentum for site index

which are *localized* around a particular lattice site $x_i = ia$ with $i = 0, \pm 1, \ldots$.

The Bloch and Wannier wave functions are complete set of functions

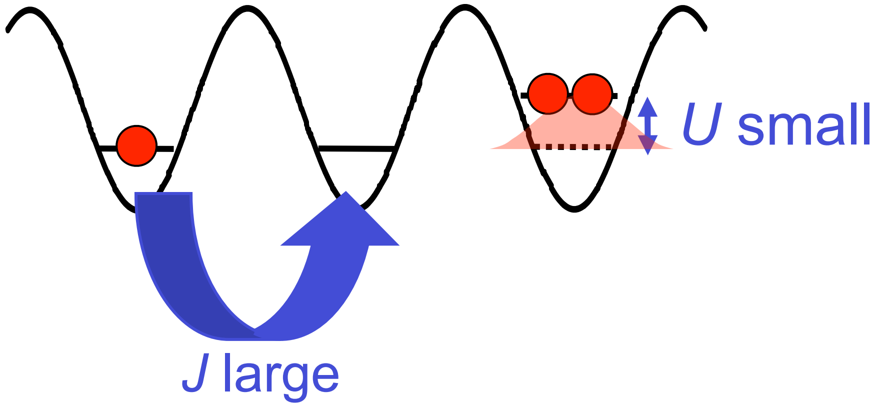


Wannier function

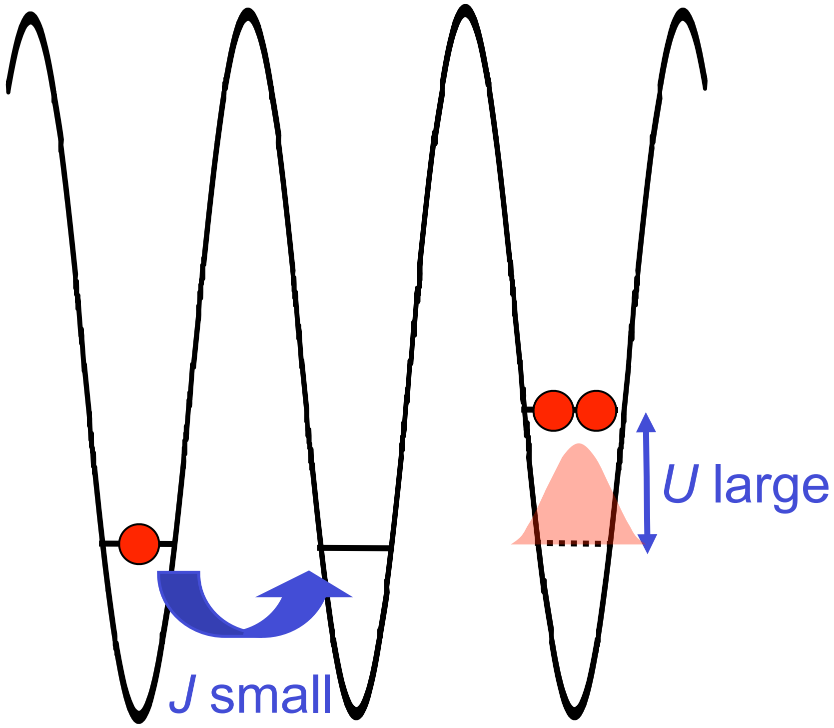
harmonic oscillator function

Laser Control: Kinetic vs. Potential Energy

- **shallow lattice** : weak laser



- **deep lattice:** intense laser



weakly interacting system:

$J >> U$

(kinetic energy >> interactions)

