Quantum Degenerate Gases

Lecture 2: Atom Cooling and Trapping

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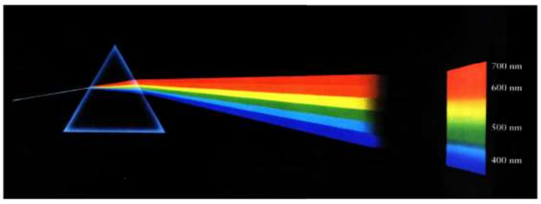
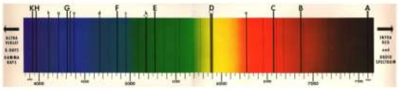
Contents

Of Light and Matter



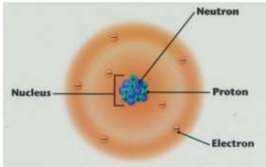
W.H. Wollaston 1766 - 1828

J. von Fraunhofer 1787 - 1826

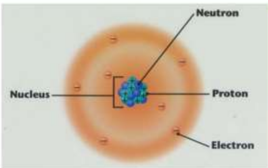


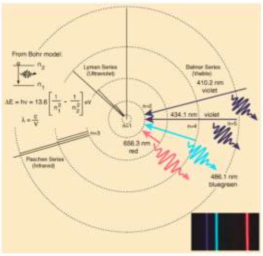
Fraunhofer Lines: discrete dark lines in the spectrum due to absorption of cold particles in the atomsphere of the Sun.

Bohr Model



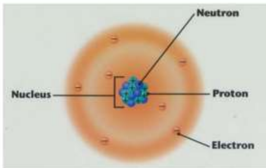
Bohr Model

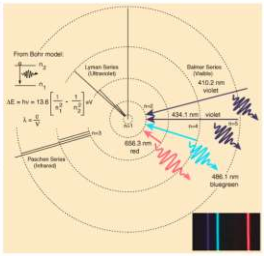




- Electrons move on a discrete set of orbits with quantized energies.
- Absorption/Emission of electromagnetic radiation quantized.
- Angular momentum quantized: $mvr = n\hbar$

Bohr Model





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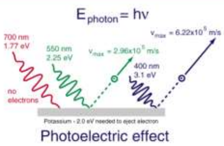
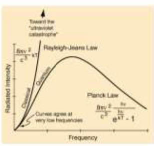
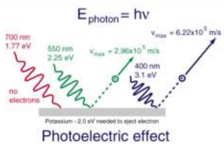
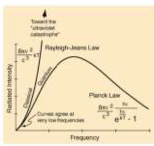
Particle-Wave Duality

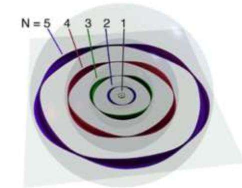




Particle-Wave Duality





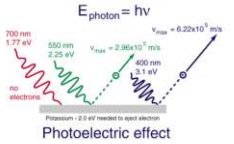


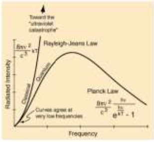
Bohr-de Broglie electron matterwave orbits shells 1-5

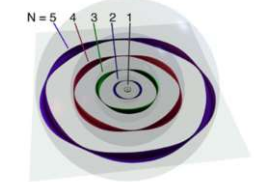
de Broglie wavelength

$$\lambda = \frac{h}{mv}$$

Particle-Wave Duality







Bohr-de Broglie electron matterwave orbits shells 1-5

de Broglie wavelength

$$\lambda = \frac{h}{mv}$$

Cast new light on light-matter interaction

Laser Spectroscopy

Measurement of energetic absorption/emission of matter using laser.

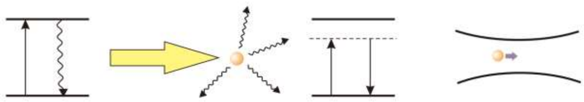
Laser Spectroscopy

Measurement of energetic absorption/emission of matter using laser.

- Gain information about structure of atoms and molecules
- Better understanding of light-matter interaction
- Line broadening etc.: need colder atoms

Interaction Between Light and Atom

Radiation pressure force | Dipole force



Atom recoils in a random direction due to spontaneous emission, gaining the momentum of the incident photon on average.
non-conservative

Atom feels a gradient force, in the direction of high(low) fields given red(blue) detuning.
conservative

Interaction between Laser and a Two-Level Atom

Complete Hamiltonian describing interaction between EM-field and a two-level atom

$$\begin{aligned} H &= \frac{\mathbf{p}^2}{2m} + E_g|g\rangle\langle g| + E_e|e\rangle\langle e| + \sum_\alpha \hbar\omega_\alpha a_\alpha^\dagger a_\alpha \\ &- \sum_\alpha \frac{\mathbf{d}\cdot\hat{\epsilon}_\alpha}{2}(|e\rangle\langle g| + |g\rangle\langle e|) \times \{i\varepsilon_\alpha a_\alpha e^{(-i\mathbf{k}_\alpha\cdot\mathbf{r}+i\omega_\alpha t)} + h.c.\} \end{aligned}$$

We want to see effects of laser on atomic motion

- Complete equations of motion too complicated
- External motion separable from internal degrees of freedom?
  Internal dynamics $\Gamma^{-1} \sim 18ns$ (^{23}Na)
  External dynamics $\omega_{recoil}^{-1} \sim 12\mu s$ (^{23}Na, $\lambda_{laser} \sim 800nm$)
  $\Gamma = \frac{1}{\pi\epsilon_0}\frac{\omega_0^3 d^2}{3\hbar c^3}$ $\quad \omega_{recoil} = \frac{\hbar k^2}{2m}$

Approximations:

- External motion decoupled from the internal dynamics
  - The internal dynamics adiabatically follows slow external motion
  - Internal degrees of freedom in quasi-steady state
- Electric-dipole approximation
- Single-mode approximation for EM-field: laser
- Markovian process: $\tau \ll \delta t \ll T_r$
  τ: correlation time in the reservoir
  δt: typical time for spontaneous decay
  T_r: total time of evolution

Lindblad master equation for a damped two-level atom

$$\begin{aligned} i\hbar\dot{\rho} &= [H', \rho] + \mathcal{L}(\rho) \\ H' &= \hbar\omega_0|e\rangle\langle e| + \frac{\hbar\Omega}{2}\{e^{i\phi(\mathbf{r})}e^{i\omega t}|g\rangle\langle e| + h.c.\} \\ \mathcal{L}(\rho) &= i\frac{\Gamma}{2}(2\sigma_-\rho\sigma_+ - \sigma_+\sigma_-\rho - \rho\sigma_+\sigma_-) \\ \sigma_- &= |g\rangle\langle e| \qquad \sigma_+ = |e\rangle\langle g| \end{aligned}$$

- $E_g = 0$, $E_e = \hbar\omega_0$, $\Omega = -\frac{\mathbf{d}\cdot\mathbf{E}(\mathbf{r})}{\hbar}$
- Trace over EM-field modes other than that of the laser
- Rotating-wave approximation (RWA): neglecting counter rotating terms

$$\frac{\Omega}{\omega_0 + \omega} \ll 1, \qquad \frac{|\delta|}{\omega_0 + \omega} \ll 1$$

Equations of motion for the density matrix

$$\begin{cases} \dot{\rho}_{ee} = -i\frac{\Omega}{2}\left(e^{-i\phi}e^{-i\omega t}\rho_{ge} - c.c.\right) - \Gamma\rho_{ee} \\ \dot{\rho}_{gg} = i\frac{\Omega}{2}\left(e^{-i\phi}e^{-i\omega t}\rho_{ge} - c.c.\right) + \Gamma\rho_{ee} \\ \dot{\rho}_{ge} = \left(i\omega_0 - \frac{\Gamma}{2}\right)\rho_{ge} - i\frac{\Omega}{2}e^{i\phi}e^{i\omega t}(\rho_{ee} - \rho_{gg}) \end{cases}$$

Transform to the rotating frame $\rho_{ge} = \tilde{\rho}_{ge}e^{i\omega t}$ to get rid of time dependence

Equations of motion in the rotating frame

$$\begin{cases} \dot{\rho}_{ee} = -i\frac{\Omega}{2}\left(e^{-i\phi}\tilde{\rho}_{ge} - c.c.\right) - \Gamma\rho_{ee} \\ \dot{\rho}_{gg} = i\frac{\Omega}{2}\left(e^{-i\phi}\tilde{\rho}_{ge} - c.c.\right) + \Gamma\rho_{ee} \\ \dot{\tilde{\rho}}_{ge} = \left(-i\delta - \frac{\Gamma}{2}\right)\tilde{\rho}_{ge} - i\frac{\Omega}{2}e^{i\phi}\left(\rho_{ee} - \rho_{gg}\right) \end{cases}$$

We are interested in steady state solution
What defines steady state?

$$\dot{\tilde{\rho}}_{ge}^{steady} = \dot{\tilde{\rho}}_{ee}^{steady} = \dot{\tilde{\rho}}_{gg}^{steady} = 0$$

Perturbative process

$$\dot{\tilde{\rho}}_{ge}^{steady} = 0 \rightarrow \tilde{\rho}_{ge}^{steady} \rightarrow \{\tilde{\rho}_{gg}^{steady}, \tilde{\rho}_{ee}^{steady}\}$$

Steady state solution

$$\begin{cases} \tilde{\rho}_{eg}^{steady} = \dfrac{-i\frac{\Omega}{2}e^{-i\phi}\left(\frac{\Gamma}{2} + i\delta\right)}{\delta^2 + \left(\frac{\Gamma}{2}\right)^2 + \frac{\Omega^2}{2}} \\ \tilde{\rho}_{ee}^{steady} = \dfrac{\frac{\Omega^2}{4}}{\delta^2 + \left(\frac{\Gamma}{2}\right)^2 + \frac{\Omega^2}{2}} \end{cases}$$

We may now incorporate kinetic energy $\frac{\mathbf{p}^2}{2m}$ into the Hamiltonian

- Density matrix elements now dependent on position (momentum) operators: $\rho_{ij}(\mathbf{r})$ $(\rho_{ij}(\mathbf{p}))$
- Derive atomic center of mass motion by quantizing position (momentum), then apply the steady-state solutions for expectation values of the external dynamics

Heisenberg equations of motion

$$\frac{d\mathbf{p}}{dt} = \frac{i}{\hbar}[H, \mathbf{p}]$$

where

$$H = \hbar\omega_0|e\rangle\langle e| + \frac{\hbar\Omega}{2}\left\{e^{i\phi(\mathbf{r})}e^{i\omega t}|g\rangle\langle e| + h.c.\right\} + \frac{\mathbf{p}^2}{2m}$$

As $[f(\mathbf{r}), \mathbf{p}] = i\hbar\nabla f(\mathbf{r})$, we have

$$\frac{d\mathbf{p}}{dt} = -\frac{\hbar}{2}\{[\nabla\Omega(\mathbf{r})e^{i\phi(\mathbf{r})}]e^{i\omega t}|g\rangle\langle e| + h.c.\}$$

Quantity we wish to evaluate

$$\mathbf{F} = \left\langle \frac{d\mathbf{p}}{dt} \right\rangle$$

Approximations:

- External motion decoupled from internal dynamics
- Internal dynamics given by steady-state solution
  $\langle |g\rangle\langle e| \rangle \sim \rho_{eg}^{steady}$
- Atom size much smaller than laser wavelength
  - Atom de Broglie wavelength small $\lambda_{laser} \gg \lambda_{atom}$
  - Spread of atomic wavefunction in time Γ^{-1} small
    $\Gamma^{-1}\frac{1}{m}\left(\frac{h}{\lambda_{atom}}\right) \ll \lambda_{laser} \Rightarrow \omega_{recoil}^{-1} \gg \Gamma^{-1}$

Semi-classical solution

$$\mathbf{F}(\mathbf{r}) \approx -\frac{\hbar}{2}\tilde{\rho}_{eg}^{steady}e^{i\phi}\Omega(\mathbf{r})\left\{\frac{\nabla\Omega(\mathbf{r})}{\Omega(\mathbf{r})} + i\nabla\phi(\mathbf{r})\right\} + c.c.$$

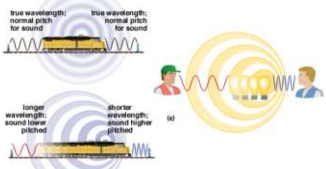
Radiation pressure force (RPF) and dipole force (DF)

$$\begin{cases} \mathbf{F} = \mathbf{F}_{RPF} + \mathbf{F}_{DF} \\ \mathbf{F}_{RPF} = -\dfrac{\hbar\Gamma}{4}\dfrac{\Omega^2}{\delta^2 + \left(\frac{\Gamma}{2}\right)^2 + \frac{\Omega^2}{2}}\nabla\phi \\ \mathbf{F}_{DF} = -\dfrac{\hbar\delta}{4}\dfrac{\nabla\Omega^2}{\delta^2 + \left(\frac{\Gamma}{2}\right)^2 + \frac{\Omega^2}{2}} \end{cases}$$

- RPF in same direction as velocity of photon $(v \propto -\nabla\phi)$
- DF is a gradient force. Atoms strong field seeking for red detuning $\delta < 0$; weak field seeking for blue detuning $\delta > 0$

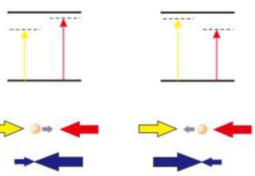
Doppler Cooling

Doppler effect

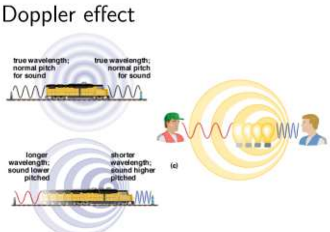


Doppler Cooling

Doppler cooling



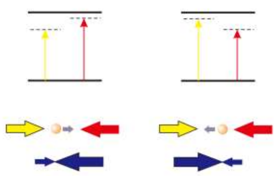
Doppler effect



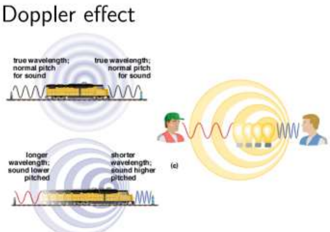
Proposed in 1975 by D.J. Wineland and H.G. Dehmelt, T.W. Hänsch and A.L. Schawlow

Doppler Cooling

Doppler cooling



Doppler effect



Proposed in 1975 by D.J. Wineland and H.G. Dehmelt, T.W. Hänsch and A.L. Schawlow

Typical Scaling (^{23}Na)
Before: 500K, $v \sim 700$m/s
After: 200μK, $v \sim 0.5$m/s

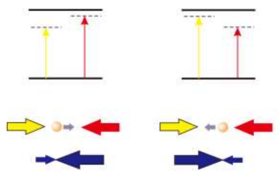
In the presence of a running wave

$$\mathbf{E}(\mathbf{r},\mathbf{t}) = \hat{\epsilon}E\cos(\omega t - \mathbf{k}\cdot\mathbf{r}) = \hat{\epsilon}E\cos(\omega t - \mathbf{k}\cdot\mathbf{v}t)$$

So that now the effective detuning seen by the atom is

$$\delta' = \delta - \mathbf{k}\cdot\mathbf{v}$$

Doppler cooling



- $\mathbf{F}_{DF} = 0$ for running waves
- $\mathbf{F}_{RPF}$ dependent on the velocity of atom and photon
- Counter propagating red-detuned fields can create effective friction

Single running wave field

$$\mathbf{F} = \frac{\hbar\mathbf{k}\Gamma}{4}\frac{\Omega^2}{(\delta-\mathbf{k}\cdot\mathbf{v})^2 + \left(\frac{\Gamma}{2}\right)^2 + \frac{\Omega^2}{2}}$$

Two counter propagating fields

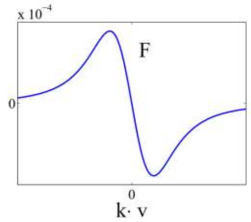
$$\begin{aligned}\mathbf{F} &= \frac{\hbar\mathbf{k}\Gamma}{4}\left\{\frac{\Omega^2}{(\delta-\mathbf{k}\cdot\mathbf{v})^2 + \left(\frac{\Gamma}{2}\right)^2 + \frac{\Omega^2}{2}} - \frac{\Omega^2}{(\delta+\mathbf{k}\cdot\mathbf{v})^2 + \left(\frac{\Gamma}{2}\right)^2 + \frac{\Omega^2}{2}}\right\} \\ &\approx \hbar\Gamma\frac{\delta\mathbf{k}(\mathbf{k}\cdot\mathbf{v})\Omega^2}{\left[\delta^2 + \left(\frac{\Gamma}{2}\right)^2 + \frac{\Omega^2}{2}\right]^2} \qquad \text{for small } \mathbf{k}\cdot\mathbf{v}\end{aligned}$$

This is the theoretical basis for the Doppler cooling. Note $\mathbf{k}(\mathbf{k}\cdot\mathbf{v})$ aligns with the direction of velocity.

For a 1-d configuration along $\hat{\mathbf{z}}$

$$F = -\eta v \qquad \eta = -\hbar k^2\Gamma\frac{\delta\Omega^2}{\left[\delta^2 + \left(\frac{\Gamma}{2}\right)^2 + \frac{\Omega^2}{2}\right]^2}$$

For red-detuned light $\delta < 0$



- Force opposite to atom velocity for red-detuned light
- The friction coefficient η maximum at $\delta = -\Gamma/2$ $(\Omega \sim \Gamma)$
- Atom absorbs a low energy photon, emits a high energy photon. Energy dissipated through spontaneous emission.

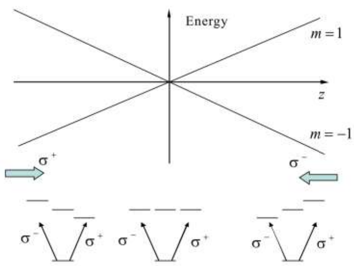
Doppler limit of laser cooling

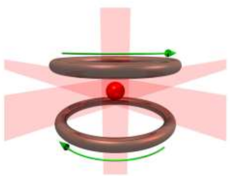
- Lower temperature, smaller detuning required
- Force on the order of spontaneous recoil effects when the temperature is within the absorption bandwidth Γ

More quantitatively

- Diffusive energy change $\frac{dE_{diff}}{dt} = \frac{\hbar^2k^2}{2m}\rho_{ee}\Gamma$
- Cooling energy change $\frac{dE_{cool}}{dt} = \mathbf{F}\cdot\mathbf{v} = -\eta v^2$
- At Doppler limit, $\delta = -\frac{\Gamma}{2}$, $\frac{dE_{cool}}{dt} + \frac{dE_{diff}}{dt} = 0$
  $k_BT_D \sim \frac{\hbar\Gamma}{16}$ (weak field limit)
- More sophisticated theory gives
  $k_BT_D \sim \frac{\hbar\Gamma}{2}$
- $T_D \sim 240\mu K$ for ^{23}Na

Combining spatially varying magnetic field and Doppler cooling lasers to cool and trap atoms simultaneously.





Magnetic field created by anti-Helmholtz coils

- Detuning now a function of position as well
- Atoms at $z < 0$ are closer to resonance of the σ^+ beam, therefore are pushed back to the origin

With quadrupole magnetic field $\mathbf{B}(\mathbf{r}) = B(x\hat{\mathbf{x}} + y\hat{\mathbf{y}} - 2z\hat{\mathbf{z}})$

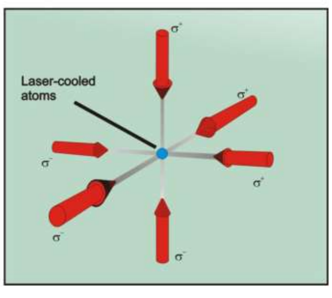
$$\delta_{\pm} = \delta \mp \mathbf{k}\cdot\mathbf{v} \mp \beta z$$

The total frictional force on the atom (for small $\mathbf{k}\cdot\mathbf{v}$ and Zeeman shfit)

$$\mathbf{F} \approx 2\hbar\Omega^2\Gamma\frac{\delta\mathbf{k}\left(\mathbf{k}\cdot\mathbf{v} + \beta z\right)}{\left[\delta^2 + \left(\frac{\Gamma}{2}\right)^2\right]^2}$$

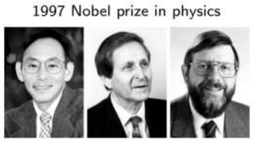
- Limitations on total atom density in the trap: atom losses due to spin-flip and excited state collisions
- Lowest temperature in principle set by the Doppler limit
- Need repumping laser for realistic atoms

Optical Molasses



$$F = -\alpha v$$

1997 Nobel prize in physics



S. Chu C.C.-Tannoudji W. Phillips

- Sub-Doppler temperature $\sim 10\mu$K
- Sisyphus cooling

Sisyphus Cooling

Theoretically for the laser setup of Doppler cooling

- Lowest achievable temperature given by the Doppler limit
  $k_BT_d = \frac{\hbar\Gamma}{2}$
- The Doppler limit occurs at $\delta = -\frac{\Gamma}{2}$

Experimentally, lower temperature at a different detuning was reached.
So, what is missing?

- Two counter propagating fields add up to something not running wave like (inhomogeneous).
- Realistic atoms have more complicated level structures.

Let us examine an idealized case.

