ADVANCED QUANTUM MECHANICS

TUTORIALS 2024–2025

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Please ask me MANY questions!

Wednesday, September 25$^{\text{th}}$, 2024

Outline of the tutorials for the first half ot the semester

- **Problem 1:** two–particle interference
- **Problem 2:** coherence and correlations in quantum gases
- **Problem 3:** lattice models, superfluid/Mott insulator transition

All problems describe experiments that have actually been performed

They all contain elements of theory and introduce calculation techniques

They all contain both standard questions and (very?) hard questions

A bird's eye view of the problem

Problem #2: Spatial Correlation Functions in Bose and Fermi gases

- One–body and two–body (reduced) density matrices
- Ideal Bose and Fermi gases at temperature $T = 0$

  Off–diagonal long–range order in bosonic systems
- Ideal quantum gases at non–zero temperature

  Description in terms of second quantisation
- First steps with interacting systems

Review: Reduced density matrix:

an example from quantum information

No identical particles in this digression.

[Nielsen & Chuang, *Quantum Computation and Quantum Information*, CUP (2000), §1.3.6]

Bipartite system: Alice's reduced density matrix

- The system comprises two parts: A (Alice) and B (Bob)

  The Hilbert space for the joint system is a tensor product: $\mathscr{H} = \mathscr{H}_A \otimes \mathscr{H}_B$

- The state of the joint system is described by a density matrix ρ acting on $\mathscr{H}$

  Pure state $|\Psi\rangle$ (e.g. ground state, not necessarily product state): $\rho = |\Psi\rangle\langle\Psi|$

  Thermal equilibrium at temperature T: $\rho = e^{-\beta H} / \mathrm{Tr}(e^{-\beta H})$

- Alice may measure any observable affecting her part of the system: $M_A = M_A \otimes \mathbb{1}_B$

  What information on the joint system does she have access to?

  Not the full ρ, but the reduced density matrix $\rho_A = \mathrm{Tr}_B(\rho)$ (partial trace over $\mathscr{H}_B$)

Local measurements on $\mathscr{H}_A$ access ρ_A only

- The complete density matrix ρ acts on $\mathscr{H} = \mathscr{H}_A \otimes \mathscr{H}_B$

  Let $\{|a_i\rangle\}$ be a basis of $\mathscr{H}_A$ and $\{|b_j\rangle\}$ a basis of $\mathscr{H}_B$

  $\rho_A = \mathrm{Tr}_B(\rho) = \sum_j \langle b_j|\rho|b_j\rangle$ acts on $\mathscr{H}_A$ only

  Show that ρ_A does not depend on the choice of the basis $\{|b_j\rangle\}$

- A local observable M_A is an observable acting only on $\mathscr{H}_A$: $M_A = M_A \otimes \mathbb{1}_B$

  $\langle M_A\rangle = \mathrm{Tr}[\,\rho\,(M_A \otimes \mathbb{1}_B)\,] = \sum_{i,j} \langle a_i,b_j|\,\rho\,(M_A \otimes \mathbb{1}_B)\,|a_i,b_j\rangle$

  Act with $(M_A \otimes \mathbb{1}_B)$ on $|a_i,b_j\rangle$: $|b_j\rangle$ is unaffected

  $$\langle M_A\rangle = \sum_i \langle a_i| \left(\sum_j \langle b_j|\rho|b_j\rangle \; M_A \right) |a_i\rangle = \sum_i \langle a_i|\,\rho_A M_A\,|a_i\rangle$$

$$\langle M_A\rangle \quad = \quad \mathrm{Tr}_A(\rho_A\, M_A) \qquad \text{with } \rho_A = \mathrm{Tr}_B(\rho)$$

The averages of all local observables are piloted by the reduced density matrix ρ_A

Example: Alice's reduced density matrix for Bell states

- Four Bell states: (maximally entangled two–particle states)
  $|\Phi_\pm\rangle = \left(|\uparrow\rangle_A |\uparrow\rangle_B \pm |\downarrow\rangle_A |\downarrow\rangle_B\right)/\sqrt{2}$ and $|\Psi_\pm\rangle = \left(|\uparrow\rangle_A |\downarrow\rangle_B \pm |\downarrow\rangle_A |\uparrow\rangle_B\right)/\sqrt{2}$

- Pure state $|\Phi_+\rangle\langle\Phi_+| = \left(|\uparrow\rangle_A |\uparrow\rangle_B + |\downarrow\rangle_A |\downarrow\rangle_B\right)\left(\langle\uparrow|_A \langle\uparrow|_B + \langle\downarrow|_A \langle\downarrow|_B\right)/2$

$$\begin{aligned}\mathrm{Tr}_B(|\Phi_+\rangle\langle\Phi_+|) &= \langle\uparrow_B|\Phi_+\rangle\langle\Phi_+|\uparrow_B\rangle + \langle\downarrow_B|\Phi_+\rangle\langle\Phi_+|\downarrow_B\rangle \\ &= (|\uparrow_A\rangle\langle\uparrow_A| + |\downarrow_A\rangle\langle\downarrow_A|)/2\end{aligned}$$

- Pure state $|\Psi_-\rangle\langle\Psi_-| = \left(|\uparrow\rangle_A |\downarrow\rangle_B - |\downarrow\rangle_A |\uparrow\rangle_B\right)\left(\langle\uparrow|_A \langle\downarrow|_B - \langle\downarrow|_A \langle\uparrow|_B\right)/2$

$$\begin{aligned}\mathrm{Tr}_B(|\Psi_-\rangle\langle\Psi_-|) &= \langle\uparrow_B|\Psi_-\rangle\langle\Psi_-|\uparrow_B\rangle + \langle\downarrow_B|\Psi_-\rangle\langle\Psi_-|\downarrow_B\rangle \\ &= (|\uparrow_A\rangle\langle\uparrow_A| + |\downarrow_A\rangle\langle\downarrow_A|)/2\end{aligned}$$

Local measurements by Alice cannot distinguish

any of the four Bell states from a statistical mixture with equal weights

Advanced Quantum Mechanics

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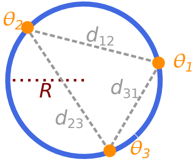
Wednesday, October 2nd, 2024

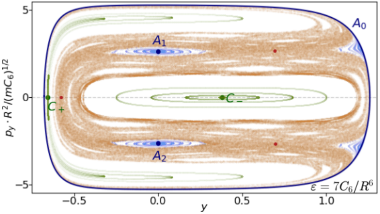
Rydberg atoms: chaos & semiclassical physics

- **Non–ergodicity** of 3 **interacting** Rydberg atoms in a circular trap



This conceptually simple system is **experimentally accessible**
due to recent progress in Rydberg atom trapping in Paris and Palaiseau

[D.J. Papoular & B. Zumer, Phys. Rev. A **107**, 022217 (2023)]
[D.J. Papoular & B. Zumer, Phys. Rev. A **110**, 012230 (2024)]



Two mechanisms impeding ergodicity in the absence of disorder:

1. quantum mechanism: **quantum scar** [Heller PRL 1984]
2. classical mechanism: **KAM tori** (**K**olmogorov, **A**rnold, **M**oser)
   [Arnold, *Mathematical Methods of Classical Mechanics*, Springer (1989)])

Both mechanisms yield quantum eigenstates
localised near classical periodic trajectories

- Telling them apart requires a detailed understanding of the **classical system** and accurate **numerical calculations** of the quantum eigenstates (not ground state!)
- **Semiclassical analysis** which goes beyond the WKB approach

  Gutzwiller's trace formula, Einstein–Brillouin–Keller theory
  [M.C. Gutzwiller, *Chaos in Classical and Quantum Mechanics*, Springer (1990)]

Spontaneous applications for a PhD position with me are welcome

Summary: Towards the one–body density matrix $\rho^{(1)}$

- Example from quantum information:

  Alice and Bob share a system defined on the Hilbert space $\mathscr{H} = \mathscr{H}_A \otimes \mathscr{H}_B$

  The complete density matrix ρ acts on $\mathscr{H}$

  Alice **only performs measurements on her part of the system:** $M_A = M_A \otimes \mathbb{1}_B$

  She cannot determine ρ, i.e. she cannot detect entanglement

  She may only access the reduced density matrix $\rho_A = \mathrm{Tr}_B(\rho)$ which acts on $\mathscr{H}_A$

  .

- **Goal:** Define analogue of the reduced density matrix for **many identical particles**

  Identify a family of experiments analogous to Young's slits

Part 1:

One–body density matrix for systems of identical particles

Definition and general properties

[C. Cohen–Tannoudji & D. Guéry–Odelin,
Advances in Atomic Physics: an overview, World Scientific (2011), §23.2]

Hilbert space for a system with given particle number N

- Start from the Hilbert space for a single particle: $\mathscr{E}$

  spin–1/2 particle frozen in space: $\dim \mathscr{E} = 2$; spin–0 particle moving in 1D: $\mathscr{E} = L^2(\mathbb{R})$

- ***N* Distinguishable particles:** $\mathscr{E}^{(N)} = \underbrace{\mathscr{E} \otimes \mathscr{E} \otimes \cdots \otimes \mathscr{E}}_{\text{tensor product of } N \text{ copies of } \mathscr{E}}$

  N frozen spin–1/2 particles: $\dim \mathscr{E} = 2^N$; N spin–0 particles in 1D: $\mathscr{E} = L^2(\mathbb{R}^N)$

- ***N* identical particles**:

Bosons

$\mathscr{E}_S^{(N)}$: **wavefunctions** are symmetric under particle exchange

density matrices operate on $\mathscr{E}_S^{(N)}$

$$\rho : \quad \mathscr{E}_S^{(N)} \longrightarrow \mathscr{E}_S^{(N)}$$

Fermions

$\mathscr{E}_A^{(N)}$: **wavefunctions** are antisymmetric under particle exchange

density matrices operate on $\mathscr{E}_A^{(N)}$

$$\rho : \quad \mathscr{E}_A^{(N)} \longrightarrow \mathscr{E}_A^{(N)}$$

Composition of the permutation operators P_σ

- **Convention used at ICFP:** (J. Dalibard and Y. Castin's notes, F. Chevy's slides, ...)

$$P_\sigma \, |u_1\rangle \otimes |u_2\rangle \otimes \cdots \otimes |u_N\rangle \quad = \quad |u_{\sigma(1)}\rangle \otimes |u_{\sigma(2)}\rangle \otimes \cdots \otimes |u_{\sigma(N)}\rangle$$

Then, $P_\sigma P_{\sigma'} = P_{\sigma' \circ \sigma}$ (note the opposite orderings of σ and σ' on either side of $=$)

Proof: $P_{\sigma'} \, |u_1\rangle \otimes |u_2\rangle \otimes \cdots \otimes |u_N\rangle = |v_1\rangle \otimes |v_2\rangle \otimes \cdots \otimes |v_N\rangle$ with $|v_j\rangle = |u_{\sigma'(j)}\rangle$

$P_\sigma \, |v_1\rangle \otimes |v_2\rangle \otimes \cdots \otimes |v_N\rangle = |w_1\rangle \otimes |w_2\rangle \otimes \cdots \otimes |w_N\rangle$ with $|w_i\rangle = |v_{\sigma(i)}\rangle$

Hence, $P_\sigma P_{\sigma'} \, |u_1\rangle \otimes |u_2\rangle \otimes \cdots \otimes |u_N\rangle = |w_1\rangle \otimes |w_2\rangle \otimes \cdots \otimes |w_N\rangle$ with $|w_i\rangle = |u_{\sigma'[\sigma(i)]}\rangle$

- **Beware:** other authors use different conventions

For example, Cohen–Tannoudji, Diu, and Laloe define $P_\sigma^{\mathrm{CDL}} = P_\sigma^{-1}$ (Vol. II, Eq. XIV.B.38)

so that $P_{\sigma'}^{\mathrm{CDL}} P_\sigma^{\mathrm{CDL}} = P_{\sigma' \circ \sigma}^{\mathrm{CDL}}$.

Density matrix is invariant under particle exchange (qu. 1)

- **For a pure state $|\Psi\rangle$,** the many–body density matrix is $\rho = |\Psi\rangle\langle\Psi|$

  Exchange the N particles through the permutation σ:

  $$\langle \mathbf{r}_{\sigma(1)},\dots,\mathbf{r}_{\sigma(N)}|\,\rho\,|\mathbf{r}'_{\sigma(1)},\dots\mathbf{r}'_{\sigma(N)}\rangle = \langle \mathbf{r}_1,\dots,\mathbf{r}_N|\;P^\dagger_\sigma|\Psi\rangle\langle\Psi|P_\sigma\;|\mathbf{r}'_1,\dots\mathbf{r}'_N\rangle$$

  for bosons, $P_{\sigma^{-1}}|\Psi\rangle = +|\Psi\rangle$; for fermions, $P_{\sigma^{-1}}|\Psi\rangle = (-)^{(\sigma^{-1})}|\Psi\rangle = (-)^{\sigma}|\Psi\rangle$

  $P^\dagger_\sigma|\Psi\rangle = P_{\sigma^{-1}}|\Psi\rangle$ appears twice (once as a ket, once as a bra): $[(-)^\sigma]^2 = 1$

  therefore $\langle \mathbf{r}_1,\dots,\mathbf{r}_N|P^\dagger_\sigma|\Psi\rangle\langle\Psi|P_\sigma|\mathbf{r}'_1,\dots\mathbf{r}'_N\rangle = +\langle \mathbf{r}_1,\dots,\mathbf{r}_N||\Psi\rangle\langle\Psi||\mathbf{r}'_1,\dots\mathbf{r}'_N\rangle$

- **Statistical mixture:** diagonalise the Hermitian operator $\rho = \sum_i p_i\;|\Psi_i\rangle\langle\Psi_i|$

  The many–particle wavefunctions $|\Psi_i\rangle$ are symmetric or antisymmetric

  The previous argument holds for each term in the sum.