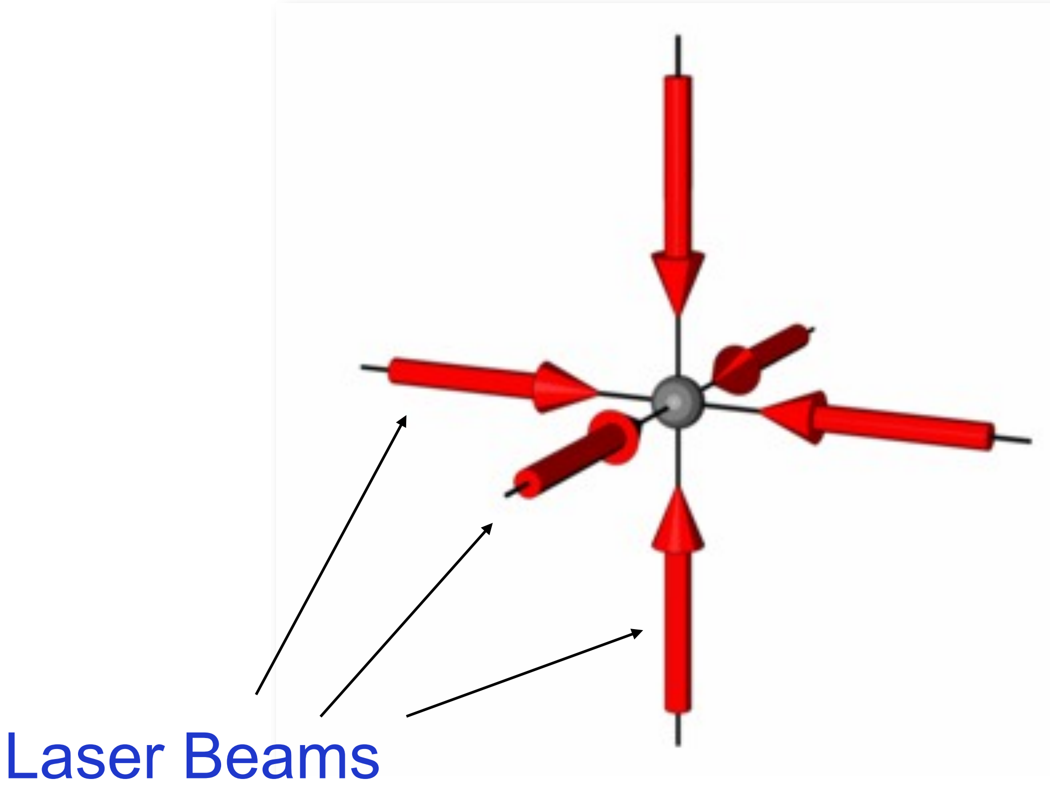
↕ laser parameters (time dependent)

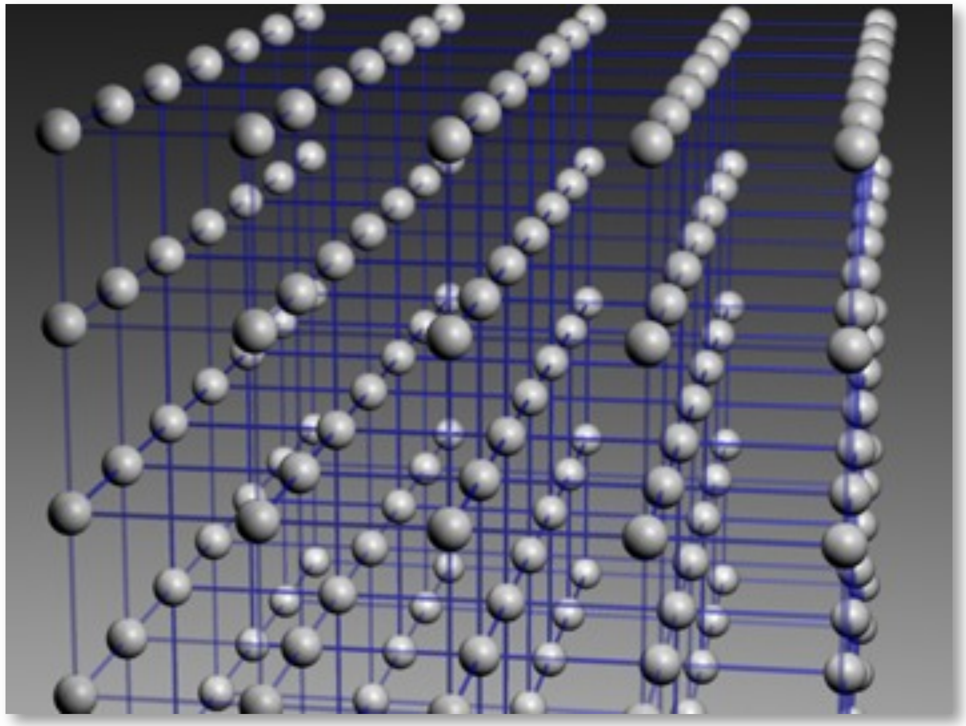
strongly interacting system:

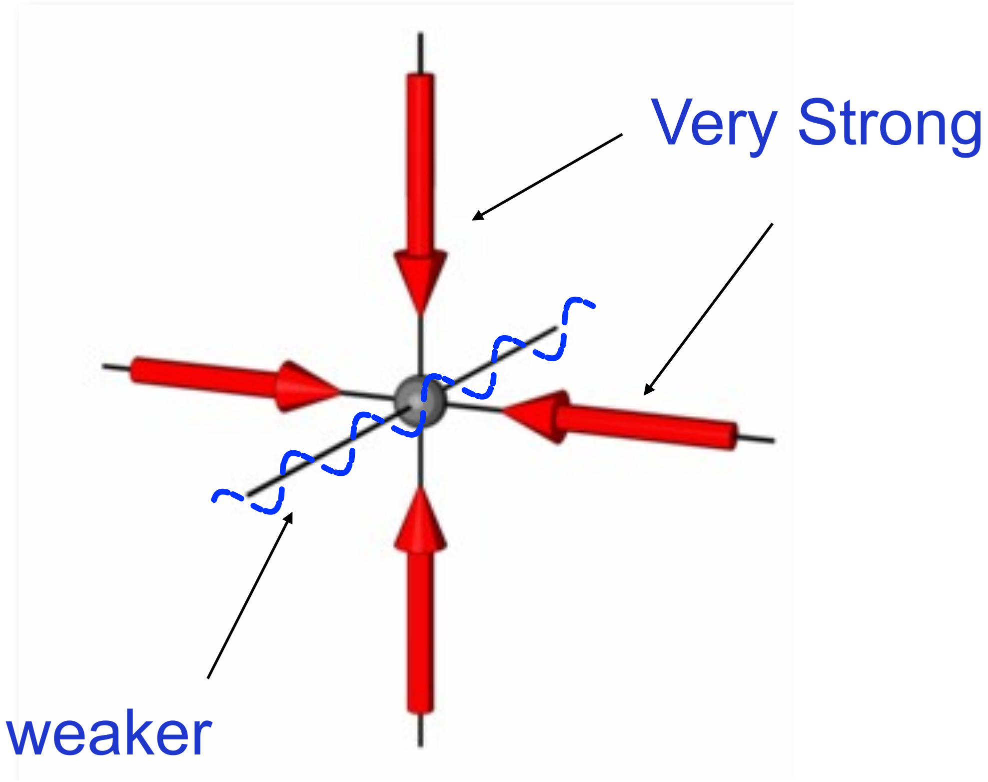
$J << U$

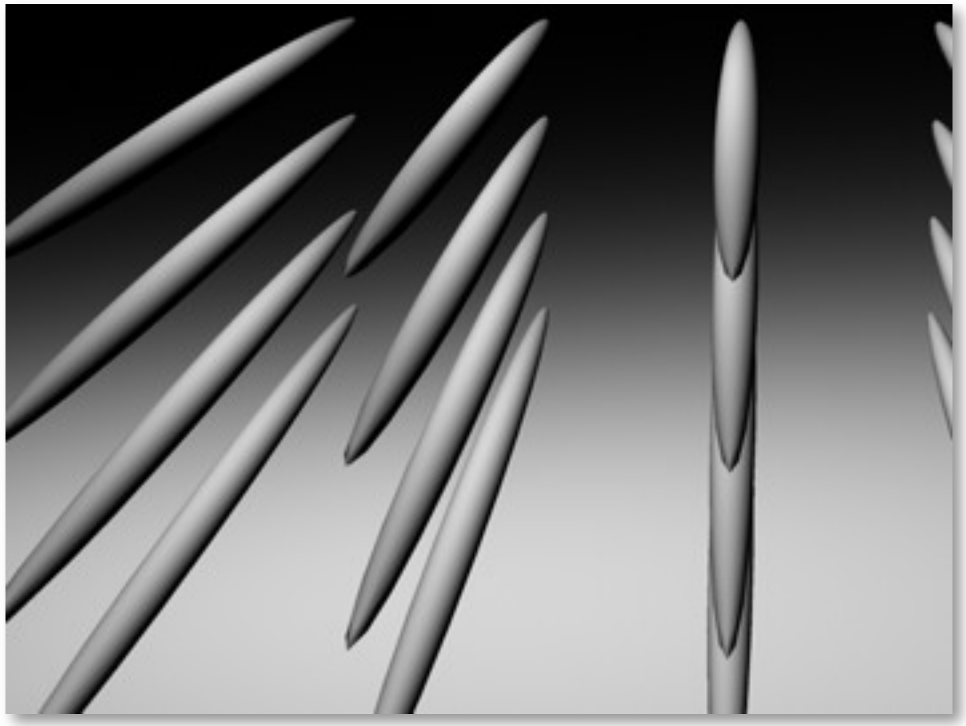
(kinetic energy << interactions)

Optical Lattice Configurations









Optical Lattice Configurations