Consider two counter progapating linearly polarized fields

$$\mathbf{E}_1 = \frac{E}{2}\hat{\epsilon}_x e^{i(kz+\omega t)} + c.c.$$
$$\mathbf{E}_2 = \frac{E}{2}\left(\cos\theta\hat{\epsilon}_x - \sin\theta\hat{\epsilon}_y\right) e^{i(-kz+\omega t)} + c.c.$$

They can be rewritten as

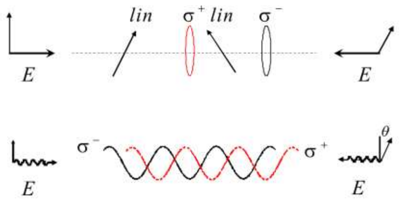
$$\mathbf{E}_1 = \frac{\sqrt{2}E}{4}\left(\hat{\epsilon}_+ + \hat{\epsilon}_-\right) e^{i(kz+\omega t)} + c.c.$$
$$\mathbf{E}_2 = \frac{\sqrt{2}E}{4}\left(e^{i\theta}\hat{\epsilon}_+ + e^{-i\theta}\hat{\epsilon}_-\right) e^{i(-kz+\omega t)} + c.c.,$$

where we have defined $\sigma^{\pm}$ polarization axis $\hat{\epsilon}_+(\hat{\epsilon}_-)$

$$\hat{\epsilon}_+ = \frac{\sqrt{2}}{2}\left(\hat{\epsilon}_x + i\hat{\epsilon}_y\right)$$
$$\hat{\epsilon}_- = \frac{\sqrt{2}}{2}\left(\hat{\epsilon}_x - i\hat{\epsilon}_y\right)$$

Polarization gradient (Lin-∠-Lin configuration)

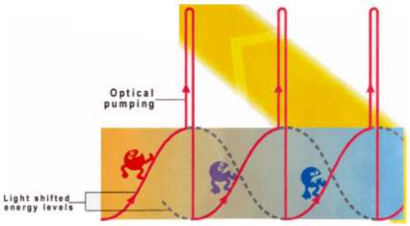
$$\mathbf{E} = \mathbf{E}_1 + \mathbf{E}_2$$
$$= \frac{\sqrt{2}}{2}Ee^{-i\omega t}\left[\cos\left(kz + \frac{\theta}{2}\right)e^{i\frac{\theta}{2}}\hat{\epsilon}_+ + \cos\left(kz - \frac{\theta}{2}\right)e^{-i\frac{\theta}{2}}\hat{\epsilon}_-\right] + c.c.$$

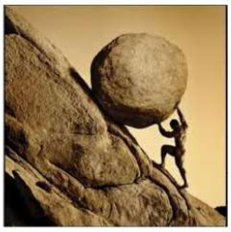


- Spatially varying polarization
- Spin-dependent lattice potentials

Sisyphus cooling (Lin-⊥-Lin configuration)

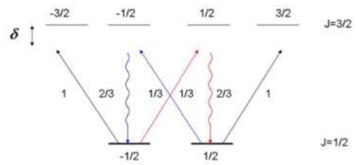
$$\mathbf{E} = \frac{\sqrt{2}E}{2}e^{-i\omega t}\left(\cos kz\hat{\epsilon}_- - i\sin kz\hat{\epsilon}_+\right) + c.c.$$





- Degenerate ground state associated with potentials with different polarization
- Atoms hop to the other ground state near maxima of potential via optical pumping

More specifically, consider relevant level schemes of an alkali atom



$$H = \frac{\mathbf{p}^2}{2m} - \delta|e_{\pm 3/2}\rangle\langle e_{\pm 3/2}| - \delta|e_{\pm 1/2}\rangle\langle e_{\pm 1/2}|$$
$$+ \frac{\sqrt{2}\hbar\Omega}{2}\cos kz\left(|e_{-3/2}\rangle\langle g_{-1/2}| + \frac{1}{\sqrt{3}}|e_{-1/2}\rangle\langle g_{1/2}|\right) + h.c.$$
$$- i\frac{\sqrt{2}\hbar\Omega}{2}\sin kz\left(|e_{3/2}\rangle\langle g_{1/2}| + \frac{1}{\sqrt{3}}|e_{1/2}\rangle\langle g_{-1/2}|\right) + h.c.$$

Need to simplify!

Simplifications

- Define collective raising/lowering operator $\{\Lambda, \Lambda^\dagger\}$

$$\Lambda = \{\cos kz\hat{\epsilon}_- - i\sin kz\hat{\epsilon}_+\} \cdot \mathbf{d}^+$$
$$H_{coupling} = \frac{\sqrt{2}\Omega}{2}\Lambda + h.c.$$

- Write down the equations of motion for the density matrix
- Adiabatic elimination of states other than $\left\{|g_{-\frac{1}{2}}\rangle, |g_{\frac{1}{2}}\rangle\right\}$

The Lindblad master equation

$$\dot{\rho} = -i[H_{eff}, \rho] + \frac{\Gamma s}{2}\sum_{q=\pm,0}\left(2J_q\rho J_q^\dagger - J_q^\dagger J_q\rho - \rho J_q^\dagger J_q\right)$$

With the satuaration parameter

$$s = \frac{\frac{(\sqrt{2}\Omega)^2}{2}}{\delta^2 + \left(\frac{\Gamma}{2}\right)^2}$$

Understanding the master equation

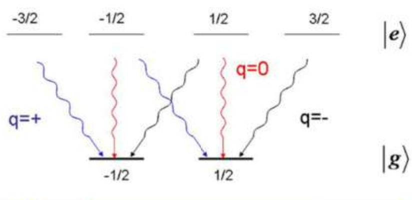
$$\dot{\rho} = -i[H_{eff}, \rho] + \frac{\Gamma s}{2}\sum_{q=\pm,0}\left(2J_q\rho J_q^\dagger - J_q^\dagger J_q\rho - \rho J_q^\dagger J_q\right)$$

The effective Hamiltonian

$$H_{eff} = \frac{\mathbf{p}^2}{2m} + \hbar\delta s\Lambda^\dagger\Lambda$$

The jump operator

$$J_q = \left(\hat{\epsilon}_q^* \cdot \mathbf{d}^-\right)\Lambda$$



Polarization gradient potential

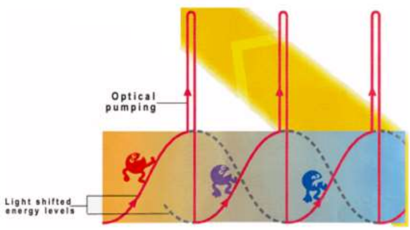
$$U = \hbar\delta s\Lambda^\dagger\Lambda$$
$$= \hbar\delta s\left\{\left(1 - \frac{2}{3}\cos^2 kz\right)|g_{\frac{1}{2}}\rangle\langle g_{\frac{1}{2}}| + \left(1 - \frac{2}{3}\sin^2 kz\right)|g_{-\frac{1}{2}}\rangle\langle g_{-\frac{1}{2}}|\right\}$$

Rate equations from master equation

$$\frac{d\rho_{g_{\frac{1}{2}},g_{\frac{1}{2}}}}{dt} = -\frac{2}{9}\Gamma s\cos^2 kz\rho_{g_{\frac{1}{2}},g_{\frac{1}{2}}} + \frac{2}{9}\Gamma s\sin^2 kz\rho_{g_{-\frac{1}{2}},g_{-\frac{1}{2}}}$$
$$\frac{d\rho_{g_{-\frac{1}{2}},g_{-\frac{1}{2}}}}{dt} = -\frac{d\rho_{g_{\frac{1}{2}},g_{\frac{1}{2}}}}{dt}$$

- For red-detuned laser $\delta < 0$
- Loss rate from $|g_{\frac{1}{2}}\rangle$ state maximum near the maximum of the polarization gradient potential
- Rate equation symmetric r.w.t. $|g_{\frac{1}{2}}\rangle$ and $|g_{-\frac{1}{2}}\rangle$

Spatially dependent decay



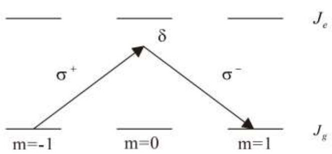
- Typical potential depth $U \sim \hbar\delta s$, as typically $s \ll 1$, atoms in the potentail should have very low temperature
- We have neglected spontaneous recoil processes in the master equation, assuming temperature much larger than the recoil energy $\frac{\hbar k^2}{2m} \sim 640nK$ ($\lambda \sim 800nm$)
- Realistic Sisyphus cooling limit for ^{23}Na: $T_s \sim 2.4\mu K$

Subrecoil Cooling

Motivation

- Temperature in previous cooling schemes limited by spontaneous recoil energy
- To go beyond this limit means to avoid spontaneous emission
- Drive atoms to a "dark state"
  - Velocity selective coherent population trapping
  - Raman sideband cooling

$J_g = 1 \to J_e = 1$



- Existence of a dark state in Λ configuration
- Treat kinetic energy as perturbation, consider internal coupling first

Counter propagating fields with orthogonal circular polarization

$$\mathbf{E}_1 = \frac{1}{2}E\left(\hat{\epsilon}_+ e^{i(kz+\omega t)} + h.c.\right)$$
$$\mathbf{E}_2 = \frac{1}{2}E\left(\hat{\epsilon}_- e^{i(kz-\omega t)} + h.c.\right)$$

Different legs of Raman process with different momentum kick.
Hamiltonian for internal states in the basis

$$\{|g_{-1}, p_z - \hbar k\rangle, |g_1, p_z + \hbar k\rangle, |e_0, p_z\rangle\}$$

$$H_{int} = \begin{pmatrix} 0 & 0 & \Omega'^*/2 \\ 0 & 0 & \Omega'^*/2 \\ \Omega'/2 & \Omega'/2 & -\delta \end{pmatrix}$$

- $\Omega' = \frac{\sqrt{2}\mathbf{d}\cdot\mathbf{E}}{2\hbar}$

Eigenvectors of H_{int}

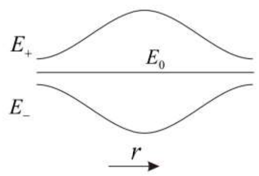
$$\begin{cases} |\Psi_\pm\rangle \propto \alpha_\pm\left(|g_{-1}, p_z - \hbar k\rangle - |g_{+1}, p_z + \hbar k\rangle\right) + \beta|e_0, p_z\rangle \\ |\Psi_0\rangle = \frac{\sqrt{2}}{2}\left(|g_{-1}, p_z - \hbar k\rangle + |g_{+1}, p_z + \hbar k\rangle\right) \end{cases}$$

The eigenvalues $E_0 = 0, E_\pm = -\delta \pm \sqrt{\delta^2 + 2|\Omega'|^2}$ give the dressed potentials that the atoms will adiabatically follow given that their velocity is small. In general however, as $|\Psi_{\pm,0}\rangle$ are not momentum eigenstates, there exist couplings between the adiabatic potentials

$$\langle\Psi_\pm|\frac{\mathbf{p}^2}{2m}|\Psi_0\rangle \propto \frac{\hbar k p_z}{m}$$

Atoms with zero momentum along $\hat{\mathbf{z}}$ ($p_z = 0$) in $|\Psi_0\rangle$ state are not coupled to other states!

Dressed potential given Gaussian field

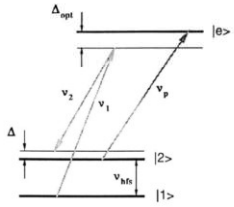


- With the spontaneous emission from the $|e_0\rangle$ states, atoms are pumped into the dark state $|\Psi_0(p_z = 0)\rangle$
- The final momentum distribution of the atoms have two narrow peaks at $\pm\hbar k$ (assuming 1-d case)
- Due to the necessity of spontaneous emission, typically $\Gamma \gg \{\delta, \Omega\}$.

Raman cooling

S. Chu group, (1992) $T \sim 100nK$

- Two counter propagating laser beams with different frequencies
- Narrow linewidth of the Raman process addresses atoms with a narrow window of velocity



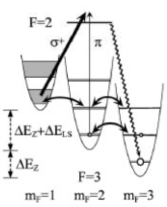
- Pulses with different negative detunings
- Optically pump atoms back
- Reverse the pulses
- Optically pump atoms back
- Engineer a velocity dependent excitation probability around $v = 0$, as in VSCPT

Side-band cooling

S. Chu group, (2000) $T \sim 290nK$

- Cooling for strongly trapped atoms
- Lamb-Dicke regime: trapping frequency much larger than the atom recoil frequency

$$\eta = \frac{1}{\lambda}\sqrt{\frac{\hbar}{2m\Omega}} \ll 1$$



- Initial state $|F = 3, m_F = 3, \nu\rangle$
- Apply magnetic field so that $|3, 3, \nu\rangle$ is degenerate with $|3, 2, \nu - 1\rangle$ and $|3, 1, \nu - 2\rangle$
- Optical pumping with strong σ^+ and a weak π pulse to drive atoms into $|3, 3, \nu - 2\rangle$
- System in the Lamb-Dicke regime, so that direct coupling matrix element between different motional sidebands are vanishingly small

1-d harmonic trap, transition probability between side-bands $\{|n_i\rangle\}$

$$P \propto |\langle n_j|e^{ik\hat{z}}|n_i\rangle|^2$$

Expanding the exponent to first order

$$e^{ik\hat{z}} \approx 1 + ik\hat{z} = 1 + ik\sqrt{\frac{\hbar}{2m\Omega}}\left(\hat{a} + \hat{a}^\dagger\right)$$

with the ladder operator $\hat{a} = \sqrt{\frac{m\Omega}{2\hbar}}\left(\hat{x} + \frac{i\hat{p}}{m\Omega}\right)$.
Therefore

$$\langle n_j|e^{ik\hat{z}}|n_i\rangle \approx \delta_{n_i,n_j} + i\eta\left(\sqrt{n_i}\delta_{n_i+1,n_j} + \sqrt{n_i+1}\delta_{n_i-1,n_j}\right)$$
$$|\langle n_j|e^{ik\hat{z}}|n_i\rangle|^2 \approx \delta^2_{n_i,n_j} + \eta^2\left(n_i\delta^2_{n_i+1,n_j} + (n_i+1)\delta^2_{n_i-1,nj}\right)$$

where the Lamb-Dicke parameter $\eta = \frac{1}{\lambda}\sqrt{\frac{\hbar}{2m\Omega}} = \sqrt{\frac{\omega_{recoil}}{\Omega}}$.

Evaporative Cooling

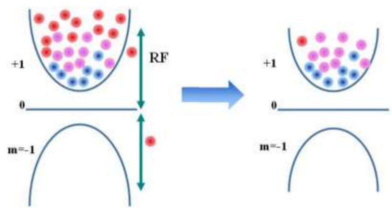
Motivation

- Doppler/Sisyphus cooling in MOT are limited by heating due to spontaneous emission
- MOT also exerts density limits due to trap losses etc.
- Subrecoil coolings have not reached the phase space densities required for a condensate

Evaporative cooling

- Remove atoms with highest energies from the trap
- Temperature lowered as atoms rethermalized via elastic collison

Evaporative cooling in a magnetic trap



- Need traps with conservative forces: magnetic trap, optical dipole trap
- Lifetime of gas much longer than collision rate
- Ineffective for identical fermions

Experimental results

Group	Atom	Eva. Cooling	N (10^6)	n (10^{12} cm^{-3})	T (μK)	ρ (10^{-6})
Rice	^{7}Li	Before	200	0.07	200	7
		After	0.1	1.4	0.4	
MIT	^{23}Na	Before	1000	0.1	200	2
		After	0.7	150	2	
JILA	^{87}Rb	Before	4	0.04	90	0.3
		After	0.02	3	0.17	

Sympathetic Cooling

- NIST (Jin), ^{40}K, ^{40}K+^{87}Rb
- LENS (Inguscio), ^{40}K+^{87}Rb
- Rice (Hulet), Paris (Salomon), ^{6}Li+^{7}Li
- MIT (Ketterle), ^{6}Li+^{23}Na
- Duke (Thomas), Innsbruck (Grimm), optical dipole trap
- Tübingen (Zimmermann), ^{6}Li+^{87}Rb
- Munich (Hänsch, Dieckmann), ^{6}Li+^{40}K+^{87}Rb
- Many more to come...

Magnetic Trap

Energy of an atomic level with quantization axis defined by the direction of the magnetic field B

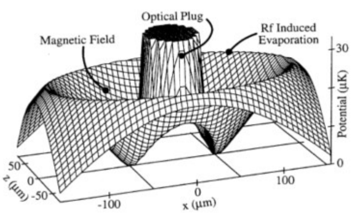
$$E = g\mu_B m_F B$$

- Quasistatic EM field cannot have local maxima in a region without charges/currents
- Atoms with $gm_F > 0$ can be trapped in the local minimum of a magnetic field (weak field seeking)
- Tight confinement
- Spin dependent

Magnetic quadruple trap

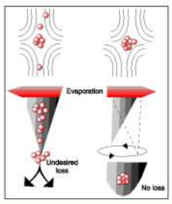
$$\mathbf{B} = B_0\left(x\hat{\mathbf{x}} + y\hat{\mathbf{y}} - 2z\hat{\mathbf{z}}\right)$$
$$|\mathbf{B}| = B_0\sqrt{x^2+y^2+4z^2}$$

Problem: non-adiabatic spin-flip at trap center (Majorana transition)
Solution I: Optical plug (MIT group)
Shine blue-detuned light at the center; repulsive barrier



Solution II: Time-orbiting trap (Boulder group)
Add a fast rotating bias field $\mathbf{B}_{bias} = B_1\left[\cos\omega t\hat{\mathbf{x}} + \sin\omega t\hat{\mathbf{y}}\right]$
Time averaged total field becomes

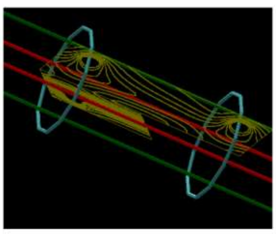
$$B_{avg} = \frac{\omega}{2\pi}\int_0^{\frac{2\pi}{\omega}} dt\sqrt{|\mathbf{B}+\mathbf{B}_{bias}|^2} \qquad \text{for } \rho B_0/B_1 \ll 1$$
$$\approx B_1 + \frac{B_0^2}{4B_1}(x^2+y^2) + 2\frac{B_0^2}{B_1}z^2$$
$$\left(\text{use } (1+x)^{\frac{1}{2}} \approx 1 + \frac{1}{2}x - \frac{1}{8}x^2 \text{ for } x \ll 1\right)$$

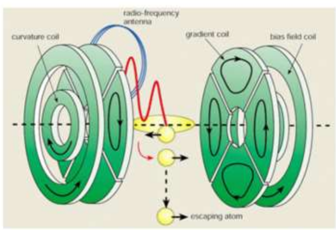


Solution III: Higher order magnetic traps with finite field at the orign
Ioffe-Pritchard trap

$$\mathbf{B} = B_0\hat{\mathbf{z}} + B_1\left[\left(z^2 - \frac{\rho^2}{2}\right)\hat{\mathbf{z}} - \rho z\hat{\rho}\right] + B_2\rho\left[\cos 2\phi\hat{\rho} - \sin 2\phi\hat{\phi}\right]$$

B_1 creates minimum at origin along $\hat{\mathbf{z}}$; B_2 creates local minimum in the traverse direction





A modern view of the magnetic trap

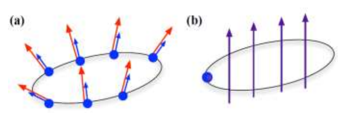
$$i\hbar\frac{\partial\psi}{\partial t} = \left[-\frac{\hbar^2}{2m}\nabla^2 + H_{\text{internal}}(\boldsymbol{r})\right]\psi$$

Local gauge transformation: $\Lambda(\boldsymbol{r}) = U^\dagger(\boldsymbol{r})H_{\text{internal}}(\boldsymbol{r})U(\boldsymbol{r})$

$$i\hbar\frac{\partial\tilde{\psi}}{\partial t} = \left[\frac{1}{2m}(i\hbar\nabla - \boldsymbol{A})^2 + \Lambda(\boldsymbol{r})\right]\tilde{\psi},$$

with $\boldsymbol{A} = -i\hbar U^\dagger\nabla U$ and and $\tilde{\psi} = U^\dagger\psi$.

- Synthetic gauge field
- Berry phase
- Majorana transition

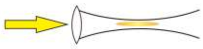


Optical Dipole Trap

Recall the dipole force

$$\mathbf{F}_{DF} = -\frac{\hbar\delta}{4}\frac{\nabla\Omega^2}{\delta^2 + \left(\frac{\Gamma}{2}\right)^2 + \frac{\Omega^2}{2}}$$

Red-detuned $\delta < 0$: strong field seeking
Blue-detuned $\delta > 0$: weak field seeking
In terms of synthetic gauge field Pros:

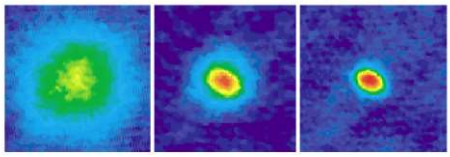


- Conservative potential, good for evaporative cooling
- Trapping multiple spin components
- Easier to implement than magnetic field traps

Cons:

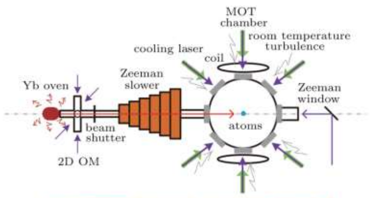
- Need large detuning to avoid spontaneous emission and heating
- Weak effective trap potential $\sim 5\mu K$
- Need very tight confinement for BEC production

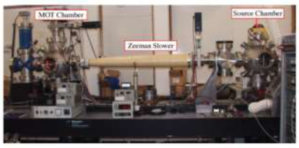
First all-optical BEC created in 2001 by Chapman's group at GIT



Summary

Overall schematics





University of Manchester

Next Lecture

Based on the understanding of interactions between laser and atoms, we have covered the basics of cooling and trapping of neutral atoms. From now on, we will focus on the properties of the cooled atoms and their applications.

Next lecture: Atom interferometry and precision measurement

- General principles of atom interferometry
- Ramsey interferometer
- Atom clock
- Other applications of atom interferometer

Quantum Degenerate Gases

Lecture 3: Precision Measurement with Cold Atoms

易为

University of Science and Technology of China

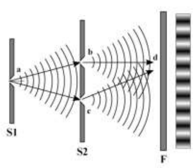
Spring 2022

中国科学技术大学

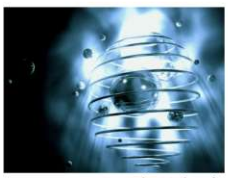
Contents

Introduction to Atom Interferometry

Double-slit interference



Matter-wave duality



- Inteferometers based on matter-wave started with electrons (1953) and neutrons (1974)
- Atom interferometers with alkali atoms since the 90s'

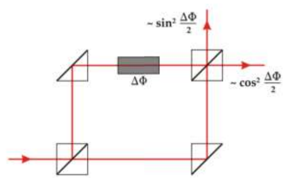
Advantages of interferometer with atoms

various species, stronger interaction with light, higher precision, better portability, lower cost etc.