The density matrix ρ is fully symmetric for bosons and for fermions

A bird's eye view of the problem

Problem #2: Spatial Correlation Functions in Bose and Fermi gases

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Single–particle operators (qu. 2)

- Start from an operator f acting on the single–particle subspace $\mathscr{E}$

e.g. kinetic energy $\mathbf{p}^2/(2m)$, trapping potential $v(\mathbf{r}) = m\omega_0^2\mathbf{r}^2/2, \ldots$ (not 2–particle interaction)

- Extend it to the N–particle Hibert space $\mathscr{E}_N$: $F^{(i)}$ acts on particle i

$$F = \sum_{i=1}^{N} F^{(i)} = \sum_{i=1}^{N} \mathbb{1}^{(1)} \otimes \ldots \otimes \mathbb{1}^{(i-1)} \otimes f^{(i)} \otimes \mathbb{1}^{(i+1)} \otimes \ldots \otimes \mathbb{1}^{(N)}$$

e.g. total kinetic energy $K = \frac{\mathbf{p}_1^2}{2m} + \cdots + \frac{\mathbf{p}_N^2}{2m}$, total trapping energy $V = v(\mathbf{r}_1) + \cdots + v(\mathbf{r}_N)$

- Average value of a single–particle operator in the state ρ?

$\langle F \rangle = \mathrm{Tr}(\rho F) = \sum_i \mathrm{Tr}(\rho\, F^{(i)})$

$\langle F \rangle = N\ \mathrm{Tr}(\rho\, F^{(1)})$ (ρ is fully symmetric)

$\langle F \rangle = N\ \mathrm{Tr}_1[\,\mathrm{Tr}_{2,\ldots,N}\,(\rho\, F^{(1)})\,]$ (take the trace first along $2, \ldots, N$, then along 1)

$\langle F \rangle = N\ \mathrm{Tr}_1[\,\mathrm{Tr}_{2,\ldots,N}\,(\rho)\ f\,]$ ($F^{(1)}$ acts only on particle 1; f acts on $\mathscr{E}$)

For any **single–particle operator** F, $\langle F \rangle = \mathrm{Tr}(\rho^{(1)} f)$ with $\rho^{(1)} = N\ \mathrm{Tr}_{2,\ldots,N}(\rho)$

- The **one–body density operator** $\rho^{(1)}$ acts on the single–particle subspace $\mathscr{E}$

It is the analog of Alice's reduced density operator

Usefulness of the one–body density operator $\rho^{(1)}$

For any **single–particle operator** F, $\langle F \rangle = \mathrm{Tr}(\rho^{(1)} f)$ with $\rho^{(1)} = N\, \mathrm{Tr}_{2,\ldots,N}(\rho)$

- ρ acts on the many–particle Hilbert space, which is huge
  $\rho^{(1)}$ acts on the single–particle subspace, which is much smaller

- In order to describe **experiments probing only single–particle observables,**
  We do not need the full density matrix ρ: we just need $\rho^{(1)}$

- Famous example: *Bose–Einstein condensate with short–ranged interactions*
  $\langle \mathbf{r} | \rho^{(1)} | \mathbf{r}' \rangle = \psi_0^*(\mathbf{r})\, \psi_0(\mathbf{r}')$, where $\psi_0(\mathbf{r})$ satisfies the *Gross–Pitaevskii equation*
  We have replaced an ***N*–particle** problem satisfying the *Schrödinger* equation
  by a **single–variable** function which obeys a *non–linear* equation
  [More on this topic next week, at the end of the presentation for Problem 2]

One–body density operator: normalisation (end of qu. 1)

- $\rho^{(1)} = N\ \mathrm{Tr}_{2,\ldots,N}\,(\rho)$ means $\langle \mathbf{r}|\rho^{(1)}|\mathbf{r}'\rangle = N \int d\mathbf{r}_2 \cdots d\mathbf{r}_N\ \langle \mathbf{r}, \mathbf{r}_2, \ldots, \mathbf{r}_N|\ \rho\ |\mathbf{r}', \mathbf{r}_2, \ldots, \mathbf{r}_N\rangle$

  no integral on $\mathbf{r}$ and $\mathbf{r}'$

- **Diagonal element:**

  $\langle \mathbf{r}|\ \rho^{(1)}\ |\mathbf{r}\rangle = N \int d\mathbf{r}_2 \cdots d\mathbf{r}_N\ \langle \mathbf{r}, \mathbf{r}_2, \ldots, \mathbf{r}_N|\ \rho\ |\mathbf{r}, \mathbf{r}_2, \ldots, \mathbf{r}_N\rangle$

  This is N times the probability of finding a particle at point $\mathbf{r}$, i.e. the density $n(\mathbf{r})$

- **Trace of $\rho^{(1)}$:** $\mathrm{Tr}(\rho^{(1)}) = N \int d\mathbf{r} d\mathbf{r}_2 \cdots d\mathbf{r}_N\ \langle \mathbf{r}, \mathbf{r}_2, \ldots, \mathbf{r}_N|\ \rho\ |\mathbf{r}, \mathbf{r}_2, \ldots, \mathbf{r}_N\rangle = N$

- Notation in terms of a function: $g^{(1)}(\mathbf{r}',\mathbf{r}) = \langle \mathbf{r}|\ \rho^{(1)}\ |\mathbf{r}'\rangle$

  Convention: opposite orderings of $\mathbf{r}$ and $\mathbf{r}'$ on either side of $=$ (justification: next slide)

  [C. Cohen–Tannoudji & D. Guéry–Odelin, *Advances in Atomic Physics: an overview*, World Scientific (2011), Eq. 23.17]

$$g^{(1)}(\mathbf{r},\mathbf{r}) = n(\mathbf{r}) \quad \text{and} \quad \int d\mathbf{r}\ g^{(1)}(\mathbf{r},\mathbf{r}) = N$$

$\rho^{(1)}$ probes **first–order coherence** (qu. 3, 4)

- Apply the general formula $\langle F \rangle = \mathrm{Tr}(\rho^{(1)} f)$ to the case where $f = |\mathbf{r}'\rangle\langle\mathbf{r}|$

  $\langle F \rangle = \mathrm{Tr}(\rho^{(1)} \, |\mathbf{r}'\rangle\langle\mathbf{r}|) = \langle\mathbf{r}|\rho^{(1)}|\mathbf{r}'\rangle = g^{(1)}(\mathbf{r}',\mathbf{r})$

  (For any single–particle operator a and single–particle states $|u\rangle$, $|v\rangle$, $\mathrm{Tr}(a\,|u\rangle\langle v|) = \langle v|a|u\rangle$)

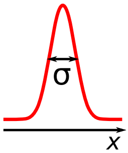
- **Single–particle case:** consider the pure state $\rho = \rho^{(1)} = |\psi\rangle\langle\psi|$

  $g^{(1)}(\mathbf{r}',\mathbf{r}) = \langle\mathbf{r}|\rho^{(1)}|\mathbf{r}'\rangle = \langle\mathbf{r}|\psi\rangle\langle\psi|\mathbf{r}'\rangle = \psi(\mathbf{r})\,\psi^*(\mathbf{r}')$

  $g^{(1)}(\mathbf{r}',\mathbf{r})$ is non–zero only if $|\mathbf{r} - \mathbf{r}'| < \sigma$

  Wavepacket extent gives coherence length

  $\langle\mathbf{r}|\rho^{(1)}|\mathbf{r}'\rangle$ probes coherence between $\mathbf{r}$ and $\mathbf{r}'$



- **Many–particle case:** F destroys a particle at point $\mathbf{r}$ and creates one at point $\mathbf{r}'$

  Equivalently: overlap in between matter waves at points $\mathbf{r}$ and $\mathbf{r}'$

  $\langle\mathbf{r}|\rho^{(1)}|\mathbf{r}'\rangle$ probes correlations between $\mathbf{r}$ and $\mathbf{r}'$

- $g^{(1)}(\mathbf{r}',\mathbf{r}) = \langle\mathbf{r}|\rho^{(1)}|\mathbf{r}'\rangle$ is called **first–order** correlation function

  First–order because it may be non–zero even for a single–particle experiment

  e.g. Young's interference experiment

Translational & rotational invariance: impact on $\rho^{(1)}$ (4)

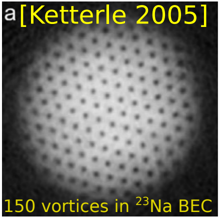
$\langle \mathbf{r}|\rho^{(1)}|\mathbf{r}'\rangle = \langle F\rangle$ with $f = |\mathbf{r}'\rangle\langle\mathbf{r}|$, and $g^{(1)}(\mathbf{r},\mathbf{r}') = \langle\mathbf{r}'|\,\rho^{(1)}\,|\mathbf{r}\rangle$ is a function of two arguments

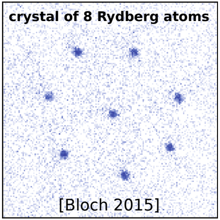
- **Quick answer:** correct, but incomplete!

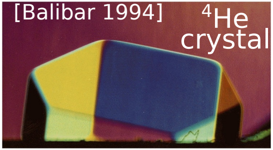
  Translational invariance yields $g^{(1)}(\mathbf{r},\mathbf{r}') = g^{(1)}(\mathbf{r}'-\mathbf{r})$

  Rotational invariance yields $g^{(1)}(\mathbf{r}'-\mathbf{r}) = g^{(1)}(|\mathbf{r}'-\mathbf{r}|)$

- But, in some experiments, **crystallisation is observed!**



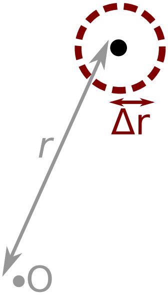




- How to reconcile these two results ? (both are correct!)

  HINT: Think about buckling; the other half of the answer is on this slide.

Kinetic energy and interaction range



- Quantum collision between a scatterer at **0** and a particle at point **r**
  Particle at **r** modelled by wavepacket with spatial extent $\Delta r < r$
  Its momentum spread Δp satisfies: $\Delta p > \hbar/\Delta r > \hbar/r$
- Kinetic energy $\sim \Delta p^2/(2m) \quad > \hbar^2/(2m\,r^2)$
  The lower bound on the kinetic energy scales with $\hbar^2/(2m\,r^2)$

[Basdevant & Dalibard, *Quantum Mechanics*, Springer (2002), §18.2.6]

- Any interaction potential which decays faster than $1/r^2$ is **short–ranged:**
  for low enough densities, kinetic energy dominates over interaction

  This holds for the van der Waals interaction C_6/r^6 between neutral atoms

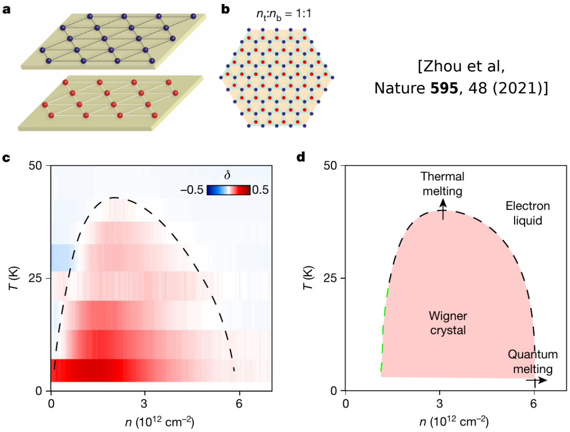
  Many atoms with repulsive interactions, at $T = 0$: crystalline phase for **high densities**

- **BEWARE:** The Coulomb interaction q^2/r is **NOT** short–ranged!

At temperature $T = 0$, is the crystal expected for high densities or for low densities ?

Wigner crystal due to repulsive Coulomb interaction

- Coulomb interaction scales like q^2/r, kinetic energy scales like $\hbar^2/(2mr^2)$
  Coulomb interaction dominates for large r, that is, for low densities
  At $T = 0$, increasing the density causes the crystal to melt!



[Zhou et al, Nature **595**, 48 (2021)]

- Predicted by Wigner in 1934, observed recently in $\mathrm{MoSe_2}$ bilayers
  Observable δ linked to photoluminescence: $\delta > 0$ means insulating (crystalline) phase

Part 2:

Two–body density matrix
for systems of identical particles

[C. Cohen–Tannoudji & D. Guéry–Odelin,
Advances in Atomic Physics: an overview, World Scientific (2011), §23.2]

Two–particle operators (qu. 5 & 18)

- Start from an operator g which acts on two different particles

  Extension to N particles: $G = \sum_i \sum_{j \neq i} g^{(i,j)}$ where $g^{(i,j)}$ acts on particles i and j

  Important example: **interaction between two particles**

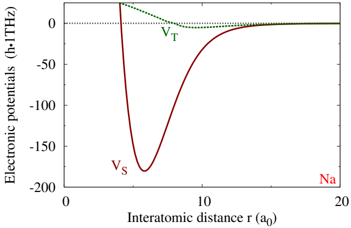
- **For two neutral atoms** (in their ground states):

  isotropic, short–ranged interaction

  Far from nucleus: C_6/r^6 van der Waals interaction

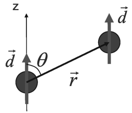
  range $l = (mC_6/\hbar^2)^{1/4} \approx 100 a_0$

  where $a_0 = 5.29 \times 10^{-11}\,m$ is the Bohr radius



- **For neutral dipolar particles:** anisotropic, longer–ranged interaction

  (magnetic atoms, heteronuclear molecules with electric dipole)



$$V_{\mathrm{DDI}}(\mathbf{r}) = \frac{\mathbf{d}_1 \cdot \mathbf{d}_2 - 3(\mathbf{d}_1 \cdot \hat{\mathbf{r}})(\mathbf{d}_2 \cdot \hat{\mathbf{r}})}{r^3}$$

$V_{\mathrm{DDI}}(\mathbf{r}) = d^2(1 - 3\cos^2\theta)/r^3$ if all dipoles point along $\mathbf{e}_z$

- **For trapped ions:** long–ranged Coulomb interactions $q_1 q_2 / r$

Two–body density operator $\rho^{(2)}$ (qu. 5)

- Calculate the expectation value of a two–body operator $G = \sum_i \sum_{j \neq i} G^{(i,j)}$

$$\langle G \rangle = \mathrm{Tr}(\rho G) \quad = \sum_i \sum_{j\neq i} \mathrm{Tr}(\rho G^{(i,j)})$$

$$\langle G \rangle = N(N-1)\ \mathrm{Tr}(\rho G^{(1,2)})$$ (ρ is fully symmetric)

$$\langle G \rangle = N(N-1)\ \mathrm{Tr}_{1,2}[\,\mathrm{Tr}_{3,\ldots,N}(\rho G^{(1,2)})\,]$$ (take trace first along $3,\ldots,N$ and then along 1,2)

$$\langle G \rangle = N(N-1)\ \mathrm{Tr}_{1,2}[\,\mathrm{Tr}_{3,\ldots,N}(\rho) g^{(1,2)}\,]$$ ($G^{1,2}$ acts on particles 1 and 2 only)

$$\langle G \rangle = \mathrm{Tr}_{1,2}(\rho^{(2)}\, g^{(1,2)}) \qquad \text{with } \rho^{(2)} = N(N-1)\,\mathrm{Tr}_{3,\ldots,N}(\rho)$$