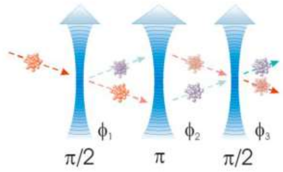
Elements of atom interferometry

- Preparation of initial state
- Coherent splitting of the wavefunction
- Free propagation, during which different phases may accumulate along different arms via interaction with the environment
- Coherent recombination of different routes to convert phase information into population difference
- Detection

Mach-Zehnder interferometer



Understanding typical atom interferometer with two-level atoms



- Two-level atoms with ground state $|g\rangle$ and excited state $|e\rangle$
- Initialize the atoms by optical pumping the population to an internal state
- π and $\pi/2$ pulses as mirrors and beamsplitters
- Atoms pick up phase shifts while propagating along different paths (via interaction with environment)
- Measure oscillation in the population of internal states as output

- Initializing the atoms: $|g\rangle$
- Application of $\frac{\pi}{2}$ pulse (beamsplitter): $\frac{\sqrt{2}}{2}\left(|g\rangle - i|e\rangle\right)$
- Free propagation for $\frac{t}{2}$, with $|e\rangle$ picking up a phase $\frac{\phi}{2}$: $\frac{\sqrt{2}}{2}\left(e^{i\omega\frac{t}{2}}|g\rangle - ie^{-i\omega\frac{t}{2}}e^{i\frac{\phi}{2}}|e\rangle\right)$
- Application of π pulse (mirror): $\frac{\sqrt{2}}{2}\left(e^{i\omega\frac{t}{2}}|e\rangle - ie^{-i\omega\frac{t}{2}}e^{i\frac{\phi}{2}}|g\rangle\right)$
- Free propagation for another $\frac{t}{2}$, with $|g\rangle$ picking up a phase $\frac{\phi}{2}$: $\frac{\sqrt{2}}{2}\left(|e\rangle - ie^{i\phi}|g\rangle\right)$
- Applicatoin of $\frac{\pi}{2}$ pulse (beamsplitter): $-\frac{i}{2}\left(1+e^{i\phi}\right)|g\rangle + \frac{1}{2}\left(1-e^{i\phi}\right)|e\rangle$
- Population in $|g\rangle$: $\frac{1}{2}\left(1+\cos\phi\right)$
  Population in $|e\rangle$: $\frac{1}{2}\left(1-\cos\phi\right)$

Note a convenient relation
$e^{-i(\mathbf{n}\cdot\sigma)\psi} = \cos\psi\mathbf{I} - i\sin\psi\left(\mathbf{n}\cdot\sigma\right)$

Precision Measurement with Atom Interferometer

Measurement of gravitational acceleration/gradient

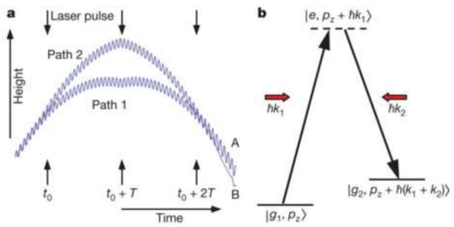
- Different paths subject to different gravitational potential
- Gratitational gradient can also be measured using two or more atom interferometers

TABLE III. List of geophysical sources of change in g (Allis *et al.*, 2000; Peters *et al.*, 2001; Sasagawa *et al.*, 2003).

Gravitation source	Magnitude
Tides at Stanford, CA	$2\times10^{-7}\,g$
1000 kg, 1.5 m away	$3\times10^{-9}\,g$
Loaded truck 30 m away	$2\times10^{-9}\,g$
Elevation variation of 1 cm	$3\times10^{-9}\,g$
Ground water fluctuation of 1 m	$5\times10^{-9}\,g$
10^8 kg of oil displacing salt at 1 km	$5\times10^{-7}\,g$

A.D. Cronin, J. Schmiedmayer, D.E. Pritchard, Rev. Mod. Phys. 81, 1051 (2009)

Measurement of gravitational pull

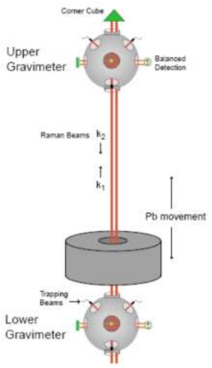


$$\Delta\Phi = -(k_1-k_2)gT^2$$

- Point-like masses in free fall
- Create different physical paths with lasers
- Deduce g from interference measurement of phase

Chu group, Berkeley (2010)

Measurement of gravitational constant



- Measure gravitational gradient caused by a single massive object
- $\delta G/G \sim 10^{-3}$

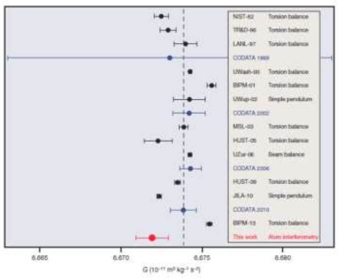
Table 1. Uncertainty limits.

Systematic	$\delta G/G$
Initial atom velocity	1.88×10^{-3}
Initial atom position	1.85×10^{-3}
Pb magnetic field gradients	1.00×10^{-3}
Rotations	0.98×10^{-3}
Source positioning	0.82×10^{-3}
Source mass density	0.36×10^{-3}
Source mass dimensions	0.34×10^{-3}
Gravimeter Separation	0.19×10^{-3}
Source mass density inhomogeneity	0.16×10^{-3}
Total	3.15×10^{-3}

Kasevich group, Stanford (2007)

Measurement of gravitational constant

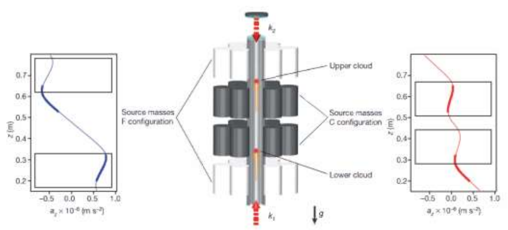
- $\delta G/G \sim 150$ p.p.m (12 p.p.m @ 2018 HUST)



Tino group, Florence (2014)

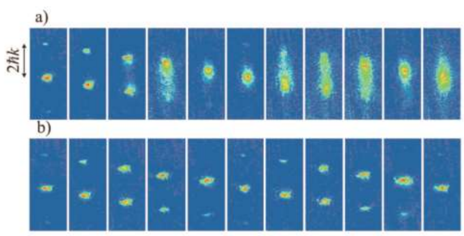
Measurement of gravitational constant

- $\delta G/G \sim 150$ p.p.m (12 p.p.m @ 2018 HUST)



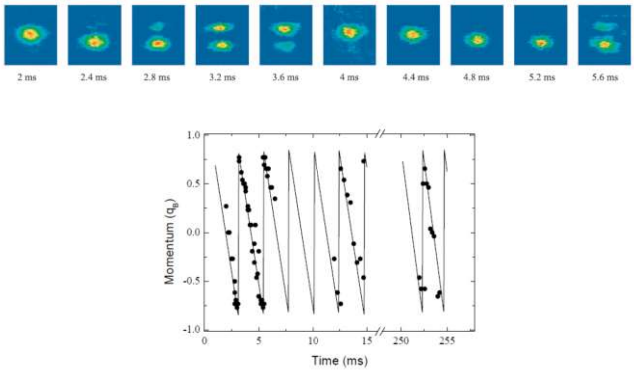
Tino group, Florence (2014)

Atom interferometer with degenerate gases (Bloch oscillation): BEC



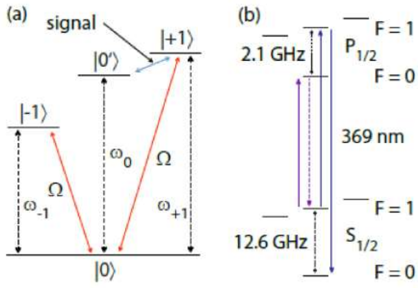
M. Fattori, et al., Phys. Rev. Lett. 100, 080405 (2008)

Atom interferometer with degenerate gases: Fermi gas



G. Roati, et al., Phys. Rev. Lett. 92, 230402 (2004)

Atomic Magnetometer (Detecting Zeeman shift via Rabi oscillations)

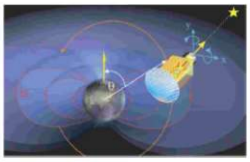


- Sensitivity: $4.6\text{pt}/\sqrt{\text{Hz}}$

Wunderlich, University Ulm

Other (possible) measurements

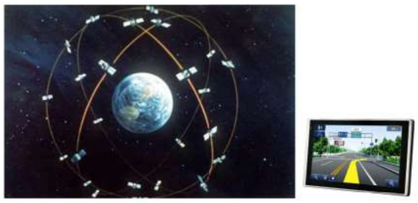
- Einstein's equivalence principle
- Test general relativity
- $1/r^2$ Newton's law
- Quantum gravity effects
- Fins structure constant
- Gravitational wave
- ...



Atomic Clock

Importance of a punctual clock

- Time is our most precisely measurable quantitiy
- Many SI units dependent on definition of 'unit time' length (m), voltage (volt), current (ampere), etc.
- Test of fundamental theory (general relativity)
- Applications in navigation with military potentials, e.g. GPS, sychronization etc.

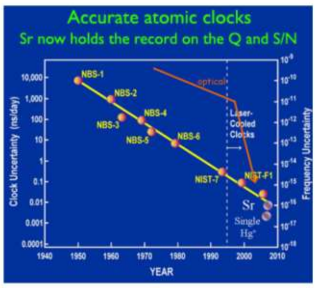


Historical milestones for atom clock

- 1949 Ramsey's separated oscillatory field technique
- 1955 First cesium atomic clock
- 1960 Hydrogen maser
- 1967 Redefinition of a second in terms of cesium
- 1975 Proposals for laser cooling of atoms and ions
- 1978 Laser cooling of trapped ions
- 1980s GPS satellite navigation introduced
- 1985 Laser cooling of atoms
- 1993 First cesium-fountain clock
- 1999 First optical-frequency measurement with femto-sec combs
- 2001 Concept of an optical clock demonstrated
- 2006 ^{87}Sr lattice clock
- 2009 Single-ion clock via quantum logic spectroscopy

How accurate are the atom clocks?

- Rubidium clock 10^{-12}
- Cesium clock 10^{-14}
- Fountain clocks 10^{-16}
- Atomic clocks in space 10^{-17}
- Lattice clocks 10^{-16}
- Single ion clocks 10^{-17}
- Current record: lattice clock with ^{87}Sr $8. \times 10^{-20}$ (Wisconsin, 2022)

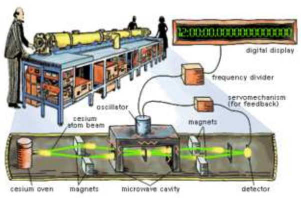


Off by one second in three hundred billion years ($\sim \times 3 \times 10^{11}$ years)

Definition (1969)

The second is the duration of 9 192 631 770 periods of the radiation corresponding to the transition between the two hyperfine levels of the ground state of the cesium 133 atom

Ramsey's separated oscillating fields method



Understanding atom clock using two-level atoms

- Two-level atoms with ground state $|g\rangle$ and excited state $|e\rangle$
- Initialize the atoms by optical pumping the population to an internal state
- Rotate the state for a time t at the beginning and the end of the free propagation
- Atoms pick up phase shifts during free propagation
- Detect oscillation in the population of the internal states

- Initializing the atoms: $|g\rangle$
- Apply rotation for a time t

$$|\psi(t)\rangle = \exp\left(-\frac{iHt}{\hbar}\right)|g\rangle$$

$$H = \hbar\begin{pmatrix} 0 & \frac{\Omega^*}{2} \\ \frac{\Omega}{2} & 0 \end{pmatrix}$$

- Free propagation for a duration τ:

$$|\psi(t+\tau) = \exp\left(-\frac{iH_0\tau}{\hbar}\right)|\psi(t)\rangle$$

$$H_0 = \hbar\begin{pmatrix} \omega & 0 \\ 0 & 0 \end{pmatrix}$$

- The other rotation

$$|\psi(t+2\tau)\rangle = \exp\left(-\frac{iHt}{\hbar}\right)|\psi(t+\tau)\rangle$$

- Calculate

$$\text{MatrixForm}\left[\text{MatrixExp}\left[-i\begin{pmatrix}0 & \frac{\text{Omega}}{2}\\ \frac{\text{Omega}}{2} & 0\end{pmatrix}t\right].\begin{pmatrix}\text{Exp}[-i*w*\text{tau}] & 0\\ 0 & 1\end{pmatrix}.\text{MatrixExp}\left[-i\begin{pmatrix}0 & \frac{\text{Omega}}{2}\\ \frac{\text{Omega}}{2} & 0\end{pmatrix}t\right].\begin{pmatrix}0\\1\end{pmatrix}\right]$$

$$-\frac{1}{4}e^{-i\,\text{Omega}\,t}\left(-1+e^{i\,\text{Omega}\,t}\right)\left(1+e^{i\,\text{Omega}\,t}\right)-\frac{1}{4}e^{-i\,\text{Omega}\,t-i\,\text{tau}\,w}\left(-1+e^{i\,\text{Omega}\,t}\right)\left(1+e^{i\,\text{Omega}\,t}\right),$$
$$\frac{1}{4}e^{-i\,\text{Omega}\,t-i\,\text{tau}\,w}\left(-1+e^{i\,\text{Omega}\,t}\right)^2+\frac{1}{4}e^{-i\,\text{Omega}\,t}\left(1+e^{i\,\text{Omega}\,t}\right)^2$$

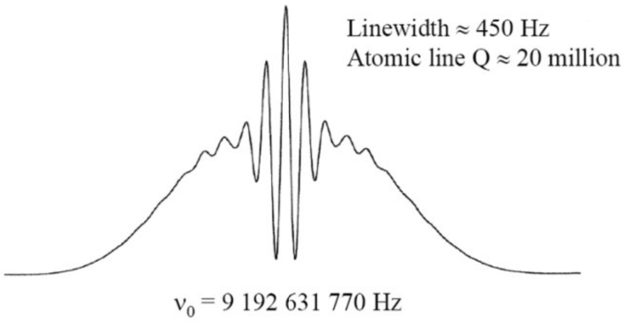
- Final population in $|e\rangle$:

$$P_e = \left|-\frac{i}{2}\sin(\Omega t)\left(1+e^{-i\tau\omega}\right)\right|^2 = \frac{\sin^2(\Omega t)}{2}\left[1+\cos(\omega\tau)\right]$$

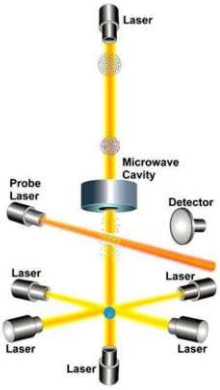
- Final population in $|g\rangle$:

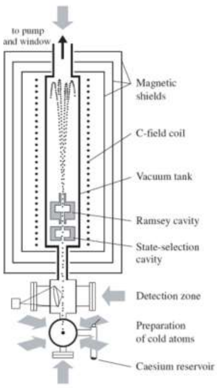
$$P_g = 1 - P_e = 1 - \frac{\sin^2(\Omega t)}{2}\left[1+\cos(\omega\tau)\right]$$

Typical data



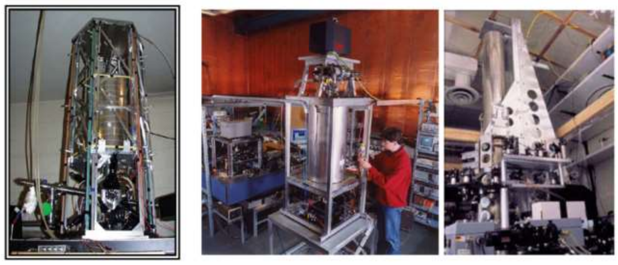
Fountain clock
Proposed by J. Zacharias in 1953, realized by M. Kasevich and S. Chu in 1989





Fountain clock

8 fountains in operation at SYRTE, PTB, NIST, USNO, Penn St, IEN, NPL, ON, with accuracy near 1 10^{-15}. More than 10 under construction.



BNM-SYRTE, FR PTB, D NIST, USA

Uncertainty

$$\sigma = \frac{1}{\pi Q}\sqrt{\frac{T_c}{\tau}}\left(\frac{1}{N}+\frac{1}{N\epsilon_c n_{ph}}+\frac{2\sigma_{\delta N}^2}{N^2}+\gamma\right)^{\frac{1}{2}}$$

Among other things

- τ is the interrogation time
- N is the total number of atoms
- $Q = \nu_0/\delta\nu$ is the atomic quality factor
  ν_0 is the cesium hyperfine splitting
  $\delta\nu$ is width of the Ramsey fringe
- $\sigma_{\delta N}$ is the uncorrelated r.m.s. fluctuation of the atom

Hence to reduce the error further, we need

- Longer interrogation time (as in single ion, space clock etc.)
- Larger atom number (atomic ensemble, BEC?)
- Larger ν_0 (optical frequencies?)
- Lower temperature, fewer collisions (isolated atoms, as in an optical lattice)

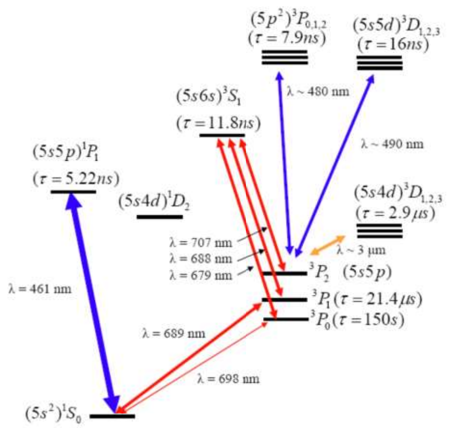
Optical lattice clock (see e.g. Thesis of Martin M. Boyd)

- $\sigma \propto \left(\frac{\nu_0}{\delta\nu}\right)^{-1}$
  microwave field: $\nu_0 \sim 10^9$, $\delta\nu \sim 1$, $Q \sim 10^9$
  opitcal field: $\nu_0 \sim 10^{14}$, $\delta\nu \sim 10^{-3}$, $Q \sim 10^{17}$
- Confine atoms in a deep optical lattice: $d \ll \lambda/2$
  longer interrogation time, fewer/no collisions
  free from Doppler effect in the Lamb-Dicke limit
  $\eta = k\sqrt{\hbar/2m\omega_k} \ll 1$
- Still benefit from the large N factor of atom ensemble

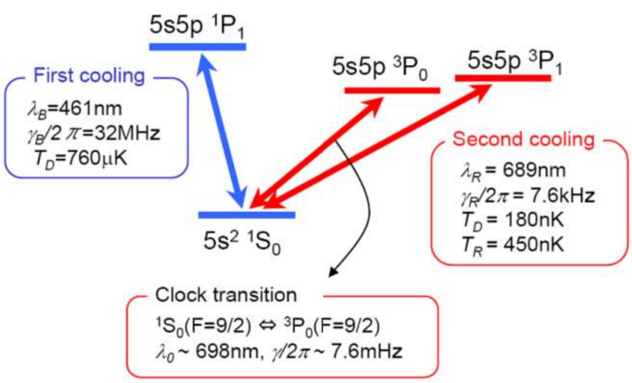
Difficulties

- Deep lattice means large energy shift (a.c. Stark shift) from optical dipole force
- Excited state has finite life-time
- Optical frequencies very difficult to register with typical electronics

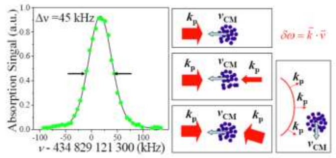
Meet ^{87}Sr (alkaline-earth like atoms in general)

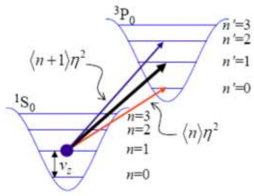


Clock transition



Suppression of Doppler effect in a deep lattice





Free space:
$\nu = \nu_c + \mathbf{k}\cdot\mathbf{v}/(2\pi) + \nu_R$
ν_R: the uncertainties (photon recoil)
In a deep harmonic potential:
$\nu = \nu_c + \Delta n\Omega/(2\pi)$
$\Omega/(2\pi)$: the trapping frequency
$\Delta n = 0, \pm 1, \cdots$: difference in the motional sideband

Condition for well-resolved sidebands

- Lamb-Dicke parameter
  $\eta = \frac{1}{\lambda}\sqrt{\frac{\hbar}{2m\Omega}} \ll 1$
- $\Gamma_{excited} \ll \hbar\Omega$

The a.c. Stark shift of state $|i\rangle$ in the presence of an electric field $\mathbf{E}$

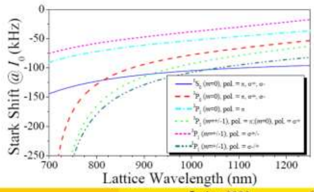
$$\delta E = -\frac{1}{2}\alpha_i|\mathbf{E}|^2$$

The a.c. polarizability α_i can be written as

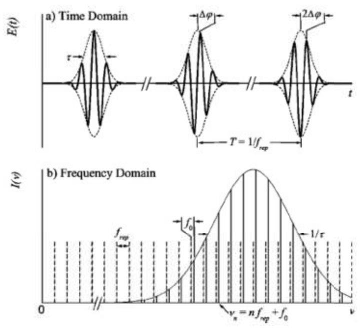
$$\alpha_i(\omega_L) = 6\pi\epsilon_0 c^3 \sum_k \frac{\Gamma_{ik}}{\omega_{ik}^2(\omega_{ik}^2 - \omega_L^2)}$$

$$\Gamma_{ik} = \frac{e^2}{4\pi\epsilon_0}\frac{4\omega_{ik}^3}{3\hbar c^3}|\langle k|\mathbf{d}\cdot\hat{\epsilon}|i\rangle|^2$$

At a magic wavelength $\lambda \sim 813nm$, the a.c. Stark shifts of $^1S_0$ and $^3P_0$ are exactly the same for ^{87}Sr



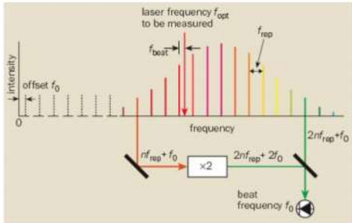
Frequency comb: gearing between optical and microwave frequencies



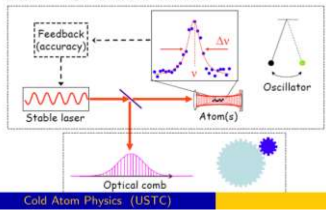
- Femto second pulse $E(t)e^{i\omega t}$ spanning the complete frequency spectrum
- Pulse recurring frequency: comb spacing
- Carrier-envelope phase: comb shift
- Optical frequency can be expressed in terms of two microwave frequencies and an integer

$$\nu_n = nf_{rep} + f_0$$

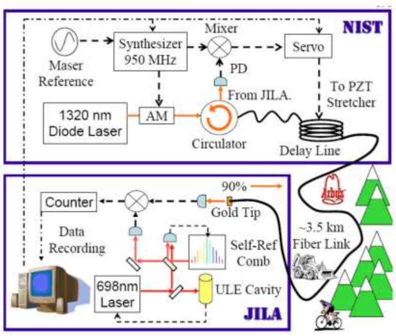
Extracting f_0 via frequency doubling



How ^{87}Sr clock works

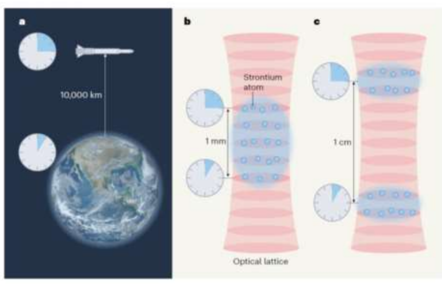


- Laser frequency fixed and stabilized by feedback from the clock transition of the atom
- The optical frequency is readout via fs frequency comb