- Notation in terms of a function: $g^{(2)}(\mathbf{r}_1,\mathbf{r}_2) = \langle \mathbf{r}_1,\mathbf{r}_2 |\, \rho^{(2)}\, | \mathbf{r}_1,\mathbf{r}_2 \rangle$

$g^{(2)}(\mathbf{r}_1,\mathbf{r}_2)$ has 2 arguments (rather than 4) because **we focus on the diagonal elements** of $\rho^{(2)}$

$\rho^{(2)}$ probes **second–order coherence** (qu. 6)

- Apply $\langle G \rangle = \mathrm{Tr}[\,\rho^{(2)}\, g\,]$ to the case where $g = |1 : \mathbf{r}_1, 2 : \mathbf{r}_2\rangle \langle 1 : \mathbf{r}_1, 2 : \mathbf{r}_2|$

  $\langle G \rangle = \langle 1 : \mathbf{r}_1, 2 : \mathbf{r}_2 | \rho^{(2)} | 1 : \mathbf{r}_1, 2 : \mathbf{r}_2 \rangle$

- **2–particle case:** consider the pure state $\rho = |\Psi\rangle \langle\Psi|$, i.e. $\rho^{(2)} = 2\,|\Psi\rangle \langle\Psi|$

  $$g^{(2)}(\mathbf{r}_1,\mathbf{r}_2) \quad = \quad \langle \mathbf{r}_1,\mathbf{r}_2 |\, \rho^{(2)}\, | \mathbf{r}_1,\mathbf{r}_2 \rangle \quad = \quad 2\, \langle \mathbf{r}_1,\mathbf{r}_2 | \Psi \rangle \, \langle \Psi | \mathbf{r}_1,\mathbf{r}_2 \rangle \quad = \quad 2 |\Psi(\mathbf{r}_1,\mathbf{r}_2)|^2$$

- **Many–particle case:**

  $g^{(2)}(\mathbf{r}_1,\mathbf{r}_2) \quad = \quad$ probability for finding one particle at $\mathbf{r}_1$ and another at $\mathbf{r}_2$

  If $\mathbf{r}_1$ and $\mathbf{r}_2$ are close by, this tests for bunching or antibunching

- $g^{(2)}(\mathbf{r}_1,\mathbf{r}_2) = \langle \mathbf{r}_1,\mathbf{r}_2 |\, \rho^{(2)}\, | \mathbf{r}_1,\mathbf{r}_2 \rangle$ is called **second–order** spatial correlation function

  Second–order because at least two particles must be present for it to be non–zero

  e.g. Hong–Ou–Mandel interference

A bird's eye view of the problem

Problem #2: Spatial Correlation Functions in Bose and Fermi systems

- One–body density matrix,   two–body density matrix
- Ideal Bose and Fermi gases at temperature $T = 0$

  Off–diagonal long–range order in bosonic systems
- Ideal quantum gases at non–zero temperature

  Description in terms of second quantisation
- First steps with interacting systems

Part 3:

Ideal gases at zero temperature

[Huang, *Statistical Mechanics*, Wiley (1987), chaps. 11 & 12]

Hamiltonian for an ideal gas of identical particles (qu. 7)

- **Hamiltonian for a single particle:** $h = \mathbf{p}^2/2m + u(\mathbf{r})$

$\mathbf{p}^2/2m$ is the kinetic energy; $u(\mathbf{r})$ is the trapping potential. No interaction in 1–particle h

- h is Hermitian: diagonalise it to get **single–particle wavefunctions and energies**

$$h\,|\phi_\alpha\rangle = \varepsilon_\alpha\,|\phi_\alpha\rangle$$

- **'Ideal gas'** means no interactions

the N–particle Hamiltonian is a one–body operator: $H = \sum_{i=1}^{N} h^{(i)}$

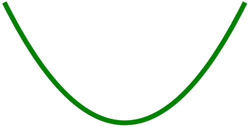
Is this slide using the first–quantised or the second–quantised formalism?

Three types of trapping potentials $u(\mathbf{r})$ (qu. 7)

- **Uniform system:** box trap

Single–particle wavefunctions are plane waves $\psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{kr}}/\sqrt{V}$

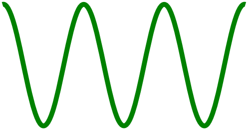
(labelled by continuous set of wavevectors)



- **Trapped system:** harmonic trap

Single–particle wavefunctions are
harmonic oscillator eigenstates $|n_x, n_y, n_z\rangle$

(labelled by 3 integers)



- **Periodic trapping potential:** optical lattice

Single–particle wavefunctions are Bloch waves $\psi_{\mathbf{k},n}(\mathbf{r}) = e^{i\mathbf{kr}} u_n(\mathbf{r})$

discrete band index n, continuous set of quasi–momenta $\mathbf{k}$

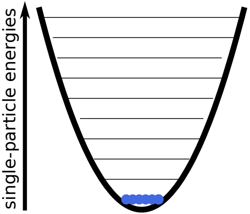
All three types of traps are routinely realised in experiments on quantum gases.

1^{st}–order coherence in an ideal Bose gas at $T = 0$ (qu. 8)

- All bosons are in the single–particle ground state $|\psi_0\rangle$

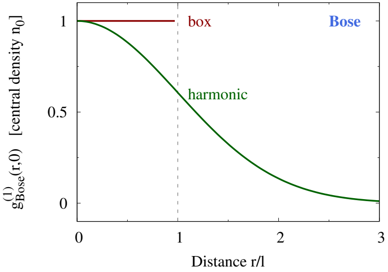
$$|\Psi\rangle = |\psi_0^{(1)}\rangle \otimes \cdots \otimes |\psi_0^{(N)}\rangle$$

[also true for distinguishable particles: where is the difference?]



- One–body density matrix: $\rho^{(1)} = N\ |\psi_0\rangle\langle\psi_0|$

$$\langle \mathbf{r}|\rho^{(1)}|\mathbf{r}'\rangle = N\ \langle \mathbf{r}|\psi_0\rangle\langle\psi_0|\mathbf{r}'\rangle = N\,\psi_0(\mathbf{r})\,\psi_0^*(\mathbf{r}')$$



- Box trap of size l:

  $\psi_0(\mathbf{r}) = 1/l^{3/2}$ and $\langle \mathbf{r}|\rho^{(1)}|\mathbf{r}'\rangle = N/l^3 \quad = \rho$

  In a very large box: $\langle \mathbf{r}|\rho^{(1)}|\mathbf{r}'\rangle \neq 0$ for $|\mathbf{r}-\mathbf{r}'| \to \infty$:

  off–diagonal long–range order

- Harmonic trap, oscillator length $l = [\hbar/(m\omega_0)]^{1/2}$:

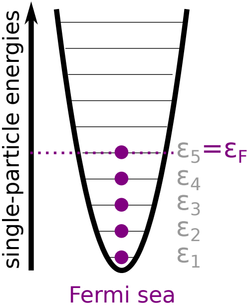
  $\psi_0(\mathbf{r}) = \exp[-r^2/(2l^2)]/(l^{3/2}\pi^{3/4})$

  $\langle \mathbf{0}|\rho^{(1)}|\mathbf{r}\rangle = N/(l^3\pi^{3/2})\exp[-r^2/(2l^2)]$

In an experiment, the coherence length l is set by the spatial volume: $l \gtrsim 1/n^{1/3}$

$n_0 = 10^{19}\,\mathrm{atoms/m^3}$, $\omega_0/(2\pi) = 100\,\mathrm{Hz}$, $m = 87\,m_{\mathrm{AMU}}$: $l = 1\,\mu\mathrm{m}$, $T_B = 0.1\,\mu\mathrm{K}$, $k_B T_B/(\hbar\omega_0) = 30$

Review: Ideal polarised Fermi gas: ground state (qu. 9)



- 1^{st} quantisation: ground–state wavefunction is a determinant

  For N particles, it involves the N lowest single–particle states

$$\Psi(\mathbf{r}_1, \ldots, \mathbf{r}_N) = \alpha \begin{vmatrix} \psi_1(\mathbf{r}_1) & \cdots & \psi_N(\mathbf{r}_1) \\ \vdots & & \vdots \\ \psi_1(\mathbf{r}_N) & \cdots & \psi_N(\mathbf{r}_N) \end{vmatrix}$$

$$= \alpha \sum_{\sigma \in \mathcal{S}_N} (-)^\sigma \, \psi_{\sigma(1)}(\mathbf{r}_1) \cdots \psi_{\sigma(N)}(\mathbf{r}_N)$$

- Calculation of the normalisation factor α:

$$1 = \int d^3 r_1 \cdots d^3 r_N \; |\alpha|^2 \sum_{\sigma, \tau \in \mathcal{S}_N} (-)^\sigma (-)^\tau \psi^*_{\sigma(1)}(\mathbf{r}_1) \cdots \psi^*_{\sigma(N)}(\mathbf{r}_N) \; \psi_{\tau(1)}(\mathbf{r}_1) \cdots \psi_{\tau(N)}(\mathbf{r}_N)$$

$$1 = |\alpha|^2 \sum_{\sigma, \tau \in \mathcal{S}_N} (-)^\sigma (-)^\tau \left(\int d^3 r_1 \, \psi^*_{\sigma(1)}(\mathbf{r}_1) \, \psi_{\tau(1)}(\mathbf{r}_1) \right) \cdots \left(\int d^3 r_N \, \psi^*_{\sigma(N)}(\mathbf{r}_N) \, \psi_{\tau(N)}(\mathbf{r}_N) \right)$$

$$1 = |\alpha|^2 \sum_{\sigma, \tau \in \mathcal{S}_N} \delta_{\sigma(1), \tau(1)} \cdots \delta_{\sigma(N), \tau(N)}$$

(the N Kronecker symbols impose $\sigma = \tau$)

$$1 = |\alpha|^2 \sum_{\sigma \in \mathcal{S}_N} 1 \quad = N! \, |\alpha|^2$$

and therefore $\alpha = 1/\sqrt{N!}$

Ideal polarised Fermi gas: $\rho^{(1)}$ for the ground state (qu. 9)

$$\rho^{(1)} = N\,\mathrm{Tr}_{2,\ldots,N}(|\Psi\rangle\langle\Psi|) \quad \text{with} \quad \Psi(\mathbf{r}_1,\ldots,\mathbf{r}_N) = \frac{1}{\sqrt{N!}}\sum_{\sigma}(-)^{\sigma}\psi_{\sigma(1)}(\mathbf{r}_1)\cdots\psi_{\sigma(N)}(\mathbf{r}_N)$$

$$\langle\mathbf{r}|\rho^{(1)}|\mathbf{r}'\rangle = N\int d^3r_2\cdots d^3r_N\;\langle\mathbf{r},\mathbf{r}_2,\ldots,\mathbf{r}_N|\Psi\rangle\;\langle\Psi|\mathbf{r}',\mathbf{r}_2,\ldots,\mathbf{r}_N\rangle \qquad \text{(no integral on } \mathbf{r} \text{ or } \mathbf{r}'\text{)}$$

$$= N\int d^3r_2\cdots d^3r_N\sum_{\sigma,\tau\in\mathcal{S}_N}\frac{(-)^{\sigma}}{\sqrt{N!}}\frac{(-)^{\tau}}{\sqrt{N!}}\psi_{\sigma(1)}(\mathbf{r})\cdots\psi_{\sigma(N)}(\mathbf{r}_N)\,\psi^*_{\tau(1)}(\mathbf{r}')\cdots\psi^*_{\tau(N)}(\mathbf{r}_N)$$

$$= \frac{N}{N!}\sum_{\sigma,\tau\in\mathcal{S}_N}(-)^{\sigma}(-)^{\tau}\;\psi_{\sigma(1)}(\mathbf{r})\,\psi^*_{\tau(1)}(\mathbf{r}')\;\left(\int d^3r_2\,\psi_{\sigma(2)}(\mathbf{r}_2)\,\psi^*_{\tau(2)}(\mathbf{r}_2)\right)\cdots$$

$$= \frac{1}{(N-1)!}\sum_{\sigma,\tau\in\mathcal{S}_N}(-)^{\sigma}(-)^{\tau}\;\psi_{\sigma(1)}(\mathbf{r})\,\psi^*_{\tau(1)}(\mathbf{r}')\;\delta_{\sigma(2),\tau(2)}\cdots\delta_{\sigma(N),\tau(N)}$$

The two permutations σ and τ coincide on $2,\ldots,N$, therefore $\sigma=\tau$

$$= \frac{1}{(N-1)!}\sum_{\sigma\in\mathcal{S}_N}[(-)^{\sigma}]^2\;\psi_{\sigma(1)}(\mathbf{r})\,\psi^*_{\sigma(1)}(\mathbf{r}')$$

To define σ, first choose $\sigma(1)=\alpha$, then there are $(N-1)!$ remaining possibilities

$$\langle\mathbf{r}|\rho^{(1)}|\mathbf{r}'\rangle = \sum_{\alpha=1}^{N}\psi_{\alpha}(\mathbf{r})\,\psi^*_{\alpha}(\mathbf{r}')$$

ADVANCED QUANTUM MECHANICS

TUTORIALS 2024–2025

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Please ask me MANY questions!