- Comb phase locked to clock laser (beat)
- Repetition rate compared to JILA signal
- The above allows the comparison of the clock transition frequency with the high accuracy microwave standards

Atomic clock and gravity



- Resolving time dilation over 1mm on Earth

NIST group (2022)

Key requirements for atom clock

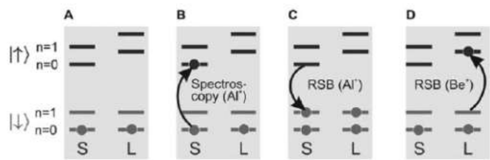
- Selection of an atom with a narrow-width transition that is immune to perturbations
- Minimizing Doppler shift (confinement, cooling)
- Reliable initial state preparation
- Efficient state detection

Conventionally, choose an atom species that satisfy all requirements
Alternatively, choose two atoms species that share these requirements

Quantum logic spectroscopy

Fractional accuracy 9.4×10^{-19} with Al$^+$-Be$^+$ single ion clock (2019)
Al$^+$, spectroscopy ion with narrow line-width
Be$^+$, logic ion providing sympathetic cooling, state initialization and detection

Coherent population mapping via motional side-band



- Initializaiton to the ground state
- Interrogation of the spectroscopy transition (B)

$$(\alpha|\downarrow\rangle_S|0\rangle_m + \beta|\uparrow\rangle_S|0\rangle_m)|\downarrow\rangle_L$$

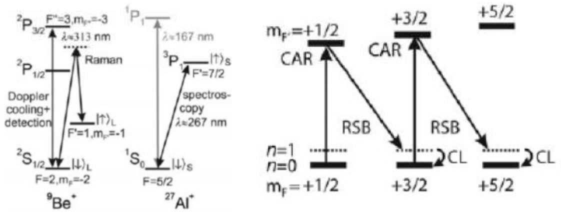
- Coherent transfer of the state of spectroscopy ion to the transfer mode via a red-side-band π pulse (C)

$$|\downarrow\rangle_S|\downarrow\rangle_L(\alpha|0\rangle_m + \beta|1\rangle_m)$$

- Coherent transfer of the transfer mode state into the state of the logic ion via a red-side-band π pulse (D)

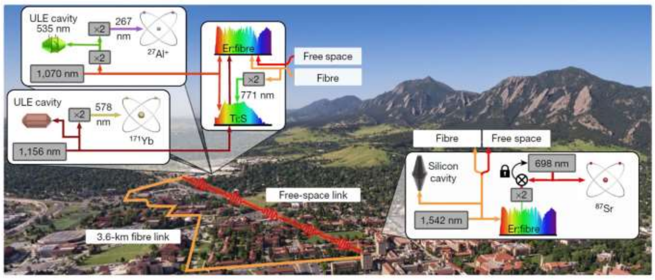
$$|\downarrow\rangle_S(\alpha|\downarrow\rangle_L + \beta|\uparrow\rangle_L)|0\rangle_m$$

Implementation with trapped Al^+ and Be^+ ions



- Initial state prepation/cooling for Al^+ ion through Be^+ ion
- Clock manipulation
- Mapping the final internal state of Al^+ ion to that of Be^+ ion
- Detection of the Be^+ ion population

Cross-Checking Atom Clocks



- $^{27}Al^+$–^{87}Sr–^{171}Yb with an accuracy $\sim 8\times 10^{-18}$

Nature 591, 564 (2021)

Next Lecture

We have covered some applications of cold atoms, including atom interferometer and atom clocks. These do not have very stringent temperature requirement of the atoms. Typical laser cooling is sufficient. Of course, we may cool the gas further given the various cooling techniques that we have discussed before. When the temperature is low enough, the atoms enter the interesting regime of quantum degeneracy. And the various intriguing properties of the quantum degenerate gases will be the main focus for the rest of this course. Next, we will start with the introduction of Bose-Einstein condensate.

Quantum Degenerate Gases

Lecture 4: Ideal Bose-Einstein Condensate

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Spring 2022

中国科学技术大学

Contents

Bose Distribution

Consider a system with eigenenergy levels $\{\epsilon_\alpha\}$, each with occupation number $\{n_\alpha\}$. The grand canonical partition function is:

$$Z=\sum_{\{n_\alpha\}}\exp\left[-\beta\sum_\alpha n_\alpha(\epsilon_\alpha-\mu)\right],$$

where $\beta=1/k_BT$, μ is the chemical potential. For bosons,

$$\begin{aligned} Z&=\sum_{n_1=0}^{\infty}\sum_{n_2=0}^{\infty}\cdots\prod_\alpha\exp\left[-\beta n_\alpha(\epsilon_\alpha-\mu)\right]\\ &=\prod_\alpha\left\{\sum_{n=0}^{\infty}\exp\left[-\beta n(\epsilon_\alpha-\mu)\right]\right\}\\ &=\prod_\alpha\frac{1}{1-\exp\left[-\beta(\epsilon_\alpha-\mu)\right]}\end{aligned}$$

Grand thermodynamic potential

$$\begin{aligned}\Omega&=-\frac{1}{\beta}\ln Z\\ &=\frac{1}{\beta}\sum_\alpha\ln\left[1-e^{-\beta(\epsilon_\alpha-\mu)}\right]\end{aligned}$$

The occupation of the αth eigenenergy level is

$$n_\alpha=\frac{\partial\Omega}{\partial\epsilon_\alpha}=\frac{1}{e^{\beta(\epsilon_\alpha-\mu)}-1}$$

The chemical potential μ is dictated by number conservation

$$N=\sum_\alpha\frac{1}{e^{\beta(\epsilon_\alpha-\mu)}-1}$$

Appearance of condensate

- For non-negative occupation number $n_\alpha\geq 0$, we must have $\mu\leq\{\epsilon_\alpha\}_{\min}=\epsilon_{\min}$
- The maximum number of particles in the excited state

$$N_{\rm ex}=\sum_{\alpha\in\text{excited}}\frac{1}{e^{\beta(\epsilon_\alpha-\epsilon_{\min})}-1}$$

- If $N_{\rm tot}>N_{\rm ex}$, the extra atoms must occupy the ground state, which has no upper-bound on occupation number
- BEC!

Neglecting the zero-point energy (shifting the zero-energy reference), we have

$$N=N_0+\sum_\alpha\frac{1}{e^{\beta\epsilon_\alpha}-1}$$

Density of state

In principle, one should carry out the discrete summations. Practically, we replace sums with integrals. Accurate for excited states here.

$$\sum_{\alpha} \rightarrow \int d\epsilon g(\epsilon)$$

where $g(\epsilon)d\epsilon$ is the number of states between ϵ and $\epsilon + d\epsilon$.
The density of state $g(\epsilon)$ is defined as

$$g(\epsilon) = \frac{dG(\epsilon)}{d\epsilon}$$

where $G(\epsilon)$ is the total number of states up to ϵ.
Note that this is just variable transformation. One may also work with the density of states in momentum space, etc.

Calculating density of states
3-D homogenous cas
Number of states in the shell between k and $k + dk$

$$\frac{L^3}{(2\pi)^3}4\pi k^2 dk$$

Plug in $\epsilon = \frac{\hbar^2 k^2}{2m}$ and $d\epsilon = \frac{\hbar^2 k dk}{m}$,

$$\frac{L^3 m^{3/2}}{\sqrt{2}\pi^2\hbar^3}\epsilon^{1/2}d\epsilon$$

Therefore

$$g(\epsilon) = \frac{L^3 m^{3/2}}{\sqrt{2}\pi^2\hbar^3}\epsilon^{1/2}$$

For d-dimensional homogeneous case,

$$\frac{L^d}{(2\pi)^d}dC_d k^{d-1}dk,$$

where $C_d = \frac{\pi^{d/2}}{\Gamma(d/2+1)}$. Plug in $\epsilon = \frac{\hbar^2 k^2}{2m}$ and $d\epsilon = \frac{\hbar^2 k dk}{m}$,

$$\frac{dC_d L^d}{2^{d/2+1}\pi^d}\left(\frac{m}{\hbar^2}\right)^{d/2}\epsilon^{d/2-1}d\epsilon$$

Therefore

$$g_d(\epsilon) \propto \epsilon^{d/2-1}$$

Special cases:
2-d case: $g_2(\epsilon) = \frac{L^2 m}{2\pi\hbar^2}$
1-d case: $g_1(\epsilon) = \frac{L m^{1/2}}{\sqrt{2}\pi\hbar}\epsilon^{-1/2}$

Density of states in a 3-d harmonic potential
Energy spectrum (zero point energy neglected)

$$E_{n_1,n_2,n_3} = \hbar(n_1\omega_1 + n_2\omega_2 + n_3\omega_3)$$

Total number of states upto E_{n_1,n_2,n_3}

$$G(E) = \frac{1}{\hbar^3\omega_1\omega_2\omega_3}\int_0^E dE_1\int_0^{E-E_1} dE_2\int_0^{E-E_1-E_2} dE_3 = \frac{E^3}{6\hbar^3\omega_1\omega_2\omega_3}$$

Therefore

$$g(E) = \frac{dG(E)}{dE} = \frac{E^2}{2\hbar^3\omega_1\omega_2\omega_3}$$

In a d-dimensional harmonic trap: $g(E) = \frac{E^{d-1}}{(d-1)!\prod_{i=1}^{d}\hbar\omega_i}$

Critical Temperature

Total particle number

$$N = N_0 + \sum_{\nu}\frac{1}{e^{\beta\epsilon_\nu} - 1}$$

At the temperature T_c where the gas starts to condense

$$N = \sum_{\nu}\frac{1}{e^{\beta_c\epsilon_\nu} - 1} = \int_0^\infty \frac{g(\epsilon)}{e^{\beta_c\epsilon} - 1}d\epsilon,$$

where $\beta_c = 1/k_B T_c$, and the density of state in general:

$$g(\epsilon) = C_\alpha\epsilon^{\alpha-1}$$

d-dimensional homogeneous case: $\alpha = d/2$
d-dimensional harmonic potential: $\alpha = d$

Hence

$$N = \int_0^\infty d\epsilon\frac{C_\alpha\epsilon^{\alpha-1}}{e^{\beta_c\epsilon} - 1} = C_\alpha (k_B T_c)^\alpha\int_0^\infty dx\frac{x^{\alpha-1}}{e^x - 1}, \quad \text{where } x = \beta_c\epsilon$$
$$= C_\alpha (k_B T_c)^\alpha\Gamma(\alpha)\zeta(\alpha)$$

where $\Gamma(\alpha) = \int_0^\infty x^{\alpha-1}e^{-x}$, $\zeta(\alpha) = \sum_{n=1}^{\infty} n^{-\alpha}$. And we have used

$$\frac{1}{e^x - 1} = e^{-x} + e^{-2x} + e^{-3x} + \cdots$$

Therefore

$$k_B T_c = \frac{N^{1/\alpha}}{[C_\alpha\Gamma(\alpha)\zeta(\alpha)]^{1/\alpha}}$$

In a 3-d harmonic potential

$$k_B T_c \approx 0.94\hbar(\omega_1\omega_2\omega_3)^{1/3}N^{1/3}$$

For a 3-d homogeneous gas

$$k_B T_c \approx 3.31\frac{\hbar^2 n^{2/3}}{m},$$

where the number density $n = N/V$.
As $\zeta(\alpha)$ only converges for $\alpha > 1$, in low dimensions, gases may not condense:

- homogenous case: no condensate for $d \leq 2$
- harmonic potential: no condensate for $d \leq 1$

From another perspective, $n\lambda_{dB}^3 \approx 2.612$, with thermal de Broglie wavelength $\lambda_{dB} = \sqrt{\frac{2\pi\hbar^2}{mk_B T}}$: low temperature, high density.

Condensate Fraction and Density Profile

Below T_c, we may take $\mu = 0$, and the particle number in the excited state is

$$N_{\text{ex}} = C_\alpha\int_0^\infty d\epsilon\frac{\epsilon^{\alpha-1}}{e^{\beta\epsilon} - 1} = C_\alpha (k_B T)^\alpha\Gamma(\alpha)\zeta(\alpha) = N\left(\frac{T}{T_c}\right)^\alpha$$

Therefore the condensate fraction is

$$N_0 = N\left[1 - \left(\frac{T}{T_c}\right)^\alpha\right]$$

How do we differentiate the condensed part from the thermal part?

Density profiles

- Condensate in 3-d harmonic trap

$$\phi_0(\mathbf{r}) = \frac{1}{\pi^{3/4}(a_1a_2a_3)^{1/2}} e^{-\frac{x^2}{2a_1^2}} e^{-\frac{y^2}{2a_2^2}} e^{-\frac{z^2}{2a_3^2}}$$

$$n_0(\mathbf{r}) = N|\phi_0(\mathbf{r})|^2 = \frac{N}{\pi^{2/3}a_1a_2a_3} e^{-\frac{x^2}{a_1^2}} e^{-\frac{y^2}{a_2^2}} e^{-\frac{z^2}{a_3^2}}$$

With $a_i^2 = \frac{\hbar}{m\omega_i}$

- Thermal gas in 3-d harmonic trap ($n \propto \int d^3\mathbf{p} e^{-\beta H(\mathbf{r},\mathbf{p})}$)

$$n_{\text{th}}(\mathbf{r}) = \frac{N}{\pi^{2/3}R_1R_2R_3} e^{-\frac{x^2}{R_1^2}} e^{-\frac{y^2}{R_2^2}} e^{-\frac{z^2}{R_3^2}}$$

With $R_i^2 = \frac{2k_BT}{m\omega_i^2}$ (temperature dependent)

$$\frac{R_i}{a_i} = \sqrt{\frac{2k_BT}{\hbar\omega_i}} \sim N^{1/6} \gg 1 \qquad \text{for } T \sim T_c$$

Velocity distribution

- Condensate in 3-d harmonic trap

$$\phi_0(\mathbf{p}) = \mathcal{F}\{\phi_0(\mathbf{r})\} = \frac{1}{\pi^{3/4}(c_1c_2c_3)^{1/2}} e^{-\frac{p_x^2}{2c_1^2}} e^{-\frac{p_y^2}{2c_2^2}} e^{-\frac{p_z^2}{2c_3^2}}$$

$$n_0(\mathbf{p}) = N|\phi_0(\mathbf{p})|^2 = \frac{N}{\pi^{3/2}c_1c_2c_3} e^{-\frac{p_x^2}{c_1^2}} e^{-\frac{p_y^2}{c_2^2}} e^{-\frac{p_z^2}{c_3^2}}$$

With $c_i = \sqrt{m\hbar\omega_i}$.
Anisotropic given anisotropic trap

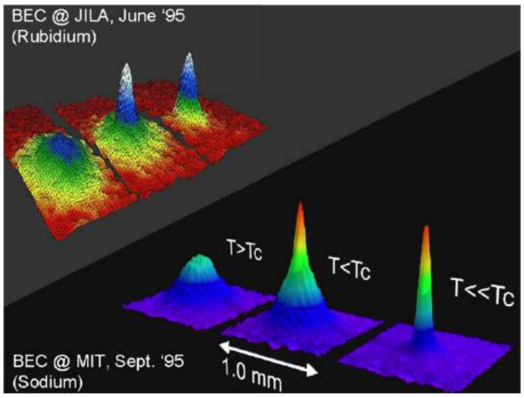
- Thermal gas in 3-d harmonic trap ($n \propto \int d^3\mathbf{r} e^{-\beta H(\mathbf{r},\mathbf{p})}$)

$$n_{\text{th}}(\mathbf{p}) = Ce^{-\frac{p^2}{2mk_BT}}$$

Isotropic

$$\sqrt{\frac{2mk_BT}{m\hbar\omega_i}} \sim N^{1/6} \gg 1 \qquad \text{for } T \sim T_c$$

Bimodal distribution



Time of flight imaging

- Release gas from the trap, let it expand freely for a long time
- Final distribution reflects the initial velocity distribution

$$n_{\text{final}}(\mathbf{r}) \propto n_0(\mathbf{v})$$

Initial condensate wavefunction

$$\phi_0(\mathbf{r}) = \frac{1}{\pi^{3/4}(a_1a_2a_3)^{1/2}} e^{-\frac{x^2}{2a_1^2}} e^{-\frac{y^2}{2a_2^2}} e^{-\frac{z^2}{2a_3^2}}$$

With its Fourier transform

$$\phi_0(\mathbf{p}) = \mathcal{F}\{\phi_0(\mathbf{r})\} = \frac{1}{\pi^{3/4}(c_1c_2c_3)^{1/2}} e^{-\frac{p_x^2}{2c_1^2}} e^{-\frac{p_y^2}{2c_2^2}} e^{-\frac{p_z^2}{2c_3^2}}$$

Evolve the wavefunction in momentum space

$$\phi_0(\mathbf{p}, t) = e^{-i\mathbf{p}^2t/2m}\mathcal{F}\{\phi_0(\mathbf{r})\}$$

Transform back to coordinate space and calculate the density distribution

$$n(\mathbf{r}, t) = |\phi_0(\mathbf{r}, t)|^2 \propto e^{-\frac{x^2}{a_1(t)^2}} e^{-\frac{y^2}{a_2(t)^2}} e^{-\frac{z^2}{a_3(t)^2}}$$

with widths $a_i(t) = \sqrt{a_i^2 + \frac{\hbar^2t^2}{m^2a_i^2}}$.
After long time of flight

$$a_i(t) \approx \frac{\hbar t}{ma_i}$$

Anisotropy and uncertainty principle

$$\frac{a_i(t)}{a_j(t)} = \frac{a_j}{a_i}$$

Long-Range Order and Order Parameter

Define single-body density matrix

$$\rho(\mathbf{r}, \mathbf{r}') = \left\langle \Psi^\dagger(\mathbf{r})\Psi(\mathbf{r}') \right\rangle,$$

where $\Psi^\dagger(\mathbf{r})$ ($\Psi(\mathbf{r})$) is the creation (annihilation) field operator satisfying the bosonic commutation relation

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

As $\Psi(\mathbf{r}) = \sum_\mathbf{k} \hat{a}_\mathbf{k} e^{-i\mathbf{k}\cdot\mathbf{r}}$, for ideal, homogeneous Bose gas

$$\begin{aligned}\rho(\mathbf{r}, \mathbf{r}') &= \sum_{\mathbf{k},\mathbf{k}'} \left\langle \hat{a}_\mathbf{k}^\dagger \hat{a}_{\mathbf{k}'} \right\rangle e^{i\mathbf{k}\cdot\mathbf{r} - i\mathbf{k}'\cdot\mathbf{r}'} \\ &= \sum_\mathbf{k} n_\mathbf{k} e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}\end{aligned}$$

For this ideal, homogeneous condensate, the condensation criterion is the macroscopic occupation of the zero momentum mode (ground state)

$$n_\mathbf{k} = \frac{N_0}{V}\delta_{\mathbf{k},0} + n'_{\mathbf{k}\neq 0}$$

Thus,

$$\rho(\mathbf{r}, \mathbf{r}') = \frac{N_0}{V} + \sum_{\mathbf{k}\neq 0} \frac{N_\mathbf{k}}{V} e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}$$

In the thermodynamic limit, $N_0/V \to$ constant, $N_{\mathbf{k}\neq 0}/V \to 0$, hence $\rho(\mathbf{r}, \mathbf{r}') = \frac{N_0}{V}$ in such a limit.
Alternatively, due to interference between different components,

$$\lim_{|\mathbf{r}-\mathbf{r}'|\to\infty} \rho(\mathbf{r}, \mathbf{r}') \to \frac{N_0}{V}$$

This is called Off Diagonal Long Range Order (ODLRO), in contrast to Diagonal Long Range Order (DLRO) as in solids.

For a general BEC, we write the field operator

$$\Psi(\mathbf{r}) = \sum_i \phi_i(\mathbf{r})\hat{a}_i$$

And the single body density matrix becomes

$$\begin{aligned}\rho(\mathbf{r}, \mathbf{r}') &= \sum_{i,j} \phi_j^*(\mathbf{r})\phi_i(\mathbf{r}') \left\langle \hat{a}_j^\dagger \hat{a}_i \right\rangle \\ &= \sum_i n_i\phi_i^*(\mathbf{r})\phi_i(\mathbf{r}')\end{aligned}$$

And we may write

$$\int d^3\mathbf{r}'\rho(\mathbf{r}, \mathbf{r}')\phi_i^*(\mathbf{r}') = n_i\phi_i^*(\mathbf{r})$$

n_i can be identified as the eigenvalues of the single body matrix element. Therefore the condensate exists if at least one of the eigenvalues of the single body density matrix is comparable to the total particle number N.

Recall the expansion

$$\Psi(\mathbf{r}) = \sum_i \phi_i(\mathbf{r})\hat{a}_i,$$

where $\hat{a}_i^\dagger$ ($\hat{a}_i$) is the creation (annihilation) operator of the i-th mode and satisfies the bosonic commutation relations

$$[\hat{a}_i, \hat{a}_j^\dagger] = \delta_{ij} \qquad [\hat{a}_i, \hat{a}_j] = [\hat{a}_i^\dagger, \hat{a}_j^\dagger] = 0$$

As we have discussed, for a general BEC (finite system or with interaction)

$$\Psi(\mathbf{r}) = \phi_0(\mathbf{r})\hat{a}_0 + \sum_{i\neq 0} \phi_i(\mathbf{r})\hat{a}_i$$

We may then identify the condensate order parameter as

$$\varphi(\mathbf{r}) = \phi_0(\mathbf{r})\langle \hat{a}_0 \rangle,$$

where $\varphi(\mathbf{r})$ can also be identified as the condensate wavefunction.

In the Hartree limit the N-body wavefunction

$$f_N(\{\mathbf{r}_i\}) \approx \prod_i \phi_0(\mathbf{r_i})$$

Fock state description of BEC

$$|N\rangle = \frac{1}{\sqrt{N!}}\int d\{\mathbf{r}_i\} f_N(\{\mathbf{r}_i\}) \prod_{i=1}^{N} \Psi^\dagger(\mathbf{r}_i)|\text{vac}\rangle$$
$$= \frac{1}{\sqrt{N!}}\left(\hat{a}_0^\dagger\right)^N |\text{vac}\rangle,$$

where we have used the expansion for the field operator

$$\Psi(\mathbf{r}) = \sum_i \phi_i(\mathbf{r})\hat{a}_i = \phi_0(\mathbf{r})\hat{a}_0 + \sum_{i\neq 0}\phi_i(\mathbf{r})\hat{a}_i$$

Note the total particle number is fixed in this description.

The Fock state description is not appropriate for the previous definition of the order parameter as $\langle N|\hat{a}_0|N\rangle = 0$. We are actually using the coherent state description of the BEC in the previous definition

$$|\alpha\rangle = e^{-\frac{1}{2}|\alpha|^2}\sum_{N=0}^{\infty}\frac{\alpha^N}{\sqrt{N!}}|N\rangle$$

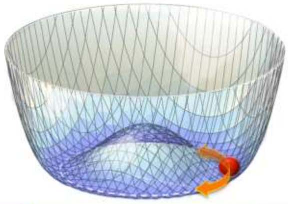
Easy to show that $\langle\alpha|\hat{a}_0|\alpha\rangle = \alpha$ and $\langle\alpha|\hat{N}|\alpha\rangle = |\alpha|^2$. Therefore the order parameter

$$\varphi(\mathbf{r}) = \alpha\phi_0(\mathbf{r}) = \sqrt{N_0}e^{i\theta}\phi_0(\mathbf{r})$$

where θ is the global phase of the condensate.

Global phase θ

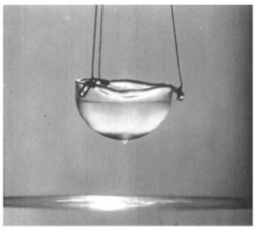
- Experimentally, trapped gases have fixed particle number, therefore not in a coherent state. The global phase of a condensate cannot be observed/measured.
- Theoretically, the global phase can take on arbitrary value for the coherent state. This is the so-called U(1) gauge symmetry.
- Spontaneous symmetry breaking
- The lowest-energy excitations above the BEC are therefore gapless (Goldstone modes)



Superfluidity and Condensate

Superfluidity is a state of matter in which viscosity of a fluid vanishes.

- ^{4}He below the lambda point
- Frictionless flow, quantized vortices
- Density of superfluid component approaches unity
- Different from condensate fraction, as we will show later



Galilean transformation

- Reference frame K: $\{E, \mathbf{P}, M\}$

$$E = \frac{\mathbf{P}^2}{2M}$$

- Reference frame K' moving relative to K with velocity $\mathbf{v}$

$$E' = \frac{(\mathbf{P} - M\mathbf{v})^2}{2M} = E - \mathbf{P}\cdot\mathbf{v} + \frac{1}{2}Mv^2$$

- The last equation generally holds

Consider an obstacle (impurity) moving with velocity $\mathbf{v}$ in a fluid of total mass m. Friction is caused by excitation of collective modes in the fluid, which can be characterized by its momentum $\mathbf{p}$ and dispersion relation ϵ_p. Consider the energy of the fluid:

Rest frame of fluid (time-dependent potential)
Initially: $E = E_0$. Finally: $E = E_0 + \epsilon_p$.

Rest frame of obstacle (static potential)
Initially: $E = E_0 + \frac{1}{2}mv^2$. Finally: $E = E_0 + \epsilon_p - \mathbf{p}\cdot\mathbf{v} + \frac{1}{2}mv^2$.

As $\epsilon_p > 0$, $\mathbf{p}\cdot\mathbf{v} > 0$, for a reduction of condensate energy (viscosity)

$$v\cos\theta > \frac{\epsilon_p}{p}, \qquad \text{where} \quad p = |\mathbf{p}|.$$

Landau criterion: if $v < v_c$, no excitations possible

$$v_c = \left(\frac{\epsilon_p}{p}\right)_{\min}$$

In the Landau criteria, there can be no excitations in the fluid for velocities below v_c, i.e. superfluid.
Example I: Phonon excitation (sound wave) $\epsilon_p = vp$

$$v_c = v$$

Example II: Ideal Bose gas $\epsilon_p = p^2/2m$

$$v_c = 0 \quad \text{at} \quad p = 0$$

Example III: Roton excitation $\epsilon_p = \Delta + (p - p_0)^2/2m$

$$v_c = \frac{\Delta}{p_c} + \frac{(p_c - p_0)^2}{2mp_c},$$

where $p_c = \sqrt{2m\Delta + p_0^2}$.

Two-fluid model (finite-T case)

- Superfluid component and normal component (thermal excitations) interpenetrating (for $v < v_c$)
- Fixed total energy. Particle exchange between two components

Consider normal components moving with velocity $\mathbf{v}$ relative to the condensate. They consist of excitations of momentum $\hbar\mathbf{k}$ in the rest frame of the condensate, with dispersion given by ϵ_k. The energy required to create the excitation is (in the normal component frame)

$$\Delta E_k = \epsilon_k - \hbar\mathbf{k}\cdot\mathbf{v}$$

The total momentum of the fluid in the frame of the condensate is

$$\langle\mathbf{p}\rangle = \sum_{\mathbf{k}} \hbar\mathbf{k}\frac{1}{e^{\beta(\Delta E_k-\mu)}-1}$$

Note:
(a) in the condensate frame only excitations contribute
(b) excitations equilibrate in the frame of normal component

For small velocities,

$$\begin{aligned}\langle\mathbf{p}\rangle &= \sum_{\mathbf{k}} \hbar\mathbf{k}\frac{1}{e^{\beta(\epsilon_k-\hbar\mathbf{k}\cdot\mathbf{v}-\mu)}-1} \\ &\approx \sum_{\mathbf{k}} \left\{\frac{\hbar\mathbf{k}}{e^{\beta(\epsilon_k-\mu)}-1} + \hbar\mathbf{k}(\beta\hbar\mathbf{k}\cdot\mathbf{v})\frac{e^{\beta(\epsilon_k-\mu)}}{(e^{\beta(\epsilon_k-\mu)}-1)^2}\right\} \\ &= \sum_{\mathbf{k}} \beta\hbar^2\frac{e^{\beta(\epsilon_k-\mu)}}{(e^{\beta(\epsilon_k-\mu)}-1)^2}\mathbf{k}(\mathbf{k}\cdot\mathbf{v})\end{aligned}$$

- $\langle\mathbf{p}\rangle = n_n V m\mathbf{v}$ (n_n is the normal component density)
- $\mathbf{k}(\mathbf{k}\cdot\mathbf{v}) = k_x^2 v_x\mathbf{e_x} + k_y^2 v_y\mathbf{e_y} + k_z^2 v_z\mathbf{e_z}$
- Symmetry in ϵ_k (homogeneous in $|\mathbf{k}|$)

We have

$$\begin{aligned}n_n &= \frac{1}{V}\sum_{\mathbf{k}}\frac{\beta\hbar^2}{m}\frac{k^2}{3}\frac{e^{\beta(\epsilon_k-\mu)}}{(e^{\beta(\epsilon_k-\mu)}-1)^2} \\ &= \frac{1}{(2\pi)^3}\int dk 4\pi k^2\frac{\beta\hbar^2}{m}\frac{k^2}{3}\frac{e^{\beta(\epsilon_k-\mu)}}{(e^{\beta(\epsilon_k-\mu)}-1)^2} \\ &= \frac{1}{(2\pi)^3}\int 4\pi k^2 dk\frac{\hbar^2k^2}{3m}\left[-\frac{\partial f(\epsilon_k-\mu)}{\partial\epsilon_k}\right],\end{aligned}$$

where $f(x) = \frac{1}{e^{\beta x}-1}$.
The simplest scenario, $\epsilon_k = \hbar^2k^2/2m$, i.e. ideal Bose gas

$$\begin{aligned}n_n &= -\frac{1}{(2\pi)^3}\int dk\frac{4\pi k^3}{3}\left[\frac{\partial f(\epsilon_k-\mu)}{\partial k}\right] \\ &= \frac{1}{(2\pi)^3}\int d^3\mathbf{k}\frac{1}{e^{\beta(\epsilon_k-\mu)}-1}\end{aligned}$$

For ideal Bose gas, $n_n = n_{ex}$, hence $n_{SF} = n_0$, i.e. superfluid density is equal to the condensate density. Contradiction?

Understanding our calculations

- Ideal BEC is not superfluid. (Landau criterion)
- We are actually considering the situation where the actual dispersion relation is very close to that of the free-particle. This is approximately the case at high temperature or for weakly interacting Bose gas, where $\epsilon_k \approx \hbar^2k^2/2m$. Therefore $n_{SF} \approx n_0$.
- For BEC with strong interaction, $\epsilon_k \neq \hbar^2k^2/2m$, the superfluid fraction can be much larger than the condensate fraction i.e. strong interaction depletes the condensate. (Quantum depletion of BEC)
- For ^{4}He, at zero temperature, $n_0 \approx 0.1 n_{tot}$, with $n_{SF} = n_{tot}$.

Next Lecture

We now know that interaction can greatly affect the overall property of the condensate. To understand the excitation spectrum, dynamical property, etc. of the BEC, we need to take interaction into consideration. At low temperatures, the major contribution to the interaction is two-body collision. To understand how one should incorporate two-body collisions into the model Hamiltonian for the BEC, we will first study the two-body scattering process in the next lecture.

Quantum Degenerate Gases

Lecture 5: Inter-atomic Interactions

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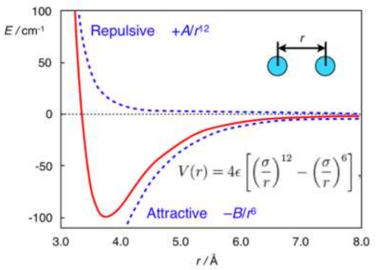
Contents

Interaction Potential between Neutral Atoms

- Neutral atoms interact via electromagnetic field. Need to go beyond ideal gas description to understand effects of interaction
- Many properties of cold atomic gases depend on interaction
  - Condensate fraction
  - Density profile
  - Dynamical properties
  - Superfluidity relies on interaction
- In dilute cold gases, three-body (or more) interactions is unlikely
- Two-body interaction is the leading order contribution
- In dilute cold atomic gases, interaction dominated by low energy, long wavelength scattering processes
- Detailed structure of the potential at short range becomes irrelevant

- At short range, potential governed by Coloumb repulsion and Pauli exclusion of eletron clouds overlap
- At long range, mainly van der Waals interaction $\sim C_6/r^6$
- Interaction in general depends on internal states (scattering channels)



Two-body Scattering

Two-body Schrödinger's equation

$$i\hbar\frac{\partial\Psi}{\partial t} = -\sum_i\left\{\frac{\hbar^2}{2m_1}\frac{\partial^2}{\partial r_{1i}^2} + \frac{\hbar^2}{2m_2}\frac{\partial^2}{\partial r_{2i}^2}\right\}\Psi + V(\mathbf{r_1}-\mathbf{r_2})\Psi \quad (i = x, y, z)$$

We may separate the center of mass motion from the relative motion and define the center of mass coordinate $\mathbf{R} = \frac{m_1\mathbf{r}_1 + m_2\mathbf{r}_2}{m_1+m_2}$, and the relative coordinate $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$. Then

$$-\frac{\hbar^2}{2}\left(\frac{1}{m_1}\frac{\partial^2}{\partial r_{1i}^2} + \frac{1}{m_2}\frac{\partial^2}{\partial r_{2i}^2}\right) = -\frac{\hbar^2}{2(m_1+m_2)}\frac{\partial^2}{\partial R_i^2} - \frac{\hbar^2}{2m_r}\frac{\partial^2}{\partial r^2},$$

where we have defined the reduced mass $\frac{1}{m_r} = \frac{1}{m_1} + \frac{1}{m_2}$, so that the relative motion can be described by a single-body Schrödinger's equation

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m_r}\nabla_r^2\Psi + V(\mathbf{r})\Psi$$

We project the wavefunction onto the basis of spherical harmonics

$$\Psi = \sum_{l,m} A_l' R_{kl}(r) Y_l^m(\theta,\varphi),$$

where m drops out of the coefficient due to the spherical symmetry of the scattering potential. Further aligning the z-axis with the direction of the incoming particle, and noting $Y_l^0 \propto P_l(\cos\theta)$, we have

$$\Psi = \sum_{l=0}^{\infty} A_l R_{kl}(r) P_l(\cos\theta)$$

Plug into the Schrödinger's equation, note

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\varphi}$$

For the derivative of the Legendre polynomial, we have used the relation

$$\int_x^1 P_l(t)dt = \frac{1-x^2}{l(l+1)}P_l'(x)$$

Therefore,

$$\begin{aligned}
&\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)P_l(\cos\theta)\\
&= \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left[-\sin^2\theta\frac{\partial}{\partial\cos\theta}P_l(\cos\theta)\right]\\
&= \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left[(-\sin^2\theta)\frac{l(l+1)}{1-\cos^2\theta}\int_{\cos\theta}^1 P_l(t)dt\right]\\
&= -l(l+1)P_l(\cos\theta)
\end{aligned}$$

Finally, we have the equation for the radial function

$$R_{kl}''(r) + \frac{2}{r}R_{kl}'(r) + \left[k^2 - \frac{l(l+1)}{r^2} - \frac{2m_r}{\hbar^2}V(r)\right]R_{kl}(r) = 0$$

We consider the low energy scattering with short range potential:

- For $r \ll R_e$, where R_e is the effective range of the interaction, k^2 term not important

$$R_l'' + \frac{2}{r}R_l' - \frac{l(l+1)}{r^2}R_l = \frac{2m_rV(r)}{\hbar^2}R_l$$

- For $R_e \ll r \ll \frac{1}{k}$, $V(r) \sim 0$

$$R_l'' + \frac{2}{r}R_l' - \frac{l(l+1)}{r^2}R_l = 0$$

with solution:

$$R_l = c_1 r^l + \frac{c_2}{r^{l+1}}$$

Note c_i contains information of details of short range interaction

For $r \sim \frac{1}{k}$,

$$R_l'' + \frac{2}{r}R_l' + \left[k^2 - \frac{l(l+1)}{r^2}\right]R_l = 0$$

With solution $R_l = c_1\frac{(2l+1)!!}{k^l}j_l(kr) - c_2\frac{k^{l+1}}{(2l-1)!!}n_l(kr)$.
In the limit of $kr \ll 1$, the spherical Bessel functions

$$j_l(kr) = (-1)^l\frac{r^l}{k^{l+1}}\left(\frac{d}{rdr}\right)^l\frac{\sin kr}{r}$$

$$n_l(kr) = (-1)^{l+1}\frac{r^l}{k^{l+1}}\left(\frac{d}{rdr}\right)^l\frac{\cos kr}{r}$$

can be simplified according to

$$\left(\frac{d}{rdr}\right)^l\frac{\sin kr}{r} \approx (-1)^l\left(\frac{d}{rdr}\right)^l\frac{k^{2l+1}r^{2l}}{(2l+1)!!} = (-1)^l\frac{k^{2l+1}}{(2l+1)!!},$$

Such that solutions for $r \sim \frac{1}{k}$ and $R_e \ll r \ll \frac{1}{k}$ are matched.

In the case of $kr \gg 1$, the spherical bessel functions become

$$j_l(kr) \approx \frac{\sin(kr - \frac{l\pi}{2})}{kr}$$

$$n_l(kr) \approx -\frac{\cos(kr - \frac{l\pi}{2})}{kr}$$

Therefore,

$$\begin{aligned}
R_l &\approx c_1\frac{(2l+1)!!}{k^l}\frac{\sin(kr-\frac{l\pi}{2})}{kr} + \frac{c_2k^{l+1}}{(2l-1)!!}\frac{\cos(kr-\frac{l\pi}{2})}{kr}\\
&= \frac{\sin(kr-\frac{l\pi}{2}+\delta_l)}{kr},
\end{aligned}$$

where the phase shift

$$\tan\delta_l = \frac{c_2}{c_1}\frac{k^{2l+1}}{(2l-1)!!(2l+1)!!} \xrightarrow{\text{low energy}} \delta_l$$

Ansatz wave function at large inter-atomic separation r

$$\Psi = e^{ikz} + f(\mathbf{k})\frac{e^{ikr}}{r},$$

which consists of an incoming plane wave and an outgoing spherical wave, with total energy given by $E = \hbar^2k^2/2m$. For spherically symmetric scatterer, $f(\mathbf{k}) = f(\theta)$, with $\cos\theta = \hat{\mathbf{k}}\cdot\hat{\mathbf{z}}$.
Matching wave functions at the far field

$$f(\theta) = \frac{1}{2ik}\sum_{l=0}^{\infty}(2l+1)\left(e^{2i\delta_l}-1\right)P_l(\cos\theta)$$

$$A_l = i^l(2l+1)e^{i\delta_l}.$$

Hence, the phase shift is closely related to the scattering amplitude $f(\theta)$ and contains information of the scattering potential at short range.

From the previous calculations, we see that for short range interactions at low energy, the phase shift for different partial waves scales as

$$\delta_l \propto k^{2l+1}$$

In reality, cold neutral atoms interact via van der Waals force at long range r^{-6}. In general, for long range interactions r^{-n},

$$\text{for} \quad l < \frac{n-3}{2}, \qquad \delta_l \propto k^{2l+1}$$
$$\text{for} \quad l \geq \frac{n-3}{2}, \qquad \delta_l \propto k^{n-2}$$

We now focus on the s-wave case, $l = 0$.

For s-wave scattering and at low energy, the scattering amplitude simplifies to

$$\begin{aligned} f(\theta) &= \frac{1}{2ik}(e^{2i\delta_0} - 1) = \frac{1}{k\cot\delta_0 - ik} \\ &= \frac{1}{2ik}(\cos 2\delta_0 + i\sin 2\delta_0 - 1) \\ &\approx \frac{\delta_0}{k} \qquad (l = 0) \end{aligned}$$

Since $\delta_0 \sim k$ for s-wave, we may define scattering length $a = -\lim_{k\to 0}\frac{\delta_0}{k}$, so that at very low energy, $f(\theta) \approx -a$ and

$$\begin{aligned} R_0(kr) &\approx \frac{1}{kr}\sin(kr + \delta_0) \\ &= \frac{\sin kr}{kr}\cos\delta_0 + \frac{\cos kr}{kr}\sin\delta_0 \\ &\approx 1 - \frac{a}{r} \end{aligned}$$

The total cross section, defined as

$$\begin{aligned} \sigma &= \int d\Omega |f(\theta)|^2 = 2\pi \int_0^\pi \sin\theta d\theta |f(\theta)|^2 \\ &= \frac{4\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)\sin^2\delta_l, \end{aligned}$$

where we have used

$$\int_{-1}^{1} P_n(x)P_m(x)dx = \frac{2}{2n+1}\delta_{mn}$$

For low energy s-wave scattering, $\sigma \approx 4\pi a^2$.

- Scattering length a depends on details of the short range potential
- Typically it is determined by fitting experimental and theoretical results
- Alternatively, details of the atomic potential are determined from spectroscopic measurements, which are then used to calculate the scattering properties by numerically solving the Schrödinger's equation.

What about identical particles?

- Need to (anti-)symmetrize the wavefunction for bosons (fermions)
- In the relative coordinate, exchanging particles amounts to the transformation $\mathbf{r} \to -\mathbf{r}$, which means $r \to r$, $\theta \to \pi - \theta$ and $\varphi \to \pi + \varphi$
- The properly (anti-)symmetrized wavefunction is

$$\Psi = e^{ikz} \pm e^{-ikz} + [f(\theta) \pm f(\pi - \theta)]\frac{e^{ikr}}{r}$$

- As the potential is spherically symmetric, we have for bosons

$$\begin{aligned} \sigma &= 2\pi \int_0^{\frac{\pi}{2}} \sin\theta d\theta |2f(\theta)|^2 \\ &\approx 8\pi a^2 \qquad (l = 0) \end{aligned}$$

- For identical fermions, the scattering length and the cross section vanishes on the s-wave level

Example: Box Potential

We consider an example to show how the scattering length is determined from the interaction potential.
Define box potential with effective range $R > 0$

$$V(r) = \begin{cases} V_0 & r < R \\ 0 & r > R \end{cases}$$

We need to solve the Schrödinger's equation

$$-\frac{\hbar^2}{m}\nabla^2\Psi + V\Psi = E\Psi,$$

where $E = \hbar^2k^2/2m_r > 0$.

Define radial wavefunction $u_l(k, r)$ such that

$$\Psi = \sum_l \frac{u_l(k,r)}{r}P_l(\cos\theta),$$

With Schrödinger's equation, $u_l(k, r)$ satisfies the equation

$$\left[\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} - \frac{2m_rV}{\hbar^2} + k^2\right]u_l(k,r) = 0$$

Solution for $l = 0$

$$\begin{cases} u_0^<(k,r) = Ae^{ik_1r} + Be^{-ik_1r} & \text{for} \quad r < R \\ u_0^>(k,r) = Ce^{ikr} + De^{-ikr} & \text{for} \quad r > R \end{cases}$$

where $k_1 = \sqrt{k^2 - 2m_rV_0/\hbar^2}$.

Consider the boundary conditions:

- At $r = 0$, $u_0^<(k,r) = 0$, hence $A = -B$
- For $r \to \infty$,

$$\Psi = \frac{\sin kr}{kr} + \frac{e^{2i\delta_0} - 1}{2ikr}e^{ikr}$$

  Hence, $C/D = -e^{2i\delta_0}$.
- Continuity condition at $r = R$ (setting $D = 1$)

$$\begin{aligned} &2iA\sin k_1R = Ce^{ikR} + e^{-ikR} \\ &A(k_1e^{ik_1R} + k_1e^{-ik_1R}) = -ke^{2i\delta_0 + ikR} - ke^{-ikR} \end{aligned}$$

Finally, we have

$$\delta_0 = -kR + \arctan\left(\frac{k\tan k_1R}{k_1}\right)$$

And the scattering length $a_s = -\lim_{k\to 0}\delta_0/k$.

Understanding scattering length

- For $V_0 > 0$, $a_s > 0$ always
- For $V_0 \to +\infty$, $a_s = R$
- For $V_0 < 0$,

$$a_s = R(1 - \frac{\tan\gamma}{\gamma}), \quad \text{with} \quad \gamma = R\sqrt{\frac{-2m_rV_0}{\hbar^2}}$$

  Therefore the scattering length may change sign.
- In fact, for $V_0 < 0$, a_s diverges for $\gamma = (n + \frac{1}{2})\pi$. This happens each time the potential becomes deep enough to support a bound state. Shape resonance.