Wednesday, October 9$^{\text{th}}$, 2024

Summary: 1–body density matrix, 1^{st}–order coherence

- One–body density operator: $\rho^{(1)} = N\,\mathrm{Tr}_{2,\ldots,N}(\rho)$

  Partial trace over any $N-1$ particles: $\rho^{(1)}$ acts on the single–particle subspace $\mathscr{E}^{(1)}$

- Average value of the single–particle operator $F = \sum f^{(i)}$ in the state ρ:

$$\langle F\rangle = \mathrm{Tr}(\rho F) \quad = \quad \mathrm{Tr}(\rho^{(1)} f)$$

- Interpretation in terms of first–order coherence between the points $\mathbf{r}$ and $\mathbf{r}'$:

$$g^{(1)}(\mathbf{r}',\mathbf{r}) \quad = \quad \langle \mathbf{r}|\rho^{(1)}|\mathbf{r}'\rangle \quad = \quad \mathrm{Tr}(\rho^{(1)}\,|\mathbf{r}'\rangle\,\langle\mathbf{r}|)$$

  Average value of the single–particle operator F defined by $f = |\mathbf{r}'\rangle\,\langle\mathbf{r}|$

  The operator f annihilates a particle at the position $\mathbf{r}$ and creates one at the position $\mathbf{r}'$

- Explicit expressions for ideal quantum gases at $T = 0$

  ideal Bose gas: off–diagonal long–range order

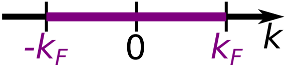
  ideal Fermi gas: $\langle \mathbf{r}|\rho^{(1)}|\mathbf{r}'\rangle = \sum_{\alpha=1}^{N} \psi_\alpha(\mathbf{r})\,\psi^*_\alpha(\mathbf{r}')$ **TODAY: calculated in simple cases**

Review: 1D uniform Fermi gas, Fermi wavevector (qu. 10)

- Large 1D box of size L, exploit translational invariance
  choose 1–particle eigenstates that are plane waves: $\psi_k(x) = e^{ikx}/\sqrt{L}$
  These are labelled by the wavevector k, corresponding to the energy $\hbar^2 k^2/(2m)$

- In a large system, "all boundary conditions give the same thermodynamical results"
  periodic boundary conditions: $\psi_k(0) = \psi_k(L)$ means $e^{ikL} = 1$
  the allowed wavevectors are $k_n = n\,2\pi/L$ (n is an integer of either sign)

- Fermi energy $\varepsilon_F =$ energy of highest–occupied 1–particle state in the ground state
  For a uniform system, define Fermi wavevector k_F through $\varepsilon_F = \hbar^2 k_F^2/(2m)$



- **Polarised** Fermi gas: each single–particle state hosts at most one particle

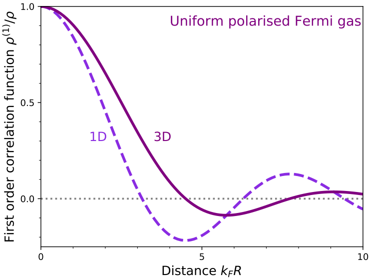
$$N = \sum_{|k_n|<k_F} 1 = \int_{-k_F}^{k_F} \frac{dk}{2\pi/L} = \frac{L}{2\pi} 2k_F = k_F L/\pi$$

$k_F = \pi\, N/L = \pi\,\rho$, where $\rho = N/L$ is the linear density: k_F is an **intensive** quantity

1D uniform Fermi gas: $\rho^{(1)}$ for the ground state (qu. 10)

$$\langle x|\rho^{(1)}|x'\rangle = \sum_{|k_n|<k_F} \psi_{k_n}(x)\,\psi^*_{k_n}(x') \quad \text{with} \quad \psi_k(x) = e^{ikx}/\sqrt{L}, \quad k_n = n2\pi/L, \quad k_F = \pi\,\rho$$

- $$\langle x|\rho^{(1)}|x'\rangle = \sum_{|k_n|<k_F} \frac{e^{ik_n(x-x')}}{L} = \int_{-k_F}^{k_F} \frac{dk}{2\pi/L}\,\frac{e^{ik(x-x')}}{L} = \frac{\sin[k_F(x-x')]}{\pi(x-x')}$$



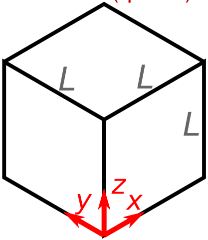
$$\langle x|\rho^{(1)}|x'\rangle = \rho\ \mathrm{sinc}[k_F(x-x')]$$

$(\mathrm{sinc}(x) = \sin(x)/x)$

- Translational symmetry and spatial parity: $\langle x|\rho^{(1)}|x'\rangle$ depends only on $|x-x'|$
- Fermi gas: the coherence length is set by k_F
  (The first zero of $\mathrm{sinc}(x)$ is for $x = \pi$)

In stark contrast to the Bose gas, the coherence length is **finite,** even at $T = 0$

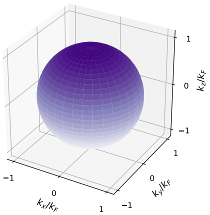
Review: 3D uniform Fermi gas, Fermi wavevector (qu. 11)



- Plane waves in 3D: $\psi_{\mathbf{k}}(\mathbf{r}) = e^{i\,\mathbf{k}\,\mathbf{r}}/L^{3/2}$, energy $\varepsilon_{\mathbf{k}} = \hbar^2 k^2/(2m)$

In real space: *cubic box* of size L with periodic boundary conditions

$$e^{i\mathbf{k}\cdot L\mathbf{e}_x} = e^{i\mathbf{k}\cdot L\mathbf{e}_y} = e^{i\mathbf{k}\cdot L\mathbf{e}_z} = 1, \quad \text{so that } \mathbf{k}_n = (2\pi/L)\,(n_x\mathbf{e}_x + n_y\mathbf{e}_y + n_z\mathbf{e}_z)$$



- **In momentum space:** the Fermi surface is a *sphere*

Fermi energy ε_F and wavevector k_F such that $\varepsilon_F = \hbar^2 k_F^2/(2m)$

Polarised Fermi gas: each 1–particle state hosts at most 1 particle

$$N = \sum_{\mathbf{k}_n < k_F} 1 = \int_{|\mathbf{k}|<k_F} \frac{d^3k}{(2\pi/L)^3} = \left(\frac{L}{2\pi}\right)^3 \frac{4}{3}\pi\, k_F^3 = \frac{(k_F L)^3}{6\pi^2}$$

$k_F = (6\pi^2\rho)^{1/3}$, where $\rho = N/L^3$ is the density (k_F is intensive)

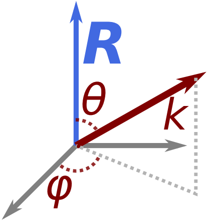
Easy question 1: Recover the 1D/3D dependence on ρ through dimensional analysis

Easy question 2: If two spin states are present, show that $k_F = (3\pi^2\rho)^{1/3}$

3D uniform Fermi gas: $\rho^{(1)}$ for the ground state (qu. 11)

$$\langle \mathbf{r}|\rho^{(1)}|\mathbf{r}'\rangle = \sum_{|\mathbf{k}_n|<k_F} \psi_{\mathbf{k}_n}(\mathbf{r})\,\psi^*_{\mathbf{k}_n}(\mathbf{r}'), \quad \psi_{\mathbf{k}}(\mathbf{r}) = \frac{e^{i\mathbf{k}\mathbf{r}}}{\sqrt{L^3}}, \quad \mathbf{k}_n = \frac{2\pi}{L}(n_x\mathbf{e}_x+n_y\mathbf{e}_y+n_z\mathbf{e}_z), \quad k_F = (6\pi^2\rho)^{1/3}$$

$$\langle \mathbf{r}|\rho^{(1)}|\mathbf{r}'\rangle = \sum_{|\mathbf{k}_n|<k_F} \frac{e^{i\mathbf{k}_n(\mathbf{r}-\mathbf{r}')}}{L^3} = \int_{|\mathbf{k}|<k_F} \frac{d^3k}{(2\pi/L)^3}\,\frac{e^{i\mathbf{k}\cdot\mathbf{R}}}{L^3} \qquad (\text{with } \mathbf{R} = \mathbf{r}-\mathbf{r}')$$



Spherical coordinates of axis **R**: $\mathbf{k}\cdot\mathbf{R} = k\,R\,\cos\theta$

$$\langle \mathbf{r}|\rho^{(1)}|\mathbf{r}'\rangle = \frac{1}{(2\pi)^3}\int_0^{k_F} dk\,k^2 \int_0^{\pi} d\theta\,\sin\theta \int_0^{2\pi} d\phi\;e^{ikR\cos\theta}$$

$$= \frac{1}{(2\pi)^2}\int_0^{k_F} dk\,k^2 \int_0^{\pi} d\theta\,\sin\theta\,e^{ikR\cos\theta}$$

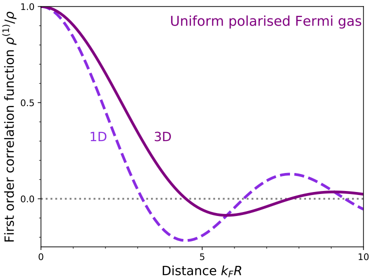
$$= \frac{1}{2\pi^2 R}\int_0^{k_F} dk\,k\sin(kR) = \frac{k_F^3}{2\pi^2(k_F R)^3}\int_0^{k_F R} du\,u\sin u$$

An integration by parts yields: $\int_0^{k_F R} du\,u\sin u = -k_F R\cos(k_F R) + \sin(k_F R)$

$$\langle \mathbf{r}|\rho^{(1)}|\mathbf{r}'\rangle = \rho\,\frac{\sin(k_F R) - k_F R\,\cos(k_F R)}{(k_F R)^3/3}$$

Show analytically that $\langle \mathbf{r}|\rho^{(1)}|\mathbf{r}\rangle = \lim_{k_F R\to 0}\langle \mathbf{r}|\rho^{(1)}|\mathbf{r}'\rangle = \rho$

3D uniform Fermi gas: $\rho^{(1)}$ for the ground state (qu. 11)



$$\langle \mathbf{r}|\rho^{(1)}|\mathbf{r}'\rangle = \rho \frac{\sin(k_F R) - k_F R \cos(k_F R)}{(k_F R)^3/3}$$

- Translational symmetry, rotational symmetry: $\langle \mathbf{r}|\rho^{(1)}|\mathbf{r}'\rangle$ depends only on $R = |\mathbf{r} - \mathbf{r}'|$
- Like in 1D, the coherence length is set by k_F
  (The first $x > 0$ such that $\tan x = x$ is $x \approx 4.5$)

- Both for the 1D Fermi gas and the 3D Fermi gas,

In stark contrast to the Bose gas, the coherence length is **finite,** even at $T = 0$

Part 4:

Calculations at non–zero temperature

Second quantisation, field operators

[Feynman, *Statistical Mechanics: a set of lectures*, W.A. Benjamin (1972), chap. 6]

Single–particle operators: second quantisation form

- $F = \sum_{i=1}^{N} f^{(i)}$ where $f^{(i)}$ acts only on particle i (F acts on each particle in the same way)

In the single–particle subspace $\mathscr{E}_1$, insert two closure relations (using a basis $\{|\alpha\rangle\}$ of $\mathscr{E}_1$)

$$f = \left(\sum_\beta |\beta\rangle\langle\beta|\right) f \left(\sum_\alpha |\alpha\rangle\langle\alpha|\right) = \sum_{\alpha,\beta} \langle\beta|f|\alpha\rangle \; |\beta\rangle\langle\alpha|$$

Kets transform like creation operators: $F = \sum_{\alpha,\beta} \langle\beta|f|\alpha\rangle \; a^\dagger_\beta \, a_\alpha$

- **Example 1:** $f = \mathbb{1}$, $F = \mathbb{1}^{(1)} + \cdots + \mathbb{1}^{(N)} = N$ **total particle number operator**

Choose any basis $\{|\alpha\rangle\}$: $\mathbb{1}^{(1)}\,|\alpha\rangle = |\alpha\rangle$, meaning that $\langle\beta|\,\mathbb{1}^{(1)}\,|\alpha\rangle = \delta_{\alpha\beta}$

$$N = \sum_\alpha a^\dagger_\alpha a_\alpha = \sum_\alpha n_\alpha$$

total particle number = sum of particle numbers in all modes

- **Example 2:** $f = h$, $H = h^{(1)} + \cdots + h^{(N)} = H$ **ideal gas Hamiltonian**

Choose a basis $\{|\alpha\rangle\}$ which diagonalises h: $h\,|\alpha\rangle = \varepsilon_\alpha\,|\alpha\rangle$, meaning that $\langle\beta|h|\alpha\rangle = \varepsilon_\alpha \delta_{\alpha\beta}$

$$H = \sum_\alpha \varepsilon_\alpha \, a^\dagger_\alpha a_\alpha = \sum_\alpha \varepsilon_\alpha \, n_\alpha$$

total energy = sum of energies in all modes

Holds regardless of quantum statistics: bosons or fermions

First quantisation versus second quantisation

- **First quantisation:**

$$\mathscr{E}^{(N)} = (\mathscr{S} \text{ or } \mathscr{A})\,[\underbrace{\mathscr{E}^{(1)} \otimes \mathscr{E}^{(1)} \otimes \cdots \otimes \mathscr{E}^{(1)}}_{\text{tensor product of } N \text{ copies of } \mathscr{E}^{(1)}}]$$

Fixed particle number N, tensor products between states for individual particles

Wavefunctions must be (anti–)symmetrised (e.g. Slater determinant for fermions)

Single–particle operators: $F = \sum_{i=1}^{N} f^{(i)}$

- **Second quantisation:** $\mathscr{H} = \mathscr{E}^{(0)} \oplus \mathscr{E}^{(1)} \oplus \cdots \oplus \mathscr{E}^{(N)} \oplus \cdots$

Arbitrary particle number, direct sum between spaces with fixed particle numbers

The direct sum $\oplus$ means that $\Psi = (|\mathrm{vac}\rangle + |\alpha\rangle + |\alpha,\beta\rangle)/\sqrt{3}$ is allowed

Wavefunctions expressed using a and $a^\dagger$ are automatically (anti–)symmetric

For fermions, the Slater determinant becomes $|\alpha_1, \ldots, \alpha_N\rangle = a^\dagger_{\alpha_1} \cdots a^\dagger_{\alpha_N} |\mathrm{vac}\rangle$

Single–particle operators: $F = \sum_{\alpha,\beta} \langle\beta|f|\alpha\rangle \; a^\dagger_\beta \, a_\alpha$

1–body density matrix, second–quantisation form (qu. 12)

$\langle \mathbf{r}|\rho^{(1)}|\mathbf{r}'\rangle = \langle F\rangle$ with $F = \sum_{i=1}^{N} f^{(i)}$ and $f = |\mathbf{r}'\rangle\langle\mathbf{r}|$; $F = \sum_{\alpha,\beta} \langle\psi_\beta|f|\psi_\alpha\rangle \; a_\beta^\dagger \, a_\alpha$

- GOAL: Extend expression for $\rho^{(1)}$ defined by density matrix ρ, **to any quantum state**
  no constraint on total particle number,
  no constraint on temperature.