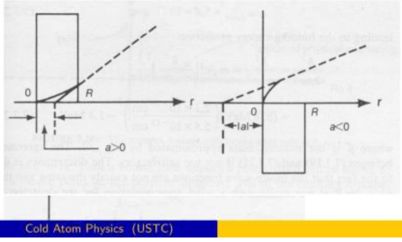
In fact, consider zero energy s-wave scattering, we have for $r > R$

$$\frac{d^2u}{dr^2} = 0$$

Therefore

$$u(r) \propto r - A$$

where A is a constant.
As $\Psi \to 1 - \frac{a}{r}$ in the $r \to \infty$ limit, we may identify $A = a$. Therefore the scattering length a is the intercept of $u(r)$, the outside radial wavefunction.



The sign change due to increased attractive interaction is due to the development of a bound state.

- For a large and positive, the radial wavefunction at $E = 0^+$ for $r > R$ is flat
- For $E = 0^-$, $r > R$, the wavefunction is $e^{-\kappa r}$. This is also flat given $\kappa \approx 0$
- For $r < R$, the radial wavefunction ($E = 0^+$ scattering state) and the $E = 0^-$ bound-state wavefunction are essentially the same
- Therefore, we may apply continuity condition at $r = R$ between the outside scattering wavefunction and the inside bound state wavefunction

$$-\left.\frac{\kappa e^{-\kappa r}}{e^{-\kappa r}}\right|_{r=R} = \left.\left(\frac{1}{r-a}\right)\right|_{r=R}$$

For $R \ll a$, $\kappa = \frac{1}{a}$, and the binding energy $E_b = \frac{\hbar^2\kappa^2}{2m_r} = \frac{\hbar^2}{2m_r a^2}$

Formal Scattering Theory

- Low energy scattering processes can be described by the scattering length
- We wish to replace the complicated short range physics with an effective interaction that has the correct low energy scattering properties

We start by writing the Hamiltonian

$$H = H_0 + V, \qquad H_0 = \frac{p^2}{2m_r}$$

We define the eigenkets for the kinetic part and the full Hamiltonian

$$H_0|\varphi\rangle = E|\varphi\rangle$$
$$H|\psi\rangle = E|\psi\rangle$$

Therefore, $|\psi\rangle \to |\varphi\rangle$ as $V \to 0$.

Similar in spirit to the previous ansatz wavefunction, we have the formal solution

$$|\psi\rangle = |\varphi\rangle + \frac{1}{E - H_0 + i\delta} V|\psi\rangle$$

This is the Lippmann-Schwinger equation, where the infinitesimal imaginary part of the energy is to make the sum convergent and to ensure only outgoing (instead of incoming) spherical waves are present.
For later applications, we may define the T-matrix $T|\varphi\rangle = V|\psi\rangle$, so that

$$T|\varphi\rangle = V|\varphi\rangle + V\frac{1}{E - H_0 + i\delta}T|\varphi\rangle$$

As $|\varphi\rangle$ is arbitrary, we have

$$T = V + V\frac{1}{E - H_0 + i\delta}T$$

Projecting the Lippmann-Schwinger equation to the coordinate basis,

$$\langle \mathbf{x}|\psi\rangle = \langle \mathbf{x}|\varphi\rangle + \int d^3\mathbf{x}' \left\langle \mathbf{x} \left| \frac{1}{E - H_0 + i\delta} \right| \mathbf{x}' \right\rangle \langle \mathbf{x}'|V|\psi\rangle$$

We define

$$G(\mathbf{x}, \mathbf{x}') = \frac{\hbar^2}{2m_r} \left\langle \mathbf{x} \left| \frac{1}{E - H_0 + i\delta} \right| \mathbf{x}' \right\rangle = -\frac{1}{4\pi}\frac{e^{ik|\mathbf{x}-\mathbf{x}'|}}{|\mathbf{x}-\mathbf{x}'|}$$

where $E = \hbar^2k^2/2m_r$, and we may identify $G(\mathbf{x}, \mathbf{x}')$ as the Green's function of the Helmholtz equation

$$(\nabla^2 + k^2)G(\mathbf{x}, \mathbf{x}') = \delta(\mathbf{x} - \mathbf{x}')$$

$$\begin{aligned}
&\frac{\hbar^2}{2m_r}\left\langle \mathbf{x} \left| \frac{1}{E - H_0 + i\delta} \right| \mathbf{x}' \right\rangle \\
&= \frac{\hbar^2}{2m_r}\int d^3\mathbf{p} d^3\mathbf{p}' \langle \mathbf{x}|\mathbf{p}\rangle \left\langle \mathbf{p} \left| \frac{1}{E - (p^2/2m_r) + i\delta} \right| \mathbf{p}' \right\rangle \langle \mathbf{p}'|\mathbf{x}'\rangle \\
&= \frac{\hbar^2}{2m_r}\int \frac{d^3\mathbf{p}}{(2\pi\hbar)^3}\frac{e^{i\mathbf{p}\cdot(\mathbf{x}-\mathbf{x}')/\hbar}}{E - (p^2/2m_r) + i\delta} \\
&= \frac{1}{(2\pi)^3}\int_0^\infty q^2dq \int_0^{2\pi} d\phi \int_{-1}^1 d(\cos\theta)\frac{e^{iq|\mathbf{x}-\mathbf{x}'|\cos\theta}}{k^2 - q^2 + i\delta} \\
&= -\frac{1}{8\pi^2}\frac{1}{i|\mathbf{x}-\mathbf{x}'|}\int_{-\infty}^\infty \frac{qdq\left(e^{iq|\mathbf{x}-\mathbf{x}'|} - e^{-iq|\mathbf{x}-\mathbf{x}'|}\right)}{q^2 - k^2 - i\delta} \\
&= -\frac{1}{4\pi}\frac{e^{ik|\mathbf{x}-\mathbf{x}'|}}{|\mathbf{x}-\mathbf{x}'|}
\end{aligned}$$

We have defined $\mathbf{p} = \hbar\mathbf{q}$. And the poles of the integrand in line 5 is $q = \pm k\sqrt{1 \pm (i\delta/k^2)} \approx \pm k \pm i\delta'$

Therefore, we have

$$\langle \mathbf{x}|\psi\rangle = \langle \mathbf{x}|\varphi\rangle - \frac{2m_r}{\hbar^2}\int d^3\mathbf{x}'\frac{e^{ik|\mathbf{x}-\mathbf{x}'|}}{4\pi|\mathbf{x}-\mathbf{x}'|}\langle \mathbf{x}'|V|\psi\rangle$$

- $\mathbf{x}$ is the vector directed towards the point of observation
- For finite range potential, $\langle \mathbf{x}'|V|\psi\rangle$ is only non-vanishing in limited regions close to the scatterer
- Observation is made typically far away from the scatterer

Therefore, we may take the limit $|\mathbf{x}| \gg |\mathbf{x}'|$, so that

$$|\mathbf{x} - \mathbf{x}'| \approx |\mathbf{x}| - \frac{\mathbf{x}\cdot\mathbf{x}'}{|\mathbf{x}|} = r - \hat{\mathbf{r}}\cdot\mathbf{x}',$$

We have defined $r = |\mathbf{x}|$, and $\hat{\mathbf{r}} = \mathbf{x}/|\mathbf{x}|$.

Hence, we make the approximations

$$e^{ik|\mathbf{x}-\mathbf{x}'|} \approx e^{ikr}e^{-i\mathbf{k}'\cdot\mathbf{x}'}$$
$$\frac{1}{|\mathbf{x}-\mathbf{x}'|} \approx \frac{1}{r},$$

where we have defined $\mathbf{k}' = k\hat{\mathbf{r}}$.
Finally, we have for large distances r,

$$\begin{aligned}
\langle \mathbf{x}|\psi\rangle &\approx \langle \mathbf{x}|\mathbf{k}\rangle - \frac{1}{4\pi}\frac{2m_r}{\hbar^2}\frac{e^{ikr}}{r}\int d^3\mathbf{x}' e^{-i\mathbf{k}'\cdot\mathbf{x}'}\langle \mathbf{x}'|V|\psi\rangle \\
&= e^{i\mathbf{k}\cdot\mathbf{x}} + \frac{e^{ikr}}{r}f(\mathbf{k}', \mathbf{k})
\end{aligned}$$

And we may identify the scattering amplitude

$$f(\mathbf{k}', \mathbf{k}) = -\frac{1}{4\pi}\frac{2m_r}{\hbar^2}\langle \mathbf{k}'|V|\psi\rangle = -\frac{2m_r}{4\pi\hbar^2}T(\mathbf{k}', \mathbf{k}; E)$$

Using

$$T(\mathbf{k}',\mathbf{k};E) = \langle \boldsymbol{k}'|T|\boldsymbol{k}\rangle = \frac{\hbar^2}{m_r k}\sum_{lm}\frac{2l+1}{4\pi}T_l(k)P_l(\hat{\boldsymbol{k}}'\cdot\hat{\boldsymbol{k}}),$$

we have

$$f(\mathbf{k}',\mathbf{k}) = f(\theta) = \sum_l (2l+1)f_l(k)P_l(\cos\theta),$$

with $f_l(k) = -\frac{T_l(k)}{8\pi^2 k}$. It follows the wave function at far field

$$\langle \boldsymbol{x}|\psi\rangle = e^{ikz} + f(\theta)\frac{e^{ikr}}{r} = \sum_l (2l+1)P_l(\cos\theta)\Big[\frac{e^{ikr}-e^{-i(kr-l\pi)}}{2ikr}\Big]$$
$$+\sum_l (2l+1)P_l(\cos\theta)f_l(k)\frac{e^{ikr}}{r}$$
$$=\sum_l (2l+1)\frac{P_l(\cos\theta)}{2ik}\Big\{\big[1+2ikf_l(k)\big]\frac{e^{ikr}}{r} - \frac{e^{-i(kr-l\pi)}}{r}\Big\}$$

Therefore recovering previous results (conservation of probability)

$$S_l(k) = 1 + 2ikf_l(k) = e^{2i\delta_l}$$
$$f_l(k) = \frac{e^{2i\delta_l}-1}{2ik}$$

Shallow bound states as poles of $S_l(k)$ ($l=0$ case)

$$\langle \boldsymbol{x}|\psi\rangle = S_0(k)\frac{e^{ikr}}{r} - \frac{e^{-ikr}}{r}$$

Translates to

$$f_{l=0}(k) = \frac{1}{k\cot\delta_0 - ik} \xrightarrow{k\to 0} \frac{1}{-1/a - ik}$$

A pole exists at $k = i\kappa$ with $\kappa = 1/a$, i.e., $E_b = -\frac{\hbar^2}{2m_r a^2}$.

Zero-range pseudo-potentials

Huang-Yang pseudo-potential (revised version)

$$V_l(r) = -\frac{(2l+1)!!}{l!2^l}\frac{\hbar^2}{2m_r}\frac{\delta(r)}{r^{l+2}}\frac{\tan\delta_l}{k^{2l+1}}\Big(\frac{\partial}{\partial r}\Big)^{2l+1}\cdot r^{l+1}$$

For the s-wave case (Fermi-Huang pseudo-potential)

$$V(\boldsymbol{r}) = \frac{2\pi\hbar^2}{m_r}a\delta(\boldsymbol{r})\Big(\frac{\partial}{\partial r}\cdot r\Big)$$

From Schrödinger's equation

$$[-\frac{\hbar^2}{2m_r}\nabla^2 + V]\psi = \frac{\hbar^2 k^2}{2m_r}\psi \quad \text{with } \psi = e^{ikz} + f(k)\frac{e^{ikr}}{r},$$

we have $f(k) = \frac{1}{-1/a-ik}$, where $-\nabla^2\frac{1}{r} = 4\pi\delta(\boldsymbol{r})$ is used.

Contact potential (s-wave case)

$$V(\boldsymbol{r}) = g\delta(\boldsymbol{r})$$

- Hermitian and convenient for many-body systems
- A constant g in momentum space
- Unphysical at short range (or large k), can lead to divergence

Renormalization (regularization): Lippmann-Schwinger equation in operator form

$$T = V + V\frac{1}{E-H_0+i\delta}T$$
$$= V + V\frac{1}{E-H_0+i\delta}V + V\frac{1}{E-H_0+i\delta}V\frac{1}{E-H_0+i\delta}V + \ldots$$

In momentum space, $E = \hbar^2k^2/2m_r = \hbar^2k'^2/2m_r$ (on-shell scattering), and

$$T(\mathbf{k}',\mathbf{k};E) = U(\mathbf{k}',\mathbf{k}) + \frac{1}{\mathcal{V}}\sum_{\mathbf{k}''}U(\mathbf{k}',\mathbf{k}'')\left(E - \frac{\hbar^2k''^2}{2m_r}+i\delta\right)^{-1}T(\mathbf{k}'',\mathbf{k};E) \implies$$

$$T(\mathbf{k}',\mathbf{k};E) = g + \frac{g}{\mathcal{V}}\sum_{\mathbf{k}''}\frac{1}{E-\frac{\hbar^2k''^2}{2m_r}+i\delta}T(\mathbf{k}'',\mathbf{k};E) \implies$$

$$\frac{1}{\mathcal{V}}\sum_{\mathbf{k}'}\frac{1}{E-\frac{\hbar^2k'^2}{2m_r}+i\delta}T(\mathbf{k}',\mathbf{k};E) = g\frac{1}{\mathcal{V}}\sum_{\mathbf{k}'}\frac{1}{E-\frac{\hbar^2k'^2}{2m_r}+i\delta}$$
$$+\frac{g}{\mathcal{V}^2}\sum_{\mathbf{k}',\mathbf{k}''}\frac{1}{E-\frac{\hbar^2k'^2}{2m_r}+i\delta}\frac{1}{E-\frac{\hbar^2k''^2}{2m_r}+i\delta}T(\mathbf{k}'',\mathbf{k};E) \implies$$

$$\frac{1}{\mathcal{V}}\sum_{\mathbf{k}'}\frac{1}{E-\frac{\hbar^2k'^2}{2m_r}+i\delta}\left[T(\mathbf{k}',\mathbf{k};E)\left(1-\frac{g}{\mathcal{V}}\sum_{\mathbf{k}''}\frac{1}{E-\frac{\hbar^2k''^2}{2m_r}+i\delta}\right)-g\right] = 0 \implies$$

$$T(\mathbf{k}',\mathbf{k};E) = T(E) = \frac{1}{\frac{1}{g}-\sum_{\mathbf{k}''}\frac{1}{E-\frac{\hbar^2k''^2}{2m_r}+i\delta}}$$

Note for s-wave scattering, $T(\mathbf{k}',\mathbf{k};E) = T(E)$.

Therefore,

$$T(E) = \frac{1}{\frac{1}{g}+\frac{1}{\mathcal{V}}\sum_{\boldsymbol{k}}\frac{1}{\frac{\hbar^2k^2}{2m_r}} - \frac{1}{\mathcal{V}}\sum_{\boldsymbol{k}}\left(\frac{1}{E-\frac{\hbar^2k^2}{2m_r}+i\delta}+\frac{1}{\frac{\hbar^2k^2}{2m_r}}\right)}$$
$$= \frac{1}{\frac{1}{g}+\frac{1}{\mathcal{V}}\sum_{\boldsymbol{k}}\frac{1}{\frac{\hbar^2k^2}{2m_r}}+\frac{ikm_r}{2\pi\hbar^2}}.$$

Compared with

$$T(E) = \frac{4\pi\hbar^2}{2m_r}\frac{1}{\frac{1}{a}+ik},$$

we need the following renormalization condition

$$\frac{1}{g} = \frac{m_r}{2\pi\hbar^2 a} - \frac{1}{\mathcal{V}}\sum_{\boldsymbol{k}}\frac{1}{\frac{\hbar^2k^2}{2m_r}}$$

Effective contact interaction

$$V(\mathbf{r},\mathbf{r}') = g\delta(\mathbf{r}-\mathbf{r}')$$

- It can lead to divergence due to the incorrect short range/high energy behavior of the contact potential
- Short distance behavior is different, but we are mostly interested in systems where particles are far apartb
- We get the same asymptotic s-wave scattering properties as with real interaction after renormalization
- The pseudopotential approximation works well for most ultra-cold quantum gases

Hamiltonian for Interacting Bose Gas

For N identical Bosons with short range s-wave interaction

$$H = \sum_{i=1}^{N}\left[\frac{p_i^2}{2m}+V(\mathbf{r}_i)\right] + U_0\sum_{i<j}\delta(\mathbf{r}_i-\mathbf{r}_j)$$

where V is the potential energy (external trapping potentia), and U_0 is related to a through renormalization.
In second quantized form

$$\hat{H}-\mu\hat{N} = \int d^3\mathbf{r}\hat{\Psi}^\dagger(\mathbf{r})\left[-\frac{\hbar^2}{2m}\nabla^2+V(\mathbf{r})-\mu+\frac{U_0}{2}\hat{\Psi}^\dagger(\mathbf{r})\hat{\Psi}(\mathbf{r})\right]\hat{\Psi}(\mathbf{r})$$

For cases where only low-energy, long-wavelength physics are involved, $U_0 = 4\pi\hbar^2 a/m$.

Next Lecture

With the basic understanding of the two-body scattering process and the effective Hamiltonian, we are in a good position to discuss the properties of interacting Boson gas.

- Mean field theory of the interacting Bose gas
- Derivation and application of Gross-Pitaevskii equation

Quantum Degenerate Gases

Lecture 6: Condensate with Interaction

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Contents

Effective Hamiltonian for Bose gas

Hamiltonian with effective contact interaction

$$H=\sum_{i=1}^{N}\left[\frac{p_i^2}{2m}+V(\mathbf{r}_i)\right]+U_0\sum_{i<j}\delta(\mathbf{r}_i-\mathbf{r}_j)$$

where V is the potential energy (external trapping potential), and $U_0=4\pi\hbar^2 a_s/m$ is given by the pseudopotential.
In second quantized form

$$\hat{H}-\mu\hat{N}=\int d^3\mathbf{r}\hat{\Psi}^\dagger(\mathbf{r})\left[-\frac{\hbar^2}{2m}\nabla^2+V(\mathbf{r})-\mu+\frac{U_0}{2}\hat{\Psi}^\dagger(\mathbf{r})\hat{\Psi}(\mathbf{r})\right]\hat{\Psi}(\mathbf{r})$$

And the creation (annihilation) operators $\hat{\Psi}^\dagger$ ($\hat{\Psi}$) satisfy the bosonic commutation relations

$$\left[\hat{\Psi}(\mathbf{r}'),\hat{\Psi}^\dagger(\mathbf{r})\right]=\delta(\mathbf{r}'-\mathbf{r})$$

Gross-Pitaevksii Equation

Different mean field approximations at zero temperature

- Hartree approximation for fixed number state: all bosons are in the same single particle state. The N- body wavefunction is therefore
$$\Psi_{\text{Hartree}}(\mathbf{r}_1,\cdots,\mathbf{r}_N)=\prod_i\phi(\mathbf{r}_i,t),$$
where $\int d\mathbf{r}|\phi(\mathbf{r})|^2=1$.
- Bogoliubov mean field expansion:
$$\hat{\Psi}=\langle\hat{\Psi}\rangle+\delta\hat{\Psi}$$
The condensate can be understood as in a coherent state under this approximation. Particle number not fixed.

These mean field approximations are equivalent in the thermodynamic limit, and both can lead to the GP equation.

Under Hartree approximation, we may calculate the energy functional of the Hamiltonian

- Kinetic energy and potential energy

$$\begin{aligned}&\int\prod_k d\mathbf{r}_k\Psi^*_{\text{Hartree}}\left\{\sum_{i=1}^{N}H_0(\mathbf{r}_i)\right\}\Psi_{\text{Hartree}}\\&=\sum_{j=1}^{N}\int d\mathbf{r}_j\phi^*(\mathbf{r}_j)H_0(\mathbf{r}_j)\phi(\mathbf{r}_j)\prod_{i\neq j}\int d\mathbf{r}_i|\phi(\mathbf{r}_i)|^2\\&=N\int d\mathbf{r}\phi^*(\mathbf{r})H_0(\mathbf{r})\phi(\mathbf{r})\end{aligned}$$

where $H_0(\mathbf{r})=-\frac{\hbar^2\nabla_{\mathbf{r}}^2}{2m}+V(\mathbf{r})$.

- Interaction energy

$$\begin{aligned}&\int\prod_{i=1}^{N}d\mathbf{r}_i\prod_{j=1}^{N}\phi^*(\mathbf{r}_j)U_0\sum_{m<n}\delta(\mathbf{r}_m-\mathbf{r}_n)\prod_{k=1}^{N}\phi(\mathbf{r}_k)\\&=C_N^2U_0\int d\mathbf{r}|\phi(\mathbf{r})|^4\end{aligned}$$

- Therefore the total energy functional is

$$\frac{E\left[\phi(\mathbf{r})\right]}{N}=\int d\mathbf{r}\left[\frac{\hbar^2}{2m}|\nabla\phi(\mathbf{r})|^2+V(\mathbf{r})|\phi(\mathbf{r})|^2+\frac{N-1}{2}U_0|\phi(\mathbf{r})|^4\right]$$

Note

$$\begin{aligned}\int d\mathbf{r}\phi^*(\mathbf{r})\nabla^2\phi(\mathbf{r})&=-\int d\mathbf{r}|\nabla\phi(\mathbf{r})|^2+\int d\mathbf{r}\nabla\cdot[\phi^*(\mathbf{r})\nabla\phi(\mathbf{r})]\\&=-\int d\mathbf{r}|\nabla\phi(\mathbf{r})|^2+\oint d\mathbf{n}\left[\phi^*(\mathbf{r})\nabla\phi(\mathbf{r})\right],\end{aligned}$$

where the surface integral vanishes and we have used $\nabla\cdot(f\nabla g)=\nabla f\cdot\nabla g+f\nabla^2 g$.

To simplify the expression, we define the condensate wavefunction

$$\psi(\mathbf{r})=N^{\frac{1}{2}}\phi(\mathbf{r})\qquad\text{with}\qquad\int d\mathbf{r}|\psi(\mathbf{r})|^2=N$$

With this, the energy functional becomes

$$E\left[\psi(\mathbf{r})\right]=\int d\mathbf{r}\left[\frac{\hbar^2}{2m}|\nabla\psi(\mathbf{r})|^2+V(\mathbf{r})|\psi(\mathbf{r})|^2+\frac{1}{2}U_0|\psi(\mathbf{r})|^4\right],$$

where we may use $(N-1)\approx N$ for large N.

- We wish to minimize the energy functional with respect to the functional variations of ψ and ψ^*
- We must minimize the energy functional while meeting the number conservation condition $\int d\mathbf{r}|\psi(\mathbf{r})|^2=N$.
- The method of Lagrange multiplier. Introduce the chemical potential μ, and minimize $E-\mu N$.