- Introduce a basis $\{|\psi_\alpha\rangle\}$ of the single–particle subspace $\mathscr{E}^{(1)}$ (any basis!)

$$F = \sum_{\alpha,\beta} \langle\psi_\beta|\mathbf{r}'\rangle \, \langle\mathbf{r}|\psi_\alpha\rangle \;\; a_\beta^\dagger \, a_\alpha = \sum_{\alpha,\beta} \psi_\alpha(\mathbf{r}) \, \psi_\beta^*(\mathbf{r}') \;\; a_\beta^\dagger \, a_\alpha$$

$$\langle\mathbf{r}|\rho^{(1)}|\mathbf{r}'\rangle = \langle F\rangle = \sum_{\alpha,\beta} \psi_\alpha(\mathbf{r}) \, \psi_\beta^*(\mathbf{r}') \;\; \langle a_\beta^\dagger \, a_\alpha\rangle$$

- We had taken the left–hand side as the first–quantised expression for $\rho^{(1)}$
  The right–hand side extends the expression to arbitrary quantum states.

- The averages $\langle a_\beta^\dagger a_\alpha\rangle$ are taken in the considered quantum state ρ

1–body density matrix, second–quantisation form (qu. 12)

$$\langle \mathbf{r}|\rho^{(1)}|\mathbf{r}'\rangle = \sum_{\alpha,\beta} \psi_\alpha(\mathbf{r})\, \psi^*_\beta(\mathbf{r}')\ \langle a^\dagger_\beta\, a_\alpha\rangle$$

- **Bose gas in its ground state:** $|N_{\psi_0}\rangle = a^{\dagger N}_{|\psi_0\rangle}\,|\mathrm{vac}\rangle\,/\sqrt{N!}$ (all particles in $|\psi_0\rangle$)

$\langle N_{\psi_0}|a^\dagger_\beta a_\alpha|N_{\psi_0}\rangle$ is the overlap of the two states $a_\alpha\,|N_{\psi_0}\rangle$ and $a_\beta\,|N_{\psi_0}\rangle$

They are non–zero only if $\alpha = \beta = 0$, and then $\langle N_{\psi_0}|a^\dagger_\beta a_\alpha|N_{\psi_0}\rangle = \langle N_{\psi_0}|n_0|N_{\psi_0}\rangle = N$

$$\langle \mathbf{r}|\rho^{(1)}|\mathbf{r}'\rangle = N\,\psi_0(\mathbf{r})\,\psi^*_0(\mathbf{r}')$$

- **Fermi gas in its ground state:** $|\mathrm{FS}\rangle = a^\dagger_1 \cdots a^\dagger_N\,|\mathrm{vac}\rangle$ (Fermi Sea FS)

$\langle \mathrm{FS}|a^\dagger_\beta a_\alpha|\mathrm{FS}\rangle$ is the overlap of $a_\alpha\,|\mathrm{FS}\rangle$ and $a_\beta\,|\mathrm{FS}\rangle$ (both proportional to number states)

Overlap is non–zero only if $\alpha = \beta$, and then $\langle \mathrm{FS}|a^\dagger_\alpha\, a_\alpha|\mathrm{FS}\rangle = \langle \mathrm{FS}|n_\alpha|\mathrm{FS}\rangle = 0$ or 1

$$\langle \mathbf{r}|\rho^{(1)}|\mathbf{r}'\rangle = \sum_{\alpha=1}^{N} \psi_\alpha(\mathbf{r})\,\psi^*_\alpha(\mathbf{r}')$$

Please wait ...

Question 13 (field operator $\Psi(\mathbf{r})$)

Question 14 (2–body density matrix $\rho^{(2)}$)

... just a few more minutes!

Nonzero–temperature $\rho^{(1)}$ for an ideal gas (qu. 15)

$\langle \mathbf{r}|\rho^{(1)}|\mathbf{r}'\rangle = \sum_{\alpha_1,\alpha_2} \psi_{\alpha_1}(\mathbf{r})\,\psi^*_{\alpha_2}(\mathbf{r}')\,\langle a^\dagger_{\alpha_2} a_{\alpha_1}\rangle$, thermal state $\rho = e^{-\beta(H-\mu N)}/Z_{GC}$ with $1/\beta = k_\mathrm{B} T$

- Grand–canonical Hamiltonian: $H - \mu N = \sum_i \varepsilon_i\,\hat{n}_i - \mu \sum_i \hat{n}_i = \sum_i (\varepsilon_i - \mu)\,\hat{n}_i$

$(H - \mu N)$ is diagonal in the Fock–state basis $\{|(n_i)\rangle\} = \{|n_1, n_2, \ldots\rangle\}$

Therefore, so is $\rho = e^{-\beta(H-\mu N)}/Z_{GC} = \sum_{(n_i)} p_{(n_i)}\ |(n_i)\rangle\langle(n_i)|$

- Calculate averages $\langle a^\dagger_{\alpha_2} a_{\alpha_1}\rangle$ in the thermal state ρ

$$\langle a^\dagger_{\alpha_2} a_{\alpha_1}\rangle = \mathrm{Tr}(\rho\, a^\dagger_{\alpha_2} a_{\alpha_1}) = \sum_{(n_i)} p_{(n_i)}\ \mathrm{Tr}(|(n_i)\rangle\langle(n_i)|\, a^\dagger_{\alpha_2} a_{\alpha_1}) = \sum_{(n_i)} p_{(n_i)}\,\langle(n_i)|a^\dagger_{\alpha_2} a_{\alpha_1}|(n_i)\rangle$$

$\langle(n_i)|a^\dagger_{\alpha_2} a_{\alpha_1}|(n_i)\rangle$ = overlap between $a_{\alpha_1}\,|(n_i)\rangle$ and $a_{\alpha_2}\,|(n_i)\rangle$, both proportional to number states

Non–zero only if $\alpha_1 = \alpha_2$, and then $\langle a^\dagger_\alpha a_\alpha\rangle = \langle \hat{n}_\alpha\rangle$

$$\langle \mathbf{r}|\rho^{(1)}|\mathbf{r}'\rangle = \sum_\alpha \psi_\alpha(\mathbf{r})\,\psi^*_\alpha(\mathbf{r}')\ \langle \hat{n}_\alpha\rangle$$ both for bosons and for fermions

Check that the conclusion is still valid in the canonical ensemble.

The role of quantum statistics (qu. 15)

$$\langle \mathbf{r}|\rho^{(1)}|\mathbf{r}'\rangle = \sum_\alpha \psi_\alpha(\mathbf{r})\,\psi^*_\alpha(\mathbf{r}')\,\langle \hat{n}_\alpha\rangle$$

In the **grand–canonical ensemble**, the averages $\langle \hat{n}_\alpha\rangle$ **reflect quantum statistics:**

- **Bose–Einstein statistics:** $$\langle \hat{n}_\alpha\rangle = \frac{1}{e^{\beta(\varepsilon_\alpha-\mu)} - 1}$$
- **Fermi–Dirac statistics:** $$\langle \hat{n}_\alpha\rangle = \frac{1}{e^{\beta(\varepsilon_\alpha-\mu)} + 1}$$
- **Boltzmann statistics:** $$\langle \hat{n}_\alpha\rangle = e^{-\beta(\varepsilon_\alpha-\mu)}$$

valid for small fugacities $z = \exp(\beta\mu) \ll 1$

Recover the quantum statistics in the grand–canonical ensemble

HINTS: The partition function Z_{GC} factorises into a product of partition functions for individual modes

Point out the link with a 1D harmonic oscillator (for bosons) and a spin–1/2 (for fermions)

$\rho^{(1)}$ for a uniform ideal Boltzmann gas (qu. 16)

$$\langle \mathbf{r}|\rho^{(1)}|\mathbf{r}'\rangle = \sum_\alpha \psi_\alpha(\mathbf{r})\, \psi^*_\alpha(\mathbf{r}')\ \langle \hat{n}_\alpha\rangle$$

- Plane wave $\psi_\mathbf{k}$ has energy $\hbar^2 k^2/(2m)$: Boltzmann weight $\langle n_\mathbf{k}\rangle = \alpha\, e^{-\beta\hbar^2k^2/(2m)}$

Calculate α using the normalisation condition $N = \sum_\mathbf{k} \langle n_\mathbf{k}\rangle = \int \frac{d^3k}{(2\pi/L)^3}\langle n_\mathbf{k}\rangle$

$$N = \alpha\left(\frac{L}{2\pi}\right)^3 \int dk\, 4\pi k^2 e^{-\beta\hbar^2k^2/(2m)} = \alpha\left(\frac{L}{\Lambda_T}\right)^3 \frac{2}{\sqrt{\pi}}\int du\, u^{1/2}e^{-u} = \alpha\left(\frac{L}{\Lambda_T}\right)^3$$

$\langle n_\mathbf{k}\rangle = \rho\Lambda_T^3 e^{-\beta\hbar^2k^2/(2m)}$ with $\rho = \frac{N}{L^3}$ and $\Lambda_T = \left(\frac{2\pi\hbar^2}{mk_\mathrm{B}T}\right)^{1/2}$ (thermal de Broglie wavelength)

- $$\langle \mathbf{r}|\rho^{(1)}|\mathbf{r}'\rangle = \sum_\mathbf{k}\langle n_\mathbf{k}\rangle \frac{e^{i\mathbf{kr}}}{L^{3/2}}\frac{e^{-i\mathbf{kr}'}}{L^{3/2}} = \sum_\mathbf{k}\langle n_\mathbf{k}\rangle\frac{e^{i\mathbf{kR}}}{L^3} \quad (\text{with } \mathbf{R} = \mathbf{r}-\mathbf{r}')$$

$$\langle \mathbf{r}|\rho^{(1)}|\mathbf{r}'\rangle = \int \frac{d^3k}{(2\pi/L)^3}\ \rho\,\Lambda_T^3\ e^{-\beta\hbar^2k^2/(2m)}\ \frac{e^{i\mathbf{kR}}}{V}$$

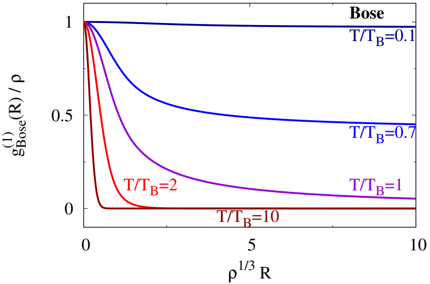
Fourier transform of a Gaussian of variance $\frac{m}{\beta\hbar^2}$ = Gaussian of variance $\frac{\beta\hbar^2}{m}$

$$\langle \mathbf{r}|\rho^{(1)}|\mathbf{r}'\rangle = \rho\, e^{-mR^2/(2\beta\hbar^2)} = \rho\, e^{-\pi R^2/\Lambda_T^2} \qquad \text{with } \rho = \frac{N}{L^3}$$

The coherence length is set by the thermal de Broglie wavelength Λ_T

1^{st}–order correlation functions for Bose & Fermi gases

- **Bosons**



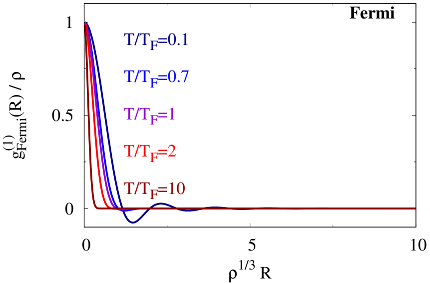
Bose condensation temperature:

$$k_B T_B = \frac{\hbar^2}{m\rho^{-2/3}} \frac{2\pi}{(\zeta(3/2))^{2/3}}$$

For $T < T_B$, $\langle \mathbf{r}|\rho^{(1)}|\mathbf{r}'\rangle \neq 0$ for $|\mathbf{r} - \mathbf{r}'| \to \infty$

Off–diagonal long–range order

- **Fermions**



Fermi temperature:

$$k_B T_F = \varepsilon_F = \frac{\hbar^2}{m\rho^{-2/3}} \frac{(6\pi)^{2/3}}{2}$$

For $T < T_F$, $\langle \mathbf{r}|\rho^{(1)}|\mathbf{r}'\rangle = 0$ for $|\mathbf{r} - \mathbf{r}'| \gtrsim 1/k_F$

No long–range order

- For $T \gg T_B$ or T_F: Boltzmann statistics, coherence length Λ_T

Spatial density of atoms in 3D: $\rho = N/L^3$

Advanced Quantum Mechanics

Tutorials 2024–2025

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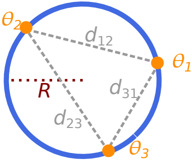
Please ask me MANY questions!

Wednesday, October 23$^{\text{th}}$, 2024

Rydberg atoms: chaos & semiclassical physics

- **Non–ergodicity** of 3 **interacting** Rydberg atoms in a circular trap

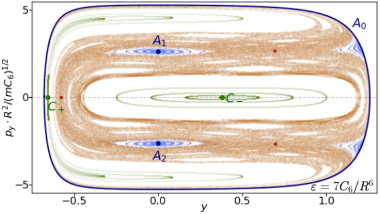


This conceptually simple system is **experimentally accessible**

due to recent progress in Rydberg atom trapping in Paris and Palaiseau

[D.J. Papoular & B. Zumer, Phys. Rev. A **107**, 022217 (2023)]

[D.J. Papoular & B. Zumer, Phys. Rev. A **110**, 012230 (2024)]



Two mechanisms impeding ergodicity in the absence of disorder:

1. quantum mechanism: **quantum scar** [Heller PRL 1984]
2. classical mechanism: **KAM tori** (**K**olmogorov, **A**rnold, **M**oser)
   [Arnold, *Mathematical Methods of Classical Mechanics*, Springer (1989)])

Both mechanisms yield quantum eigenstates **localised near classical periodic trajectories**

- Telling them apart requires a detailed understanding of the **classical system** and accurate **numerical calculations** of the quantum eigenstates (not ground state!)
- **Semiclassical analysis** which goes beyond the WKB approach

Gutzwiller's trace formula, Einstein–Brillouin–Keller theory

[M.C. Gutzwiller, *Chaos in Classical and Quantum Mechanics*, Springer (1990)]

Spontaneous applications for a PhD position with me are welcome

Summary: 1^{st}–order coherence in ideal gases

- One–body density operator: $\rho^{(1)} = N\,\mathrm{Tr}_{2,\ldots,N}(\rho)$

  Interpretation in terms of first–order coherence between the points $\mathbf{r}$ and $\mathbf{r}'$:

  $$g^{(1)}(\mathbf{r}',\mathbf{r}) = \langle \mathbf{r}|\rho^{(1)}|\mathbf{r}'\rangle = \mathrm{Tr}(\rho^{(1)}\,|\mathbf{r}'\rangle\,\langle\mathbf{r}|)$$

The operator $f = |\mathbf{r}'\rangle\,\langle\mathbf{r}|$ annihilates a particle at the position $\mathbf{r}$ and creates one at the position $\mathbf{r}'$

- Second–quantised expression of one–body operators: $F = \sum_{\alpha,\beta} \langle\beta|f|\alpha\rangle\; a^\dagger_\beta\, a_\alpha$

  $$\langle \mathbf{r}|\rho^{(1)}|\mathbf{r}'\rangle = \psi_\alpha(\mathbf{r})\,\psi^*_\beta(\mathbf{r}')\;\langle a^\dagger_\beta\, a_\alpha\rangle$$

- **Bose gases:**

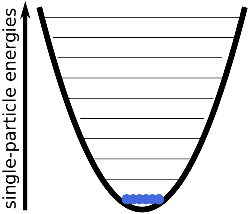
  off-diagonal long–range order for $T < T_B$ (T_B = Bose condensation temperature)

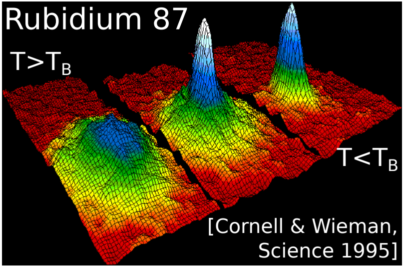
  $$\langle \mathbf{r}|\rho^{(1)}|\mathbf{r}'\rangle \neq 0 \quad \text{for } |\mathbf{r}-\mathbf{r}'| \to \infty$$

Bose–Einstein Condensation (BEC)

- For an ideal Bose gas at temperature $T = 0$: all particles in the same state

$$|\Psi\rangle = |\psi_0^{(1)}\rangle \otimes \cdots \otimes |\psi_0^{(N)}\rangle$$





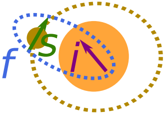
[M.H. Anderson et al, Science **269**, 198 (1995)]

- For $0 < T < T_B$, or in the presence of interactions: **Off–Diagonal Long Range Order**

$$\langle \mathbf{r}|\rho^{(1)}|\mathbf{r}'\rangle \neq 0 \quad \text{for } |\mathbf{r}-\mathbf{r}'| \to \infty$$

Experimental investigation: [Bloch, Hänsch, & Esslinger, Nature **403**, 166 (2000)] (next 3 slides)

Experiment probing 1^{st}–order coherence of a BEC (1/3)



- The alkali $^{87}\mathrm{Rb}$ has electron spin $s = 1/2$ and nuclear spin $i = 3/2$

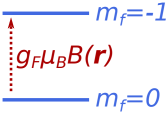
Hyperfine structure: $\mathbf{f} = \mathbf{s} + \mathbf{i}$ ($f = 1$ or 2) focus on $f = 1$

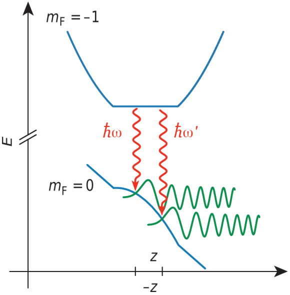
Potential energy in a magnetic field: $-\boldsymbol{m} \cdot \mathbf{B}(\mathbf{r}) = g_F \mu_B \, m_f \, B(\mathbf{r})$

$g_F = -1/2 < 0$: atoms with $m_f = -1$ are trapped; atoms with $m_f = 0$ are untrapped.

- Tune radio wave frequency $\hbar\omega_{\mathrm{RF}}$ to Zeeman splitting $g_F \mu_B \, B(\mathbf{r})$

to flip spin projection from $m_f = -1$ (trapped) to $m_f = 0$ (untrapped)





- $B(z)$ depends on z and traps many atoms in a 'cigar'

2 RF frequencies: $\hbar\omega_1 = g_F \mu_B \, B(z_1)$, $\hbar\omega_2 = g_F \mu_B \, B(z_2)$

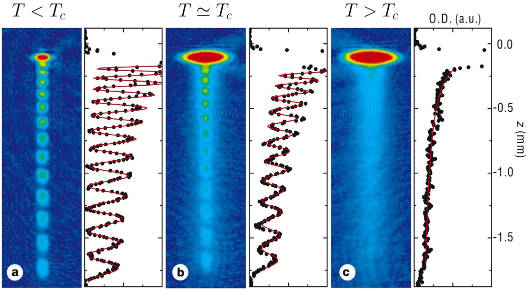
yield 2 matter waves with energies $E_1 = mgz_1$, $E_2 = mgz_2$

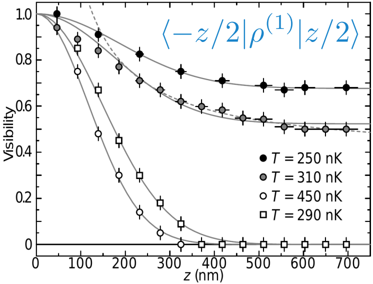
very small outcoupling rates to probe single–particle physics

Do these matter waves interfere? i.e. are they coherent?

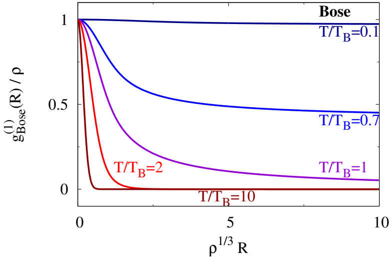
Experiment probing 1st–order coherence of a BEC (2/3)

- **2 matter waves extracted from 2 different points of a Bose gas overlap**





- Cold, but not ultracold, Bose gas ($T > T_c$): no interference fringes, $\langle \mathbf{r}_1|\rho_1|\mathbf{r}_2\rangle = 0$
- **B**ose–**E**instein **C**ondensate ($T < T_c$): interference fringes, $\langle \mathbf{r}_1|\rho_1|\mathbf{r}_2\rangle \neq 0$
- For $T < T_c$, what sets the fringe distribution?



[Bloch, Hänsch, & Esslinger, Nature **403**, 166 (2000)]

Experiment probing 1^{st}–order coherence of a BEC (3/3)

- **A single radio wave,** frequency ω_1 resonant with $B(z_1)$

  yields a **stationary matter wave** $\psi_1(z)$ with energy $E_1 = mgz_1$

- **Two different radio waves,** frequencies resonant with $B(z_1)$ and $B(z_2)$

  yield **2 matter waves** $\psi_1(z)$, $\psi_2(z)$ with **different energies** $E_1 = mgz_1$**,** $E_2 = mgz_2$

The superposition state is not stationary: $\psi(z,t) = \psi_1(z)e^{-iE_1 t/\hbar} + \psi_2(z)e^{-iE_2 t/\hbar}$

- **At zero temperature** $T = 0$, the density profile may be shown to satisfy:

$$n(z,t) \propto \frac{1 + \cos\left[q\left(|z|^{1/2} - (gt^2/2)^{1/2}\right)\right]}{|z|^{1/2}} \qquad \text{with} \qquad q = m\,(z_1 - z_2)\,(2g)^{1/2}\,/\hbar$$

Schrödinger equation for a particle in a linear potential (e.g. gravity) leads to Airy function [NIST Dynamic Library of Mathematical Functions, §9.2 & §9.7, `https://dlmf.nist.gov`]

[Bloch, Hänsch, & Esslinger, Nature **403**, 166 (2000)]

The field operator $\hat{\Psi}(\mathbf{r})$ (qu. 13)

- Annihilation operator in a **continuous basis,** e.g. at point $\mathbf{r}$: $\hat{\Psi}(\mathbf{r}) = a_{\langle \mathbf{r}|}$

  $\hat{\Psi}(\mathbf{r})$ is an operator mapping $\mathscr{E}^{(N)}$ onto $\mathscr{E}^{(N-1)}$ ($\mathbf{r}$ is *not* an operator)

$$|\mathbf{r}\rangle = \sum_\alpha |\psi_\alpha\rangle \langle \psi_\alpha | \mathbf{r}\rangle = \sum_\alpha \psi^*_\alpha(\mathbf{r})\, |\psi_\alpha\rangle, \qquad \text{therefore} \qquad \hat{\Psi}^\dagger(\mathbf{r}) = \sum_\alpha \psi^*_\alpha(\mathbf{r})\, a^\dagger_\alpha$$

$$[\hat{\Psi}(\mathbf{r}), \hat{\Psi}(\mathbf{r}')]_\pm = 0, \qquad [\hat{\Psi}^\dagger(\mathbf{r}), \hat{\Psi}^\dagger(\mathbf{r}')]_\pm = 0, \qquad [\hat{\Psi}(\mathbf{r}), \hat{\Psi}^\dagger(\mathbf{r}')]_\pm = \delta(\mathbf{r}-\mathbf{r}')$$

Express the many–body Hamiltonian in terms of the operators $\hat{\Psi}(\mathbf{r})$ and $\hat{\Psi}^\dagger(\mathbf{r})$

- 1–body trapping term: $u = \int d^3r\, |\mathbf{r}\rangle\, u(\mathbf{r})\, \langle \mathbf{r}|$, hence $U = \int d^3r\, u(\mathbf{r})\, \hat{\Psi}^\dagger(\mathbf{r})\, \hat{\Psi}(\mathbf{r})$

- Kinetic energy: $k = \int d^3r\, |\mathbf{r}\rangle \left(\frac{\mathbf{p}^2}{2m}\right) \langle \mathbf{r}|$, hence $K = \int d^3r\, \hat{\Psi}^\dagger(\mathbf{r}) \left(\frac{\mathbf{p}^2}{2m}\right) \hat{\Psi}(\mathbf{r})$

$$\mathbf{p}\, \hat{\Psi}(\mathbf{r}) = -i\hbar\, \nabla \hat{\Psi}(\mathbf{r}) \quad \text{and} \quad \hat{\Psi}^\dagger(\mathbf{r})\, \mathbf{p} = \left(\mathbf{p}\, \hat{\Psi}(\mathbf{r})\right)^\dagger = +i\hbar\, \nabla \hat{\Psi}^\dagger(\mathbf{r})$$

Therefore $$K = \frac{1}{2m} \int d^3r \left(\hat{\Psi}^\dagger(\mathbf{r})\, \mathbf{p}\right) \left(\mathbf{p}\, \hat{\Psi}(\mathbf{r})\right) = \frac{\hbar^2}{2m} \int d^3r \left(\nabla \hat{\Psi}\right)^\dagger \left(\nabla \hat{\Psi}\right)$$

- **Total ideal–gas Hamiltonian:** $H = \int d^3r \left[\frac{\hbar^2}{2m} \left(\nabla \hat{\Psi}\right)^\dagger \left(\nabla \hat{\Psi}\right) + u(\mathbf{r})\, \hat{\Psi}^\dagger \hat{\Psi}\right]$

Same form as single–particle Hamiltonian, but **replace wavefunction by the field operator**

1–body density $\rho^{(1)}$: 2^{nd}–quantised expression (qu. 13)

- As usual for $\rho^{(1)}$, consider the 1–body operator $f = |\mathbf{r}'\rangle \langle \mathbf{r}|$ and $F = \sum_{i=1}^{N} f^{(i)}$

- Average the one–body operator F in some quantum state:
  $\langle F \rangle \quad = \quad \mathrm{Tr}[\, \rho^{(1)} f \,] \quad = \quad \mathrm{Tr}[\, \rho^{(1)} \, |\mathbf{r}'\rangle \langle \mathbf{r}| \,] \quad = \quad \langle \mathbf{r}|\rho^{(1)}|\mathbf{r}'\rangle$

- Express F in terms of second–quantised operators:
  $f = |\mathbf{r}'\rangle \langle \mathbf{r}|$ means that $F = \hat{\Psi}^{\dagger}(\mathbf{r}') \, \hat{\Psi}(\mathbf{r})$

$$\langle \mathbf{r}|\rho^{(1)}|\mathbf{r}'\rangle \quad = \quad \langle \, \hat{\Psi}^{\dagger}(\mathbf{r}') \, \hat{\Psi}(\mathbf{r}) \, \rangle$$

Answers the question: Does the system remain coherent if one particle is destroyed at point **r** and another one is created at point **r**′ ?

Two–body operators

- Second–quantised form
- Application 1: Pair correlation function (qu. 14)
- Application 2: Pair–wise interaction (qu. 18)

Two–body operators: second–quantised form (qu. 14)

- **Beware!** for **fermions,** the ordering of the labels in the bras and kets matters
  $|\alpha,\beta\rangle = a^\dagger_\alpha a^\dagger_\beta\,|\mathrm{vac}\rangle$ but $|\beta,\alpha\rangle = a^\dagger_\beta a^\dagger_\alpha\,|\mathrm{vac}\rangle$ so that $|\alpha,\beta\rangle = -\,|\beta,\alpha\rangle$

  The fermionic ket is a **stack:** "Last In, First Out", just like a stack of plates

  $|\alpha,\beta\rangle^\dagger = \langle\alpha,\beta|$ always holds true. No problem for bosons ($a^\dagger_\alpha$ and $a^\dagger_\beta$ commute).