Minimizing the energy functional $\frac{\delta E[\psi]}{\delta \psi^*}=0$, we have

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r})+V(\mathbf{r})\psi(\mathbf{r})+U_0|\psi(\mathbf{r})|^2\psi(\mathbf{r})=\mu\psi(\mathbf{r}),$$

where we have used $\frac{\delta F[f(r')]}{\delta f(r)}=\frac{\partial F}{\partial f}\delta(r-r')$.

- Time independent Gross-Pitaevskii equation (GPE), which describes the static properties of a dilute, interacting BEC.
- GPE has the form of Schrödinger equation, with the potential given by the external potential and a non-linear mean field term $U_0|\psi|^2$ exerted by other bosons.
- For a uniform BEC, $\mu=U_0|\psi|^2=nU_0$. In fact, for an interacting gas, the chemical potential is the energy it takes to add one particle into the ensemble while keeping the entropy constant, which for a static condensate is just the mean field energy.

Alternatively, GPE can be derived starting from the second quantized Hamiltonian and applying the Bogoliubov approximation

$$\hat{H}=\int d^3\mathbf{r}\hat{\Psi}^\dagger(\mathbf{r},t)\left[-\frac{\hbar^2}{2m}\nabla^2+V(\mathbf{r},t)\right]\hat{\Psi}(\mathbf{r},t)$$
$$+\frac{1}{2}\int\hat{\Psi}^\dagger(\mathbf{r}',t)\hat{\Psi}^\dagger(\mathbf{r},t)U(\mathbf{r}-\mathbf{r}')\hat{\Psi}(\mathbf{r},t)\hat{\Psi}(\mathbf{r}',t)d^3\mathbf{r}d^3\mathbf{r}'$$

The Heisenberg equation for the field operator gives

$$i\hbar\frac{\partial}{\partial t}\hat{\Psi}(\mathbf{r},t)=\left[\hat{\Psi}(\mathbf{r},t),\hat{H}\right]$$
$$=\left[-\frac{\hbar^2}{2m}\nabla^2+V(\mathbf{r},t)+\int d^3\mathbf{r}'\hat{\Psi}^\dagger(\mathbf{r}',t)U(\mathbf{r}-\mathbf{r}')\hat{\Psi}(\mathbf{r}',t)\right]\hat{\Psi}(\mathbf{r},t)$$

- Bogoliubov approximation $\hat{\Psi}\approx\langle\hat{\Psi}\rangle=\psi$, where we have left out the fluctuation $\delta\hat{\Psi}$ of the mean field expansion.
- Pseudopotential $U(\mathbf{r}-\mathbf{r}')=\frac{4\pi\hbar^2 a_s}{m}\delta(\mathbf{r}-\mathbf{r}')$.

We arrive at the Time-Dependent Gross-Pitaevskii Equation (TDGPE)

$$i\hbar\frac{\partial}{\partial t}\psi(\mathbf{r},t)=\left[-\frac{\hbar^2}{2m}\nabla^2+V(\mathbf{r},t)+U_0|\psi(\mathbf{r},t)|^2\right]\psi(\mathbf{r},t)$$

Consider the stationary case $\psi(\mathbf{r},t)=\psi(\mathbf{r})e^{-i\mu t}$, with static external potential $V(\mathbf{r})$

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r})+V(\mathbf{r})\psi(\mathbf{r})+U_0|\psi(\mathbf{r})|^2\psi(\mathbf{r})=\mu\psi(\mathbf{r})$$

Note we may identify the dynamic phase in the mean field wave function as the chemical potential.

Ground State Properties

Interaction energy scales with particle number. For sufficiently large number of particles with repulsive interaction, the kinetic energy can be negligible, which amounts to the Thomas-Fermi (TF) approximation

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

Solution

$$n(\mathbf{r})=|\psi(\mathbf{r})|^2=\begin{cases}\frac{\mu-V(\mathbf{r})}{U_0} & \mu>V(\mathbf{r})\\ 0 & \mu\le V(\mathbf{r})\end{cases}$$

The energy to put one particle into the atom cloud μ is the sum of trapping potential $V(\mathbf{r})$ and the local interaction mean field $n(\mathbf{r})U_0$. This, together with the number constraint can lead to the solution of the chemical potential.

The boundary of the cloud is given by $\mu=V(\mathbf{r})$.

Consider an anisotropic harmonic trap

$$V(\mathbf{r})=\frac{1}{2}m\omega_x^2x^2+\frac{1}{2}m\omega_y^2y^2+\frac{1}{2}m\omega_z^2z^2$$

Scale the spatial coordinate according to

$$r_i=\sqrt{\frac{2\mu}{m\omega_i^2}}r_i',\qquad(i=x,y,z)$$

where $\sqrt{\frac{2\mu}{m\omega_i^2}}$ is the radius of the cloud in the i-th direction, and the external potentail becomes $V(\mathbf{r}')=\mu r'^2$. Hence

$$N=\int d^3\mathbf{r}\frac{\mu-V(\mathbf{r})}{U_0}$$
$$=\frac{1}{\omega_x\omega_y\omega_z}\left(\frac{2\mu}{m}\right)\int d^3\mathbf{r}'\frac{\mu-\mu r'^2}{U_0}$$
$$=\frac{8\pi}{15}\left(\frac{2\mu}{m\bar{\omega}^2}\right)^{\frac{3}{2}}\frac{\mu}{U_0},\quad\text{with}\quad\bar{\omega}=(\omega_x\omega_y\omega_z)^{\frac{1}{3}}$$

The chemical potential can be expressed as

$$\mu=\frac{15^{\frac{2}{5}}}{2}\left(\frac{Na_s}{\bar{a}}\right)^{\frac{2}{5}}\hbar\bar{\omega},\quad\text{with}\quad\bar{a}=\sqrt{\frac{\hbar}{m\bar{\omega}}}$$

The average spatial extent of the cloud can be characterized by

$$\bar{R}=\left(\prod_{i=x,y,z}\sqrt{\frac{2\mu}{m\omega_i^2}}\right)^{\frac{1}{3}}=15^{\frac{1}{5}}\left(\frac{Na_s}{\bar{a}}\right)^{\frac{1}{5}}\bar{a}$$

- Spatial extent of the cloud in TF approximation larger than that of the ground state of the trap in the non-interacting case (repulsive interaction tends to broaden the density distribution)
- One needs $\frac{Na_s}{\bar{a}}\gg 1$ for the TF approximation to be valid
- TF approximation breaks down near the boundary of the cloud

Is the gas too dilute to apply TF approximation?

- Diluteness condition $na_s^3\ll 1$ at the trap center (which features maximum n)

$$na_s^3=\frac{\mu}{U_0}a_s^3=\frac{15^{\frac{2}{5}}}{8\pi}\left(\frac{N^{\frac{1}{6}}a_s}{\bar{a}}\right)^{\frac{12}{5}}$$

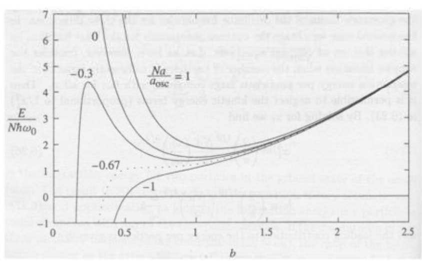
Dilutness condition $\frac{N^{\frac{1}{6}}a_s}{\bar{a}}\ll 1$

- TF approximation condition $\frac{Na_s}{\bar{a}}\gg 1$
- Realistic experimental paramters for ^{87}Rb, $N=10^5$, $\omega\approx 2\pi\times 200\text{Hz}$, $a_s=100a_0$ ($a_0\approx 0.53\mathring{A}$)

$$\frac{Na_s}{\bar{a}}\approx 738\gg 1\qquad\frac{N^{\frac{1}{6}}a_s}{\bar{a}}\approx 0.05\ll 1$$

Attracitve interaction

- The gas becomes unstable when the interaction is large, hence Thomas Fermi approximation is not valid
- One can estimate the energy using variational method, with the wavefunction ansatz given as Gaussian $\psi(\mathbf{r})=\frac{N^{\frac{1}{2}}}{b^{\frac{3}{2}}\pi^{\frac{3}{4}}}e^{-\frac{r^2}{2b^2}}$
- Numerical solution of the GPE reveals a metastable local minimum for $N|a_s|/\bar{a}<0.57$



Healing length

- Consider a condensate in a box with infinitely hard walls. The healing length ξ characterizes the distance over which the wavefunction approaches its bulk value from the wall.
- Suppose the potential is $+\infty$ at $x=0$, and 0 for $x>0$, and the gas is uniform in other directions. The GPE gives

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x)+U_0|\psi(x)|^2\psi(x)=\mu\psi(x)$$

The chemical potential can be determined from the bulk GPE $\mu=U_0|\psi_0|^2$, we have

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x)=U_0\left(|\psi_0|^2-|\psi(x)|^2\right)\psi(x)\,,$$

with boundary condition $\psi(0)=0, \psi(\infty)=\psi_0$. Solution:

$$\psi(x)=\psi_0\tanh\left(\frac{2}{\sqrt{2}\xi}\right)\,,\quad \text{with}\quad \xi=\sqrt{\frac{\hbar^2}{2mn_0U_0}}=\sqrt{\frac{1}{8\pi n_0 a_s}}$$

Dynamics of BEC

Time dependent GPE (TDGPE)

$$i\hbar\frac{\partial}{\partial t}\psi(\mathbf{r},t)=\left[-\frac{\hbar^2}{2m}\nabla^2+V(\mathbf{r},t)+U_0|\psi(\mathbf{r},t)|^2\right]\psi(\mathbf{r},t)$$

- To be consistent with GPE, the stationary condition should be $\psi(\mathbf{r},t)=e^{-i\mu t/\hbar}\psi(\mathbf{r})$
- Formally, one may start from the action

$$S=\int Ldt=\int dtd^3\mathbf{r}\left\{\frac{i\hbar}{2}\left(\psi^*\frac{\partial\psi}{\partial t}-\psi\frac{\partial\psi^*}{\partial t}\right)-E[\psi]\right\}\,,$$

TDGPE can then be derived from $\frac{\delta S}{\delta\psi^*}=0$.

Separate the wavefunction into the density part and the phase part $\psi=\sqrt{n(\mathbf{r},t)}e^{i\varphi(\mathbf{r},t)}$. Applying the TDGPE, we have

$$m\frac{\partial\mathbf{v}}{\partial t}+\nabla\left(V+nU_0-\frac{\hbar^2}{2m\sqrt{n}}\nabla^2\sqrt{n}+\frac{1}{2}mv^2\right)=0$$
$$\frac{\partial n}{\partial t}+\nabla\cdot(n\mathbf{v})=0$$

The velocity is defined as the gradient of the phase

$$\mathbf{v}=\frac{\hbar}{m}\nabla\varphi=\frac{\hbar}{2mi}\left(\frac{\psi^*\nabla\psi-\psi\nabla\psi^*}{|\psi|^2}\right)$$

Compare with the hydrodynamic equation for perfect fluids

$$\frac{\partial\mathbf{v}}{\partial t}-\mathbf{v}\times(\nabla\times\mathbf{v})=-\frac{1}{mn}\nabla p-\nabla\left(\frac{v^2}{2}\right)-\frac{1}{m}\nabla V$$

As $\nabla\times\mathbf{v}=0$, $dp=nd\mu=nd(nU_0)$, the difference lies in the additional term $\frac{1}{m}\nabla\left(\frac{\hbar^2}{2m\sqrt{n}}\nabla^2\sqrt{n}\right)$, the so-called quantum pressure term.

- Condensate is irrotational $\nabla\times\mathbf{v}=0$
- The quantum pressure term describes a force derived from spatial variation of the condensate wavefunction
- Suppose the wavefunction varies over a spatial scale of η, let's estimate magnitude of the quantum pressure term and the usual pressure term in the hydrodynamic equation

$$\frac{1}{mn}\nabla p=\frac{1}{m}\nabla(nU_0)\sim\frac{nU_0}{m\eta}$$
$$\frac{1}{m}\nabla\left(\frac{\hbar^2}{2m\sqrt{n}}\nabla^2\sqrt{n}\right)\sim\frac{\hbar^2}{2m^2\eta^3}$$

Therefore the quantum pressure term becomes negligible if the spatial variation of the wavefunction occurs on length scale η much larger than healing length $\xi=\sqrt{\frac{\hbar^2}{2mnU_0}}$. In this case, the dynamics of the condensate can be described by the hydrodynamic equation.

Variant form of the TDGPE

$$m\frac{\partial\mathbf{v}}{\partial t}+\nabla\left(V+nU_0-\frac{\hbar^2}{2m\sqrt{n}}\nabla^2\sqrt{n}+\frac{1}{2}mv^2\right)=0$$
$$\frac{\partial n}{\partial t}+\nabla\cdot(n\mathbf{v})=0$$

To study excitations, we apply linear response theory and expand the density around its equilibrium value

$$n(\mathbf{r},t)=n_0(\mathbf{r})+\delta n(\mathbf{r},t)$$

Plug it into the equations above, treating $\mathbf{v}$ and δn as small quantities, we have

$$\frac{\partial(n_0+\delta n)}{\partial t}=-\nabla\cdot[(n_0+\delta n)\mathbf{v}]\rightarrow$$
$$\frac{\partial\delta n}{\partial t}\approx-\nabla\cdot(n_0\mathbf{v})$$

And

$$m\frac{\partial\mathbf{v}}{\partial t}=-\nabla\delta\tilde{\mu}\,,$$

where

$$\tilde{\mu}=V+nU_0-\frac{\hbar^2}{2m\sqrt{n}}\nabla^2\sqrt{n}$$

Combining the two equations, we have the equations of motion

$$m\frac{\partial^2\delta n}{\delta t^2}\approx\nabla\cdot(n_0\nabla\delta\tilde{\mu})\,,$$

which describes excitations of a Bose gas in an arbitrary potential. We will now consider the simple case of a uniform gas, with travelling wave excitations:

$$n_0=\text{constant}\,,\qquad \delta n=Ae^{i\mathbf{q}\cdot\mathbf{r}-i\omega t}$$

Hence we have

$$\delta\tilde{\mu}\approx\delta nU_0-\delta\left[\frac{\hbar^2}{2m\sqrt{n}}\right]\nabla^2\sqrt{n_0}-\frac{\hbar^2}{2m\sqrt{n_0}}\delta\left[\nabla^2\sqrt{n}\right]$$
$$\approx\delta nU_0-\frac{\hbar^2}{2m\sqrt{n_0}}\frac{1}{2\sqrt{n_0}}\nabla^2\delta n$$
$$=\left(U_0+\frac{\hbar^2q^2}{4mn_0}\right)\delta n$$

Plug into the equations of motion

$$m\omega^2\delta n=\left(n_0U_0q^2+\frac{\hbar^2q^4}{4m}\right)\delta n$$

Defining $|\omega|=\frac{\epsilon_q}{\hbar}$, we have the dispersion relation for the excitation

$$\epsilon_q=\sqrt{2n_0U_0\epsilon_0+\epsilon_0^2}\,,$$

where $\epsilon_0=\frac{\hbar^2q^2}{2m}$ is the free particle energy.

- For small q, i.e. long-wavelength limit

$$\epsilon_q\approx s\hbar q\,,$$

where $s=\sqrt{n_0U_0/m}$ is the sound speed for the Bogoliubov phonons
- For large q, i.e. short-wavelength limit

$$\epsilon_q\approx n_0U_0+\frac{\hbar^2q^2}{2m}\,,$$

which is a free particle spectrum with a mean field shift.
- The transition between the two limiting case roughly takes place at $\frac{\hbar^2q_c^2}{2m}\sim n_0U_0$. Hence $q_c\sim\frac{\sqrt{2mn_0U_0}}{\hbar}=\xi^{-1}$. This implies that excitations with length scales larger than the healing length are collective excitations while those smaller than ξ behave like free particles.
- Different from the roton part of the superfluid ^{4}He excitation.

Excitation for attractive interaction

- Notice the sound speed $s = \sqrt{n_0 U_0/m}$ becomes purely imaginary for attractive interaction. This implies instability.
- Condensate with attractive interaction stabilizes by balancing the attractive interaction with kinetic energy.
- The lowest wavenumber for the excitation in an attractive condensate is determined from $\frac{\hbar^2 q_c^2}{2m} + 2n_0U_0 = 0$. Therefore $q_c = \frac{\sqrt{4mn_0|U_0|}}{\hbar} = \sqrt{16\pi n_0 |a|} = \sqrt{2}\xi^{-1}$.
- Excitations in an attractive condensate with length scales larger than the order of the healing length is unstable.
- Consider a trapped cloud of condensate with radius R. The lowest wavenumber of a mode is $\sim 1/R$, while the density is on the order of N/R^3. Therefore, the maximum particle number in the trap before the cloud becomes unstable and collapses is $N_c \sim R/|a|$.

Microscopic Theory of BEC

Hamiltonian in second quantized form

$$\hat{H} = \int d^3\mathbf{r} \hat{\Psi}^\dagger(\mathbf{r}) \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r}) + \frac{U_0}{2}\hat{\Psi}^\dagger(\mathbf{r})\hat{\Psi}(\mathbf{r}) \right] \hat{\Psi}(\mathbf{r})$$

- Two-body interaction kicks atom out of the condensate (quantum depletion)
- We now explicitly consider fluctuations around the mean field,

$$\hat{\Psi}(\mathbf{r}) = \psi(\mathbf{r}) + \delta\hat{\Psi}(\mathbf{r})$$

- We will start with uniform gas at zero temperature, in which case we can take the Fourier transform of the field operator $\hat{a}_\mathbf{k} = \frac{1}{\sqrt{V}} \int d^3\mathbf{r} \hat{\Psi}(\mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{r}}$
- We will then discuss situations with general external potential and at finite temperature, respectively

For a uniform gas the Hamiltonian in momentum space becomes

$$\hat{H} = \sum_\mathbf{k} \frac{\hbar^2 k^2}{2m} \hat{a}^\dagger_\mathbf{k} a_\mathbf{k} + \frac{U_0}{2V} \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} \hat{a}^\dagger_{\mathbf{k}+\mathbf{q}} \hat{a}^\dagger_{\mathbf{k}'-\mathbf{q}} \hat{a}_{\mathbf{k}'} \hat{a}_\mathbf{k} \,,$$

where creation (annihilation) operators satisfy the bosonic commutation relations.
Suppose the state with $k = 0$ is the only macroscopically occupied state, as

$$\hat{a}^\dagger_0 \hat{a}_0 |N_0\rangle = N_0 |N_0\rangle \,, \qquad \hat{a}_0 \hat{a}^\dagger_0 |N_0\rangle = (N_0+1)|N_0\rangle \,,$$

we may consider $\left[\hat{a}_0, \hat{a}^\dagger_0\right] \approx 0$, and take them to be complex numbers. In fact, setting the global phase to be zero, we may take $\hat{a}_0$ and $\hat{a}^\dagger_0$ to be $\sqrt{N_0}$, which is equivalent to taking $\langle \hat{\Psi} \rangle \approx \sqrt{\frac{N_0}{V}}$ in the Bogoliubov approximation.

Keeping terms up to quadratic order in $\hat{a}_\mathbf{k}$ and $\hat{a}^\dagger_\mathbf{k}$ ($\mathbf{k} \neq 0$), the interaction can either have two or four a_0 ($a^\dagger_0$).

- All operators in the interaction term have zero momentum, i.e. $k = k' = q = 0$, we have $\frac{N_0^2 U_0}{2V}$
- Only two operators have zero momentum:
  - $k = q = 0$, $k' \neq 0$, we have $\frac{N_0U_0}{2V} \sum_{\mathbf{k}' \neq 0} \hat{a}^\dagger_{\mathbf{k}'} a_{\mathbf{k}'}$
  - $k' = q = 0$, $k \neq 0$, we have $\frac{N_0U_0}{2V} \sum_{\mathbf{k} \neq 0} \hat{a}^\dagger_{\mathbf{k}} a_{\mathbf{k}}$
  - $\mathbf{k} = -\mathbf{q} \neq 0$, $k' = 0$, we have $\frac{N_0U_0}{2V} \sum_{\mathbf{k} \neq 0} \hat{a}^\dagger_{\mathbf{k}} a_{\mathbf{k}}$
  - $\mathbf{k}' = \mathbf{q} \neq 0$, $k = 0$, we have $\frac{N_0U_0}{2V} \sum_{\mathbf{k}' \neq 0} \hat{a}^\dagger_{\mathbf{k}'} a_{\mathbf{k}'}$
  - $\mathbf{k} = -\mathbf{q} = -\mathbf{k}' \neq 0$, we have $\frac{N_0U_0}{2V} \sum_{\mathbf{k} \neq 0} \hat{a}_{-\mathbf{k}} a_{\mathbf{k}}$
  - $\mathbf{q} \neq 0$, $k = k' = 0$, we have $\frac{N_0U_0}{2V} \sum_{\mathbf{q} \neq 0} \hat{a}^\dagger_{\mathbf{q}} a^\dagger_{-\mathbf{q}}$

The effecitive Hamiltonian

$$\hat{H} = \frac{N_0^2 U_0}{2V} + \sum_{\mathbf{k}\neq 0} (\epsilon_0 + 2n_0U_0) \hat{a}^\dagger_\mathbf{k} \hat{a}_\mathbf{k} + \frac{n_0U_0}{2} \sum_{\mathbf{k}\neq 0} (\hat{a}^\dagger_\mathbf{k} \hat{a}^\dagger_{-\mathbf{k}} + \hat{a}_\mathbf{k} \hat{a}_{-\mathbf{k}}) \,,$$

where $n_0 = N_0/V$, $\epsilon_0 = \hbar^2 k^2/2m$. Note the term $\epsilon_0 + 2n_0U_0$ describes the Hartee-Fock mean field.
We introduce the chemical potential μ to fix total particle number

$$\begin{aligned}\hat{H} - \mu\hat{N} = \hat{H} - \mu \left(N_0 + \sum_{\mathbf{k}\neq 0} \hat{a}^\dagger_\mathbf{k} \hat{a}_\mathbf{k} \right) &:= \mathcal{K} \\ = \frac{N_0^2 U_0}{2V} - \frac{N_0^2 U_0}{V} & \\ + \sum_{\mathbf{k}\neq 0} \left[(\epsilon_0 + 2n_0U_0 - n_0U_0) \hat{a}^\dagger_\mathbf{k} \hat{a}_\mathbf{k} + \frac{n_0U_0}{2} (\hat{a}^\dagger_\mathbf{k} \hat{a}^\dagger_{-\mathbf{k}} + \hat{a}_\mathbf{k} \hat{a}_{-\mathbf{k}}) \right] \,, &\end{aligned}$$

where we have taken $\mu = n_0 U_0$.