- 2–body operator: g acts on $\mathscr{E}^{(2)}$ (two different particles), $G = \sum_i \sum_{j\neq i} g^{(i,j)}$

  Choose basis $\{|\alpha\rangle\}$ for $\mathscr{E}^{(1)}$, expand g in 2–particle basis $\{|1:\alpha\rangle \otimes |2:\beta\rangle\}$

$$g = \left(\sum_{\alpha\beta} |\alpha,\beta\rangle\,\langle\alpha,\beta|\right) g \left(\sum_{\gamma\delta} |\gamma,\delta\rangle\,\langle\gamma,\delta|\right) = \sum_{\alpha,\beta,\gamma,\delta} \langle\alpha,\beta|\,g\,|\gamma,\delta\rangle\;|\alpha,\beta\rangle\langle\gamma,\delta|$$

$$G = \sum_{\alpha,\beta,\gamma,\delta} \langle\alpha,\beta|\,g\,|\gamma,\delta\rangle\;\; a^\dagger_\alpha\, a^\dagger_\beta\, a_\delta\, a_\gamma$$

The ordering of the operators matches that of the labels of the matrix element:

First destroy a particle in $|\gamma\rangle$, **then** destroy a particle in $|\delta\rangle$,
then create a particle in $|\beta\rangle$, **then** create a particle in $|\alpha\rangle$.

Pair correlation function: 2^{nd}–quantised form (qu. 14)

- Start from the 2–body operator $g = |\mathbf{r}, \mathbf{r}'\rangle\langle\mathbf{r}, \mathbf{r}'|$ and $G = \sum_{i \neq j} g^{(i,j)}$

- Average the two–body operator G in some quantum state:

$$\langle G \rangle = \mathrm{Tr}[\,\rho^{(2)} g\,] = \mathrm{Tr}[\,\rho^{(2)}\,|\mathbf{r}, \mathbf{r}'\rangle\langle\mathbf{r}, \mathbf{r}'|\,] = \langle \mathbf{r}, \mathbf{r}'|\rho^{(2)}|\mathbf{r}, \mathbf{r}'\rangle$$

Diagonal elements of the two–body density $\rho^{(2)}$

- Express G in terms of second–quantised operators:

$g = |\mathbf{r}, \mathbf{r}'\rangle\langle\mathbf{r}, \mathbf{r}'|$ means that $G = \hat{\Psi}^\dagger(\mathbf{r})\hat{\Psi}^\dagger(\mathbf{r}')\,\hat{\Psi}(\mathbf{r}')\,\hat{\Psi}(\mathbf{r})$

$$\langle \mathbf{r}, \mathbf{r}'|\,\rho^{(2)}\,|\mathbf{r}, \mathbf{r}'\rangle = \langle\,\hat{\Psi}^\dagger(\mathbf{r})\,\hat{\Psi}^\dagger(\mathbf{r}')\,\hat{\Psi}(\mathbf{r}')\,\hat{\Psi}(\mathbf{r})\,\rangle$$

- **Hanbury–Brown and Twiss effect with ideal Bose and Fermi gases:**

  • Ideal Bose gas at $T = 0$: $\langle \mathbf{r}, \mathbf{r}'|\rho^{(2)}|\mathbf{r}, \mathbf{r}'\rangle = \langle \mathbf{r}|\,\rho^{(1)}\,|\mathbf{r}\rangle\;\langle \mathbf{r}'|\,\rho^{(1)}\,|\mathbf{r}'\rangle$

• Ideal Bose gas above T_B, or ideal Fermi gas always, grand–canonical ensemble:

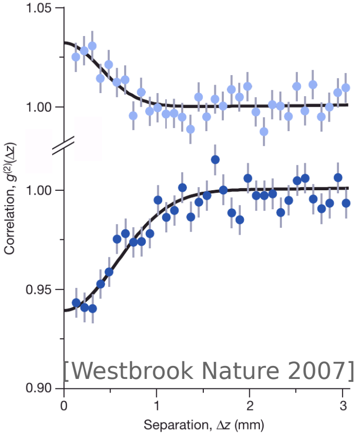
$$\langle \mathbf{r}, \mathbf{r}'|\rho^{(2)}|\mathbf{r}, \mathbf{r}'\rangle = \langle \mathbf{r}|\,\rho^{(1)}\,|\mathbf{r}\rangle\,\langle \mathbf{r}'|\,\rho^{(1)}\,|\mathbf{r}'\rangle \pm |\,\langle \mathbf{r}|\,\rho^{(1)}\,|\mathbf{r}'\rangle\,|^2 \qquad \text{(+ bosons, - fermions)}$$

[see e.g. Naraschewski & Glauber, Phys. Rev. A **59**, 4595 (1999), part III]

Experiment: atomic Hanbury–Brown & Twiss effect

- A cloud of gaseous $^4\mathrm{He}$ (above T_B) or $^3\mathrm{He}$ falls onto a detector plate:

  Position– and time–resolved detection yields $\dfrac{\langle \mathbf{r}, \mathbf{r}' | \rho^{(2)} | \mathbf{r}, \mathbf{r}' \rangle}{\langle \mathbf{r} | \, \rho^{(1)} \, | \mathbf{r} \rangle \, \langle \mathbf{r}' | \, \rho^{(1)} \, | \mathbf{r}' \rangle}$



- Which curve corresponds to the bosonic isotope? to the fermionic isotope?

[Jeltes et al, Nature **445**, 402 (2007)]

Part 5:

Interacting systems

pair–wise interaction, dispersion relation

[Pitaevskii & Stringari, *Bose–Einstein Condensation and Superfluidity*, OUP (2016), chs. 2 & 4]

[Wilks, *An Introduction to Liquid Helium*, Clarendon Press (Oxford, 1970), ch. 7]

Pair–wise interactions: second–quantised form (qu. 18)

(See slide 23 for various types of pair–wise interactions)

- 2–particle operator $V = \sum_i \sum_{j \neq i} \frac{v^{(i,j)}}{2}$ $v^{(i,j)} = v^{(j,i)}$ and 2 additional properties:

  1. Diagonal in terms of 2–particle states: $v = \int d^3 r_1 d^3 r_2 \; |\mathbf{r}_1, \mathbf{r}_2\rangle \; v(\mathbf{r}_1, \mathbf{r}_2) \; \langle \mathbf{r}_1, \mathbf{r}_2|$

  2. Translational invariance: $v(\mathbf{r}_1, \mathbf{r}_2) = v(\mathbf{r}_1 - \mathbf{r}_2)$

- Using these properties, expand v in the 2–particle basis involving plane waves $|\mathbf{k}\rangle$:

$$v = \int \frac{d^3k_1}{(2\pi/L)^3} \frac{d^3k_2}{(2\pi/L)^3} \frac{d^3q}{(2\pi/L)^3} \; |\mathbf{k}_1 + \mathbf{q}, \mathbf{k}_2 - \mathbf{q}\rangle \; v(\mathbf{q}) \; \langle \mathbf{k}_1, \mathbf{k}_2| \quad \text{with} \quad v(\mathbf{q}) = \int \frac{d^3r}{L^3} \, e^{-i\mathbf{qr}} \, v(\mathbf{r})$$

  and interpret this expression in terms of momentum conservation.

- Express V using the field operator $\Psi(\mathbf{k})$ destroying a particle in the plane wave $|\mathbf{k}\rangle$:

$$V = \frac{1}{2} \int \frac{d^3k_1}{(2\pi/L)^3} \frac{d^3k_2}{(2\pi/L)^3} \frac{d^3q}{(2\pi/L)^3} \; v(\mathbf{q}) \; \hat{\Psi}^\dagger(\mathbf{k}_1 + \mathbf{q}) \, \hat{\Psi}^\dagger(\mathbf{k}_2 - \mathbf{q}) \, \hat{\Psi}(\mathbf{k}_2) \, \hat{\Psi}(\mathbf{k}_1)$$

- For the contact interaction $v(\mathbf{r}_1 - \mathbf{r}_2) = g\,\delta(\mathbf{r}_1 - \mathbf{r}_2)$:

$$V = \frac{1}{2} \frac{g}{L^3} \int \frac{d^3k_1}{(2\pi/L)^3} \frac{d^3k_2}{(2\pi/L)^3} \frac{d^3q}{(2\pi/L)^3} \; \hat{\Psi}^\dagger(\mathbf{k}_1 + \mathbf{q}) \, \hat{\Psi}^\dagger(\mathbf{k}_2 - \mathbf{q}) \, \hat{\Psi}(\mathbf{k}_2) \, \hat{\Psi}(\mathbf{k}_1)$$

Diagonal form of $\rho^{(1)}$ for an interacting system (qu. 19)

- For an ideal (Bose or Fermi) gas, $\langle \mathbf{r}|\rho^{(1)}|\mathbf{r}'\rangle = \sum_\alpha \langle \hat{n}_\alpha \rangle \; \psi_\alpha(\mathbf{r}) \, \psi^*_\alpha(\mathbf{r}')$

Diagonal means sum over a *single index* α; $h = \sum_\alpha \varepsilon_\alpha \, |\psi_\alpha\rangle\langle\psi_\alpha|$

The diagonal form holds in the presence of **interactions,** for suitable functions $\{|\phi_\alpha\rangle\}$

- We are used to expectation values for Hermitian operators M: then, $\langle M \rangle$ is real

  $\langle \mathbf{r}|\rho^{(1)}|\mathbf{r}'\rangle$ = average of non–hermitian operator $M = \hat{\Psi}^\dagger(\mathbf{r}') \, \hat{\Psi}(\mathbf{r})$, may be complex

- $$\begin{aligned} \langle M^\dagger \rangle &= \mathrm{Tr}[\,\rho\, M^\dagger\,] = \mathrm{Tr}[\,(M\,\rho^\dagger)^\dagger\,] = \mathrm{Tr}[\,(M\,\rho)^\dagger\,] \\ &= \mathrm{Tr}[\,M\,\rho\,]^* = \mathrm{Tr}[\,\rho\,M\,]^* = \langle M \rangle^* \end{aligned}$$

- $$\langle \mathbf{r}'|\rho^{(1)}|\mathbf{r}\rangle = \langle \hat{\Psi}^\dagger(\mathbf{r}) \, \hat{\Psi}(\mathbf{r}') \rangle = \langle \left(\hat{\Psi}^\dagger(\mathbf{r}') \, \hat{\Psi}(\mathbf{r}) \right)^\dagger \rangle = \langle \mathbf{r}|\rho^{(1)}|\mathbf{r}'\rangle^*$$

The operator $\rho^{(1)}$ is Hermitian, so it may be diagonalised: $\rho^{(1)} = \sum_\alpha \nu_\alpha \; |\phi_\alpha\rangle\langle\phi_\alpha|$

$$\langle \mathbf{r}|\rho^{(1)}|\mathbf{r}'\rangle = \sum_\alpha \nu_\alpha \;\; \phi_\alpha(\mathbf{r}) \, \phi^*_\alpha(\mathbf{r}')$$

- **Bose–Einstein condensate** if (at least) one of the populations ν_α is of order N

Dilute Bose gas versus liquid Helium 4 (qu. 20)

Dilute Bose gas

- Dilute: $nR^3 \ll 1$

  $[R = (mC_6/\hbar^2)^{1/4} = \text{interaction range}]$

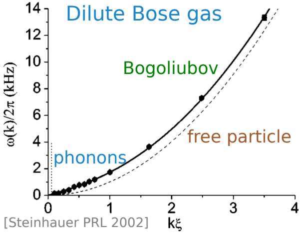
- Weak interactions: $na^3 \ll 1$

  [scattering length a sets interaction strength]

- At $T \sim 0$, all atoms in condensate

  [depletion $1 - n_0/N = 1.5(na^3)^{1/3} \approx 0.01$]

- Excitation spectrum



- Superfluid (phonons at low T: $\varepsilon = c\,k$)

Liquid Helium 4

- Liquid with $nR^3 \sim 1$

  [The motion of a given atom is not ballistic]

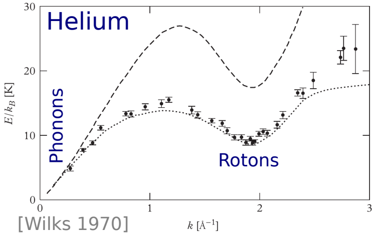
- Strong, nonzero–ranged interactions

  [roton minimum in excitation spectrum]

- At $T \sim 0$, few atoms in condensate

  [depletion $1 - n_0/N \approx 0.9$]

- Excitation spectrum



- Superfluid (phonons at low T: $\varepsilon = c\,k$)

Bose condensate present: **Bogoliubov prescription**

- Diagonalise $\rho^{(1)}$ to get the single–particle basis $\{|\phi_i\rangle\}$: $\quad \rho^{(1)} = \sum_i n_i \, |\phi_i\rangle \, \langle\phi_i|$
- Expand the field operator onto the basis $\{|\phi_i\rangle\}$: $\quad \hat{\Psi}(\mathbf{r}) = \sum_i a_i \, \phi_i(\mathbf{r})$

$$\langle \mathbf{r}|\rho^{(1)}|\mathbf{r}'\rangle = \langle \, \hat{\Psi}^\dagger(\mathbf{r}')\hat{\Psi}(\mathbf{r}) \, \rangle = \sum_{i,j} \langle a_i^\dagger a_j\rangle \; \phi_i^*(\mathbf{r}') \, \phi_j(\mathbf{r})$$

Compare the two expressions for $\rho^{(1)}$: $\quad \langle a_i^\dagger a_j\rangle = n_i \, \delta_{i,j}$

- If a condensate is present: $\quad n_0$ is of the order of N

$\langle a_0^\dagger a_0\rangle = n_0$ and $\quad \langle a_0 a_0^\dagger\rangle = \langle a_0^\dagger a_0 + 1\rangle = n_0 + 1$

Bogoliubov prescription: **Neglect commutator,** replace a_0 by a **number**

$$a_0 = \sqrt{n_0} \quad \text{and} \quad \hat{\Psi}(\mathbf{r}) = \sqrt{n_0} \, \phi_0(\mathbf{r}) + \sum_{i \neq 0} a_i \, \phi_i(\mathbf{r})$$

- In the presence of a condensate, the average $\langle \hat{\Psi}(\mathbf{r})\rangle$ is non–zero!

$$\langle \hat{\Psi}(\mathbf{r})\rangle = \sqrt{n_0} \, \phi_0(\mathbf{r}) = \Psi_0(\mathbf{r})$$

Applicable both in the absence and in the presence of interactions

The **order parameter** $\Psi_0(\mathbf{r}) = \langle \hat{\Psi}(\mathbf{r}) \rangle$

$$\hat{\Psi}(\mathbf{r}) = \sqrt{n_0}\,\phi_0(\mathbf{r}) + \sum_{i\neq 0} a_i\,\phi_i(\mathbf{r}) = \Psi_0(\mathbf{r}) + \sum_{i\neq 0} a_i\,\phi_i(\mathbf{r})$$

- **Order parameter:** $\Psi_0(\mathbf{r}) \neq 0$ only in presence of a condensate (and $\int d^3r\,|\Psi_0^2| = N_0$)

  just like magnetisation in the para–to–ferromagnetic phase transition

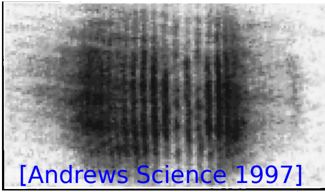
  Give a simple argument why $\langle\hat{\Psi}(\mathbf{r})\rangle$ vanishes in the absence of a condensate!

- **Symmetry breaking:**

  $\Psi_0(\mathbf{r})$ may be multiplied by arbitrary $e^{i\theta}$

  The condensate phase θ varies from realisation to realisation

  measurable by interference, pilots Josephson oscillations



[Andrews Science 1997]

- **Time dependence:** Start from a pure state $|\Psi_N\rangle$ with $N \gg 1$ particles

  Destroy a particle **from the condensate:**

  $a_0\,|\Psi_N\rangle = \sqrt{n_0}\,|\Psi_N\rangle$ has $(N-1)$ particles **and** non–zero overlap with $|\Psi_N\rangle$

  $$\langle\Psi_N|\,\hat{\Psi}(\mathbf{r})\,|\Psi_N\rangle = \langle\Psi_N|\,a_0^\dagger\,\hat{\Psi}(\mathbf{r})\,|\Psi_N\rangle\,/\sqrt{n_0} \neq 0$$

  The time dependence of $|\Psi_N\rangle$ is $\exp[-iE_Nt/\hbar]$; that of $a_0\,|\Psi_N\rangle$ is $\exp[-iE_{N-1}t/\hbar]$

  The complete time dependence is $\exp[-i(E_N - E_{N-1})t/\hbar] = \exp[-i\,\mu\,t/\hbar]$

  Time dependence of $\Psi_0(\mathbf{r})$ is determined by chemical potential $\mu = E_N - E_{N-1}$

Weakly–interacting bosons, $T = 0$: **Gross–Pitaevskii**

- Many–body Hamiltonian for the contact interaction $v(\mathbf{r}-\mathbf{r}') = g\,\delta(\mathbf{r}-\mathbf{r}')$

$$H = \int d^3r_1 \left[\hat{\Psi}^\dagger(\mathbf{r}_1)\left(\frac{p^2}{2m}+u\right)\hat{\Psi}(\mathbf{r}_1) + \frac{g}{2}\hat{\Psi}^\dagger(\mathbf{r}_1)\hat{\Psi}^\dagger(\mathbf{r}_1)\hat{\Psi}(\mathbf{r}_1)\hat{\Psi}(\mathbf{r}_1)\right]$$

- Time dependence of the field operator: $i\hbar\,\partial\hat{\Psi}(\mathbf{r})/\partial t = [\,\hat{\Psi}(\mathbf{r}), H\,]$

$$i\hbar\frac{\partial\hat{\Psi}}{\partial t} = \left(-\frac{\hbar^2\Delta}{2m}+u(\mathbf{r})\right)\hat{\Psi}(\mathbf{r}) + g\,\hat{\Psi}^\dagger(\mathbf{r})\hat{\Psi}(\mathbf{r})\hat{\Psi}(\mathbf{r})$$

- **Approximation:** replace $\hat{\Psi}(\mathbf{r})$ by $\Psi_0(\mathbf{r})$ **“fully condensed system”**

The field operator becomes a *classical field* satisfying the *non–linear* Gross–Pitaevskii equation

$$i\hbar\,\frac{\partial\Psi_0}{\partial t} = \left(-\frac{\hbar^2\Delta}{2m}+u(\mathbf{r})\right)\Psi_0(\mathbf{r}) + g\,|\Psi_0(\mathbf{r})|^2\,\Psi_0(\mathbf{r})$$

- Stationary state (i.e. ground state) $\Psi_0(\mathbf{r},t) = \Psi_0(\mathbf{r})\,e^{-i\mu t/\hbar}$

$$\mu\,\Psi_0 = \left(-\frac{\hbar^2\Delta}{2m}+u(\mathbf{r})\right)\Psi_0(\mathbf{r}) + g\,|\Psi_0(\mathbf{r})|^2\,\Psi_0(\mathbf{r})$$

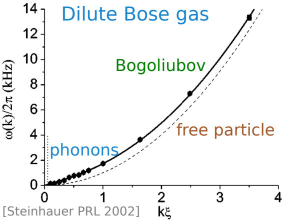
- **Uniform gas:** $\Psi_0 = \sqrt{n}$, chemical potential $\mu = gn$, energy $E = gn^2\,V/2$

Bosonic Bogoliubov theory: excitations in Bose gas

1. Using the Bogoliubov prescription,
replace the full Hamiltonian by an approximate quadratic one
in terms of $a^\dagger_{\mathbf{k}}$ and $a_{\mathbf{k}}$ creating and annihilating plane waves with $\mathbf{p} = \hbar\,\mathbf{k}$

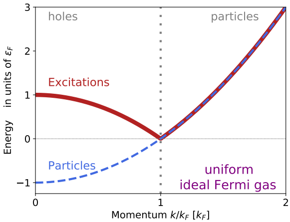
2. "Diagonalise the quadratic Hamiltonian",
i.e. introduce new operators $b_{\mathbf{k}}$ annihilating the ground state
such that $H = E_0 + \sum_{\mathbf{k}} \varepsilon(\mathbf{k})\, b^\dagger_{\mathbf{k}}\, b_{\mathbf{k}}$ and $\varepsilon(\mathbf{k}) > 0$:
E_0 is the ground state energy and $\varepsilon(\mathbf{k})$ is the dispersion relation for the excitations

weakly–interacting Bose gas



$$\varepsilon(k) = \left[\left(\frac{\hbar^2 k^2}{2m}\right)^2 + 2\,\frac{\hbar^2 k^2}{2m}\,gn\right]^{(1/2)}$$

ideal Fermi gas



$$\varepsilon(k) = \left|\frac{\hbar^2 k^2}{2m} - E_F\right|$$

Step 1: **Bogoliubov prescription**

- Many–body Hamiltonian involving the contact interaction $v(\mathbf{r_1} - \mathbf{r}_2) = g\delta(\mathbf{r}_1 - \mathbf{r}_2)$

$$H = \sum_{\mathbf{p}} \frac{p^2}{2m} a^\dagger_{\mathbf{p}} a_{\mathbf{p}} + \frac{g}{2L^3} \sum_{\mathbf{p}_1+\mathbf{p}_2+\mathbf{p}_3+\mathbf{p}_4=0} a^\dagger_{-\mathbf{p}_3} a^\dagger_{-\mathbf{p}_4} a_{\mathbf{p}_2} a_{\mathbf{p}_1}$$

- Approximation for the interaction term exploiting Bogoliubov criterion:

  Replace $a_0 = \sqrt{N_0}$ by a number, keep non–condensed modes up to 2^{nd} order

If none of the momenta $\mathbf{p}_i$ are $\mathbf{0}$: order 4; if only 1 momentum $\mathbf{p}_i = \mathbf{0}$: order 3

2 non–zero momenta: $a^\dagger_0 a^\dagger_0 a_{-\mathbf{p}} a_{\mathbf{p}},\ a^\dagger_0 a^\dagger_{\mathbf{p}} a_0 a_{\mathbf{p}},\ a^\dagger_{\mathbf{p}} a^\dagger_0 a_0 a_{\mathbf{p}},\ a^\dagger_0 a^\dagger_{\mathbf{p}} a_{\mathbf{p}} a_0,\ a^\dagger_{\mathbf{p}} a^\dagger_0 a_{\mathbf{p}} a_0,\ a^\dagger_{\mathbf{p}} a^\dagger_{-\mathbf{p}} a_0 a_0$

1 non–zero momentum: does not conserve momentum

All momenta are 0: $a^\dagger_0 a_0 = N - \sum_{\mathbf{p}\neq 0} a^\dagger_{\mathbf{p}} a_{\mathbf{p}}$ $\quad a^\dagger_0 a^\dagger_0 a_0 a_0 \approx (a^\dagger_0 a_0)^2 = N^2 - 2N \sum_{\mathbf{p}\neq 0} a^\dagger_{\mathbf{p}} a_{\mathbf{p}}$

For $a^\dagger_0 a^\dagger_0 a_0 a_0$, we have implemented particle number conservation: $N = N_0 + N_{\text{thermal}}$

- The resulting quadratic Hamiltonian conserves momentum: $(n = N/V)$

$$H_{\text{Bogo}} = \frac{gN^2}{2L^3} + \sum_{\mathbf{p}} \left[\left(\frac{p^2}{2m} + gn \right) a^\dagger_{\mathbf{p}} a_{\mathbf{p}} + \frac{gn}{2} \left(a_{-\mathbf{p}} a_{\mathbf{p}} + a^\dagger_{\mathbf{p}} a^\dagger_{-\mathbf{p}} \right) \right]$$

The particle number is not conserved: the condensate acts as a reservoir

Step 2: **Diagonalise the quadratic Hamiltonian**

$$H_{\rm Bogo} = \frac{gN^2}{2L^3} + \sum_{\mathbf{p}} H_{\mathbf{p}} \qquad \text{where} \quad H_{\mathbf{p}} = \left(\frac{p^2}{2m} + gn \right) a^\dagger_{\mathbf{p}} \, a_{\mathbf{p}} \quad + \quad \frac{gn}{2} \left(a_{\mathbf{p}} \, a_{-\mathbf{p}} \; + \; a^\dagger_{\mathbf{p}} \, a^\dagger_{-\mathbf{p}} \right)$$

- Introduce new bosonic operators $b_{\mathbf{p}}$ and $b^\dagger_{\mathbf{p}}$: $\quad [\, b_{\mathbf{p}}, b^\dagger_{\mathbf{p}'} \,] = \delta_{\mathbf{p},\mathbf{p}'} , \quad [\, b_{\mathbf{p}}, b_{\mathbf{p}'} \,] = 0$

  Look for them in the form: $\quad a_{\mathbf{p}} = u_p b_{\mathbf{p}} + v_p b^\dagger_{-\mathbf{p}}$, $\quad$ hence $a^\dagger_{\mathbf{p}} = u_p b^\dagger_{\mathbf{p}} + v_p b_{-\mathbf{p}}$

  where u_p, v_p are real and depend only on $p = |\mathbf{p}|$

  $[\, a_{\mathbf{p}}, a^\dagger_{\mathbf{p}} \,] = 1$ yields $u_p^2 - v_p^2 = 1$: $\quad$ take $u_p = \cosh \theta_p$ and $v_p = \sinh \theta_p$

- $$\begin{aligned}
a^\dagger_{\mathbf{p}} a_{\mathbf{p}} &= u_p^2 \, b^\dagger_{\mathbf{p}} b_{\mathbf{p}} + u_p v_p \, b^\dagger_{\mathbf{p}} b^\dagger_{-\mathbf{p}} + u_p v_p \, b_{-\mathbf{p}} b_{\mathbf{p}} + v_p^2 \, b_{-\mathbf{p}} b^\dagger_{-\mathbf{p}} \\
a_{\mathbf{p}} a_{-\mathbf{p}} &= u_p^2 \, b_{\mathbf{p}} b_{-\mathbf{p}} + u_p v_p \, b_{\mathbf{p}} b^\dagger_{\mathbf{p}} + u_p v_p \, b^\dagger_{-\mathbf{p}} b_{-\mathbf{p}} + v_p^2 \, b^\dagger_{-\mathbf{p}} b^\dagger_{\mathbf{p}} \\
a^\dagger_{\mathbf{p}} a^\dagger_{-\mathbf{p}} &= u_p^2 \, b^\dagger_{\mathbf{p}} b^\dagger_{-\mathbf{p}} + u_p v_p \, b_{-\mathbf{p}} b^\dagger_{-\mathbf{p}} + u_p v_p \, b^\dagger_{\mathbf{p}} b_{\mathbf{p}} + v_p^2 \, b_{-\mathbf{p}} b_{\mathbf{p}}
\end{aligned}$$

- Set coefficient of $b^\dagger_{\mathbf{p}} \, b^\dagger_{-\mathbf{p}}$ (which is the same as for $b_{-\mathbf{p}} \, b_{\mathbf{p}}$) to zero:

$$\frac{\sinh(2\theta_p)}{2} \left(\frac{p^2}{2m} + gn \right) + \frac{gn}{2} \cosh(2\theta_p) = 0, \quad \text{hence} \quad \tanh(2\theta_p) = -\frac{gn}{p^2/(2m) + gn}$$

Bosonic Bogoliubov: **Result**

$$\cosh\theta = \left[\frac{\cosh(2\theta)+1}{2}\right]^{1/2}, \quad \sinh\theta = -\left[\frac{\cosh(2\theta)-1}{2}\right]^{1/2}, \quad \cosh(2\theta) = 1/\sqrt{1-\tanh^2(2\theta)}$$

- $u_p = \left[\frac{p^2/(2m)+gn}{2\,\varepsilon(p)} + \frac{1}{2}\right]^{1/2}$ and $v_p = -\left[\frac{p^2/(2m)+gn}{2\,\varepsilon(p)} - \frac{1}{2}\right]^{1/2}$

- Diagonal form of the many–body Hamiltonian: $H = E_0 + \sum_{\mathbf{p}} \varepsilon(p)\, b^\dagger_{\mathbf{p}}\, b_{\mathbf{p}}$

  Ground–state energy: $E_0 = \frac{gN^2}{2L^3} + \frac{1}{2}\sum_{\mathbf{p}}\left(\varepsilon(p) - \frac{p^2}{2m} - gn\right)$

  (More accurate than the Gross–Pitaevskii result, but not the whole story)

  Bogoliubov dispersion relation $\varepsilon(p) = \left[\left(\frac{p^2}{2m}\right)^2 + 2\,\frac{p^2}{2m}\,gn\right]^{1/2}$

- Justify that the non–condensed modes are populated even at $T=0$

  Show that, at $T=0$, the condensate density is: $n_0 = \frac{N}{V}\left[1 - \frac{8}{3\sqrt{\pi}}\,(na^3)^{1/2}\right]$

($g = 4\pi\hbar^2 a/m > 0$, where $a > 0$ is the scattering length encoding repulsive interactions)