Assuming $N \approx N_0$, the Hamiltonian can be written as

$$\mathcal{K} = -\frac{N^2 U_0}{2V} + \sum_{\mathbf{k}\neq 0} \left[(\epsilon_0 + n_0U_0) \hat{a}^\dagger_\mathbf{k} \hat{a}_\mathbf{k} + \frac{n_0U_0}{2} (\hat{a}^\dagger_\mathbf{k} \hat{a}^\dagger_{-\mathbf{k}} + \hat{a}_\mathbf{k} \hat{a}_{-\mathbf{k}}) \right] \,,$$

The task is to diagonalize the Hamiltonian. Note that after the expansion and by neglecting higher order terms, the remaining Hamiltonian is quadratic in the creation/annihilation operators, and therefore can be diagonlaized analytically.
The Bogoliubov transformation

- Introduce a new set of creation/annihilation operators via canonical transformation, with the new operators satisfying the bosonic commutation relations
- Solve for the transformation cofficients by requiring that the Hamiltonian be diagonal in the new creation/annihilation operators
- One may then read out ground state energy and excitaiton spectrum from the diagonalized Hamiltonian

Bogoliubov transformation

$$\begin{aligned}\hat{a}_\mathbf{k} &= u_k \hat{\alpha}_\mathbf{k} - v_k \hat{\alpha}^\dagger_{-\mathbf{k}} \\ \hat{a}_{-\mathbf{k}} &= u_k \hat{\alpha}_{-\mathbf{k}} - v_k \hat{\alpha}^\dagger_\mathbf{k}\end{aligned}$$

Reverse transformation

$$\hat{\alpha}^\dagger_\mathbf{k} = \frac{u_k}{|u_k|^2 - |v_k|^2} \hat{a}^\dagger_\mathbf{k} + \frac{v_k^*}{|u_k|^2 - |v_k|^2} \hat{a}_{-\mathbf{k}}$$

- The coefficients are independent of the direction of $\mathbf{k}$
- For $\hat{\alpha}_\mathbf{k}$ ($\hat{\alpha}^\dagger_\mathbf{k}$) to satisfy the bosonic commutation relation, we need $|u_k|^2 - |v_k|^2 = 1$

Now we perform the transformation on the effective quadratic Hamiltonian

$$\begin{aligned}\mathcal{K} = &-\frac{N^2 U_0}{2V} + \sum_{\mathbf{k}\neq 0} \xi_k \left(u_k^* \hat{\alpha}^\dagger_\mathbf{k} - v_k^* \hat{\alpha}_{-\mathbf{k}} \right) \left(u_k \hat{\alpha}_\mathbf{k} - v_k \hat{\alpha}^\dagger_{-\mathbf{k}} \right) \\ &+ \frac{n_0U_0}{2} \sum_{\mathbf{k}\neq 0} \left(u_k^* \hat{\alpha}^\dagger_\mathbf{k} - v_k^* \hat{\alpha}_{-\mathbf{k}} \right) \left(u_k^* \hat{\alpha}^\dagger_{-\mathbf{k}} - v_k^* \hat{\alpha}_\mathbf{k} \right) \\ &+ \frac{n_0U_0}{2} \sum_{\mathbf{k}\neq 0} \left(u_k \hat{\alpha}_\mathbf{k} - v_k \hat{\alpha}^\dagger_{-\mathbf{k}} \right) \left(u_k \hat{\alpha}_{-\mathbf{k}} - v_k \hat{\alpha}^\dagger_\mathbf{k} \right) \\ &= \sum_{\mathbf{k}\neq 0} \left\{ \xi_k (|u_k|^2 + |v_k|^2) - n_0U_0 (v_k^* u_k^* + v_k u_k) \right\} \hat{\alpha}^\dagger_\mathbf{k} \hat{\alpha}_\mathbf{k} \\ &+ \sum_{\mathbf{k}\neq 0} \left\{ -\xi_k u_k^* v_k + \frac{n_0U_0}{2} \left[(u_k^*)^2 + v_k^2 \right] \right\} \hat{\alpha}^\dagger_\mathbf{k} \hat{\alpha}^\dagger_{-\mathbf{k}} \\ &+ \sum_{\mathbf{k}\neq 0} \left\{ -\xi_k u_k v_k^* + \frac{n_0U_0}{2} \left[(v_k^*)^2 + u_k^2 \right] \right\} \hat{\alpha}_\mathbf{k} \hat{\alpha}_{-\mathbf{k}} \\ &- \frac{N^2 U_0}{2V} - \sum_{\mathbf{k}\neq 0} \left\{ \xi_k |v_k|^2 - \frac{n_0U_0}{v}{}^*_k u_k^* - \frac{n_0U_0}{2} u_k v_k \right\}\end{aligned}$$

with $\xi_k = \epsilon_0 + n_0 U_0$

Therefore,

$$
\begin{aligned}
&-\xi_k u_k^* v_k + \frac{n_0 U_0}{2}(u_k^*)^2 + \frac{n_0 U_0}{2} v_k^2 = 0 \\
&-\xi_k u_k v_k^* + \frac{n_0 U_0}{2}(u_k)^2 + \frac{n_0 U_0}{2}(v_k^*)^2 = 0 \\
&|u_k|^2 - |v_k|^2 = 1
\end{aligned}
$$

Since only the relative sign between u_k and v_k is relevant, we may assume v_k to be real. u_k is then given

$$
u_k = \frac{\xi_k \pm \sqrt{\xi_k^2 - n_0^2 U_0^2}}{n_0 U_0} v_k
$$

As $\xi_k^2 - n_0^2 U_0^2 \geq 0$, u_k must be real too. It is then straightforward to solve for u_k and v_k.

Thus we have

$$
\mathcal{K} = -\frac{N^2 U_0}{2V} + \sum_{\mathbf{k}\neq 0} \epsilon_k \hat{\alpha}_{\mathbf{k}}^\dagger \hat{\alpha}_{\mathbf{k}} - \frac{1}{2}\sum_{\mathbf{k}\neq 0}(\epsilon_0 + n_0 U_0 - \epsilon_k),
$$

with the excitation spectrum $\epsilon_k = \sqrt{2n_0 U_0 \epsilon_0 + \epsilon_0^2}$, and ground state energy $-\frac{N^2 U_0}{2V} - \frac{1}{2}\sum_{\mathbf{k}\neq 0}(\epsilon_0 + n_0 U_0 - \epsilon_k)$. The transformation coefficients are given as

$$
\begin{aligned}
|u_k|^2 &= \frac{1}{2}\left(\frac{\xi_k}{\epsilon_k} + 1\right) \\
|v_k|^2 &= \frac{1}{2}\left(\frac{\xi_k}{\epsilon_k} - 1\right)
\end{aligned}
$$

with $\xi_k = \epsilon_0 + n_0 U_0$.

- Ground state is the vacuum state for $\hat{\alpha}_{\mathbf{k}}$ ($\hat{\alpha}_{\mathbf{k}}^\dagger$)operators
- Excitations above this ground state are gapless collective motion

The total particle operator

$$
\begin{aligned}
\hat{N} &= N_0 + \sum_{\mathbf{k}\neq 0} \hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}} \\
&= N_0 + \sum_{\mathbf{k}\neq 0} |v_k|^2 + \sum_{\mathbf{k}\neq 0}(|u_k|^2 + |v_k|^2)\hat{\alpha}_{\mathbf{k}}^\dagger \hat{\alpha}_{\mathbf{k}} \\
&- \sum_{\mathbf{k}\neq 0} u_k v_k \left(\hat{\alpha}_{\mathbf{k}}^\dagger \hat{\alpha}_{-\mathbf{k}}^\dagger + \hat{\alpha}_{-\mathbf{k}}\hat{\alpha}_{\mathbf{k}}\right)
\end{aligned}
$$

At zero temperature (in the ground state),

$$
\begin{aligned}
n_{\text{ex}} &= \frac{1}{V}\sum_{\mathbf{k}\neq 0}|v_k|^2 = \frac{1}{(2\pi)^3}\int d^3\mathbf{k}\frac{1}{2}\left(\frac{\xi_k}{\epsilon_k} - 1\right) \\
&= \frac{1}{4\pi^2}\left(\frac{2mn_0U_0}{\hbar^2}\right)^{\frac{3}{2}}\int_0^\infty t^2 dt \frac{t^2 + 1 - \sqrt{(t^2+1)^2 - 1}}{\sqrt{(t^2+1)^2 - 1}} \\
&= \frac{1}{3\pi^2}\left(\frac{m}{\hbar}\sqrt{\frac{n_0 U_0}{m}}\right)^3
\end{aligned}
$$

We find that n_{ex} characterizes the quantum depletion of the condensate at zero temperature due to interaction. As $U_0 = \frac{4\pi\hbar^2 a_s}{m}$,

$$
\frac{n_{\text{ex}}}{n_0} = \frac{8}{3\sqrt{\pi}}(n_0 a_s^3)^{\frac{1}{2}}
$$

For $n_0 a_s^3 \ll 1$, quantum depletion is small and we may replace n_0 with n in the expression above:

$$
\frac{n_{\text{ex}}}{n} \approx \frac{8}{3\sqrt{\pi}}(n a_s^3)^{\frac{1}{2}}
$$

This is the case for most of the experiments. Therefore the quantum depletion is small so long as the scattering length is much smaller than the inter-particle separation.

Ground state energy ($\langle H\rangle$)

$$
E_g = \frac{N^2 U_0}{2V} - \frac{1}{2}\sum_{\mathbf{k}\neq 0}(\epsilon_0 + n_0 U_0 - \epsilon_k)
$$

- For large k, $\xi_k - \sqrt{\xi_k^2 - n_0^2 U_0^2} \sim n_0^2 U_0^2/(2\xi_k) \sim 1/k^2$, therefore, the summation/intergral diverges
- The contact interaction we adopted is constant in momentum space, which is unphysical at large momenta
- To fix this, we need to introduce an effective interaction instead of the bare contact interaction

Recall the renormalization relation

$$
\begin{aligned}
\frac{1}{U_0} &= \frac{1}{U_p} - \frac{1}{\mathcal{V}}\sum_{\boldsymbol{k}}\frac{1}{2\epsilon_0} \quad \Rightarrow \\
U_0 &= U_p + \frac{U_p U_0}{V}\sum_{\boldsymbol{k}}\frac{1}{2\epsilon_0},
\end{aligned}
$$

where $U_p = 4\pi\hbar^2 a_s/m$. Retaining second-order in U_p

$$
U_0 = U_p + \frac{U_p^2}{V}\sum_{\boldsymbol{k}}\frac{1}{2\epsilon_0}
$$

We subsequently derive the ground-state energy accurate to the second order in U_p.

Explicitly, the ground state energy is

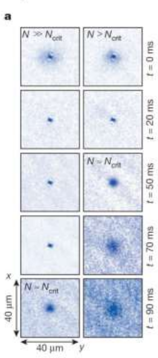
$$
\begin{aligned}
E_g &= \frac{N^2 U_0}{2V} - \frac{1}{2}\sum_{\boldsymbol{k}}(\epsilon_0 + n_0 U_0 - \epsilon_k) \\
&\approx \frac{N^2 U_p}{2V} - \frac{1}{2}\sum_{\boldsymbol{k}}\left[\frac{(nU_p)^2}{\epsilon_0 + nU_p + \epsilon_k} - \frac{(nU_p)^2}{2\epsilon_0}\right],
\end{aligned}
$$

where we used $n_0 \approx n$. It follows

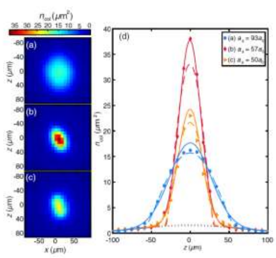
$$
\frac{E_g}{V} \approx \frac{n^2 U_p}{2}\left[1 + \frac{128}{15\pi^{\frac{1}{2}}}(na_s^3)^{\frac{1}{2}}\right]
$$

T.D. Lee and C.N. Yang, Phys. Rev. 105, 1119 (1957)

Impact of LHY–Quantum Droplet



^{164}Dy (2016)

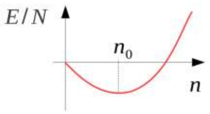


^{166}Er (2016)

Question:

- Beyond mean field!
- Few-body or many-body effect?

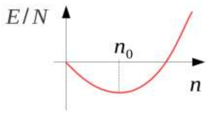
Possible explanations



$$\frac{E}{N} \sim g_2 n + g_{\alpha+1} n^{\alpha}$$

- Three-body effects: $\alpha = 2$ (Bulgac 2002; Petrov 2014)
- LHY $\alpha = 3/2$: (Petrov 2015)

Possible explanations



$$\frac{E}{N} \sim g_2 n + g_{\alpha+1} n^{\alpha}$$

Important for small N

$$E = E_{kin} + E_{MF} + E_{LHY}$$

$$\frac{g_{11} n_1^2 + g_{22} n_2^2 + 2 g_{12} n_1 n_2}{2} \qquad \frac{8}{15\pi^2} m_1^{3/2} (g_{11} n_1)^{5/2} f\left(\frac{m_2}{m_1}, \frac{g_{12}^2}{g_{11} g_{22}}, \frac{g_{22} n_2}{g_{11} n_1}\right)$$

$\delta g = g_{12} + \sqrt{g_{11} g_{22}} < 0$

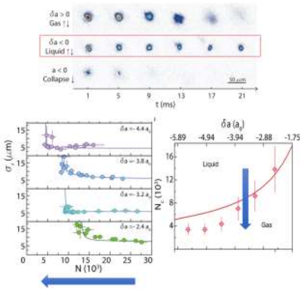
$\frac{n_2}{n_1} \sim \sqrt{g_{11}/g_{22}}$

$$\sim \delta g\, n^2 < 0 \qquad \sim g\, n^{5/2} > 0$$

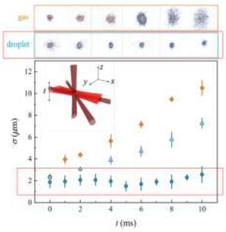
- Three-body effects: $\alpha = 2$ (Bulgac 2002; Petrov 2014)
- LHY $\alpha = 3/2$: (Petrov 2015)
- Should work for a two-component BEC in the mean-field unstable regime

D. Petrov, Phys. Rev. Lett. 115, 155302 (2015)

Experimental confirmation



Barcelona (Science 2018)



Florence (PRL 2018)

^{39}K, ^{41}K–^{87}Rb, ^{23}Na–^{87}Rb

An early study

THE
PHYSICAL REVIEW
A journal of experimental and theoretical physics established by E. L. Nichols in 1893
SECOND SERIES, VOL. 115, NO. 4 AUGUST 15, 1959

Energy Levels of a Bose-Einstein System of Particles with Attractive Interactions*

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(Received March 17, 1959)

An N-body Bose-Einstein system of particles with long-range attraction and hard-sphere repulsion between particles is considered. It is shown that if the constants of the interaction have values within a certain range it is possible to calculate the ground-state energy of the system as a function of Ω/N, where Ω is the volume of the box containing the system, in the limit $N \to \infty$, $\Omega \to \infty$, with $N/\Omega = \rho$ fixed. The results show that the system can possess an N-body bound state, which has an equilibrium density and negative energy, and that the interactions can be saturating. Excited states are also considered. It is shown that low-lying excitations consist purely of phonons, whose velocity agrees with that computed from the macroscopic compressibility, furnished by the ground-state energy. The formula for the general excited energy levels suggests that thermodynamically the system may have a "gas" phase and two "liquid" phases, the transition between the two "liquid" phases being the analog of the Bose-Einstein condensation of the ideal gas. Thermodynamic considerations are, however, not contained in this paper.

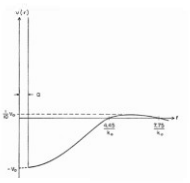
N-body bound state in 1959

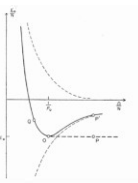
- Long-range attraction and hard-core repulsion

$$V(r) = 8\pi a \delta(r) \frac{\partial}{\partial r} r + w(r)$$

- Energy per particle

$$\frac{E}{N} = -4\pi b n + 4\pi a n \frac{128}{15} \left(\frac{n a^3}{\pi}\right)^{\frac{1}{2}}$$





Fluctuations in a Trapped Gas

With an external trap, k is no longer a good quantum number. We therefore return to the original Bogoliubov expansion in the real space

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

With Hamiltonian

$$\hat{H} - \mu\hat{N} = \int d^3\mathbf{r} \hat{\Psi}^\dagger(\mathbf{r}) \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r}) - \mu + \frac{U_0}{2}\hat{\Psi}^\dagger(\mathbf{r})\hat{\Psi}(\mathbf{r})\right] \hat{\Psi}(\mathbf{r})$$

- The idea is to substitute the field operator with this expansion in the Hamiltonian and arrange together terms that are first (second) order in $\delta\hat{\Psi}$
- Zeroth order term should be the mean field Hamiltonian
- The coefficient of the first order in $\delta\hat{\Psi}$ should vanish if the $\psi(\mathbf{r})$ satisfies GPE
- Second order terms give the fluctuations around the mean field

Second order Hamiltonian

$$\begin{aligned}\hat{K}^{(2)} &= (\hat{H} - \mu\hat{N})^{(2)} \\ &= \int d^3\mathbf{r} \{-\delta\hat{\Psi}^\dagger \frac{\hbar^2}{2m}\nabla^2\delta\hat{\Psi} + \left[V(\mathbf{r}) + 2U_0|\psi|^2 - \mu\right]\delta\hat{\Psi}^\dagger\delta\hat{\Psi} \\ &+ \frac{U_0}{2}\left[\psi^2\left(\delta\hat{\Psi}^\dagger\right)^2 + (\psi^*)^2\left(\delta\hat{\Psi}\right)^2\right]\}\end{aligned}$$

Heisenberg equations of motion

$$i\hbar\frac{\partial\delta\hat{\Psi}}{\partial t} = [\delta\hat{\Psi}, \hat{K}^{(2)}]$$

$$i\hbar\frac{\partial\delta\hat{\Psi}^\dagger}{\partial t} = [\delta\hat{\Psi}^\dagger, \hat{K}^{(2)}]$$

Note the fluctuations satisfy the bosonic commutation relation. In particular,

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

We then have the coupled equations

$$i\hbar\frac{\partial\delta\hat{\Psi}}{\partial t} = \left(-\frac{\hbar^2}{2m}\nabla^2 + V + 2n_0U_0 - \mu\right)\delta\hat{\Psi} + U_0\psi^2\delta\hat{\Psi}^\dagger$$

$$-i\hbar\frac{\partial\delta\hat{\Psi}^\dagger}{\partial t} = \left(-\frac{\hbar^2}{2m}\nabla^2 + V + 2n_0U_0 - \mu\right)\delta\hat{\Psi}^\dagger + U_0(\psi^*)^2\delta\hat{\Psi}$$

Apply the transformation

$$\delta\hat{\Psi} = \sum_i \left[u_i(\mathbf{r})\hat{\alpha}_i e^{-i\epsilon_i t/\hbar} - v_i^*(\mathbf{r})\hat{\alpha}_i^\dagger e^{i\epsilon_i t/\hbar}\right]$$

$\hat{\alpha}_i^\dagger$ ($\hat{\alpha}_i$) are the creation (annihilation) operators for the ith state in the expansion.

Bogoliubov-de Gennes equation (BdG)

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r}) + 2n_0(\mathbf{r})U_0 - \mu - \epsilon_i\right] u_i(\mathbf{r}) - n_0(\mathbf{r})U_0 v_i(\mathbf{r}) = 0$$
$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r}) + 2n_0(\mathbf{r})U_0 - \mu + \epsilon_i\right] v_i(\mathbf{r}) - n_0(\mathbf{r})U_0 u_i(\mathbf{r}) = 0$$

- Orthogonality of different eigenstates
$$\int d^3\mathbf{r}\left(u_i u_j^* - v_i v_j^*\right) = 0$$
- Canonical transformation condition (commutation relation conserving)
$$\int d^3\mathbf{r}\left(|u_i|^2 - |v_i|^2\right) = 1$$
- $\hat{K}^{(2)}$ is diagonalized by the transformation in the sense that $\hat{K}^{(2)} = \sum_i \epsilon_i \hat{\alpha}_i^\dagger \hat{\alpha}_i +$ constant, where ϵ_i is the excitation spectrum.

Simple example of BdG for uniform gas

- For a uniform condensate, n_0 is a constant
- As k is good quantum number, we may perform the expansion in momentum space, i.e. $u_i(\mathbf{r}) = u_k e^{-i\mathbf{k}\cdot\mathbf{r}}$ and $v_i(\mathbf{r}) = v_k e^{-i\mathbf{k}\cdot\mathbf{r}}$

The BdG equation becomes ($\mu = n_0 U_0$)

$$\left[\frac{\hbar^2 k^2}{2m} + 2n_0U_0 - \mu - \epsilon_k\right] u_k - n_0U_0 v_k = 0$$
$$\left[\frac{\hbar^2 k^2}{2m} + 2n_0U_0 - \mu + \epsilon_k\right] v_k - n_0U_0 u_k = 0$$

In matrix form

$$\begin{pmatrix} \frac{\hbar^2k^2}{2m} + n_0U_0 - \epsilon_k & -n_0U_0 \\ -n_0U_0 & \frac{\hbar^2k^2}{2m} + n_0U_0 + \epsilon_k \end{pmatrix}\begin{pmatrix} u_k \\ v_k \end{pmatrix} = 0$$

Determinant of the coefficient matrix should be zero

$$(\epsilon_0 + n_0U_0 - \epsilon_k)(\epsilon_0 + n_0U_0 + \epsilon_k) = n_0^2U_0^2$$

We then recover the Bogoliubov dispersion relation

$$\epsilon_k = \sqrt{\epsilon_0(\epsilon_0 + 2n_0U_0)}$$

- For general trapping potential, it is convenient to expand onto the eigen-basis of $-\frac{\hbar^2}{2m}\nabla^2 + V$
- In that case, one needs to make a cutoff in the expansion at a high energy eigenstate, and diagonalize the coefficient matrix in the subspace, often numerically
- Note that in general there will be off-diagonal matrix elements

Finite Temperature Theories

- At finite temperatures, in addition to the quantum depletion, there will be thermal depletion of the condensate
- We wish to introduce a simple treatment at finite temperature based on Bogoliubov mean field description in free space
- Post-Bogoliubov-transformation effective Hamiltonian
$$\mathcal{K} = -\frac{N^2U_0}{2V} + \sum_{\mathbf{k}\neq 0}\epsilon_k \hat{\alpha}_\mathbf{k}^\dagger \hat{\alpha}_\mathbf{k} - \frac{1}{2}\sum_{\mathbf{k}\neq 0}(\epsilon_0 + n_0U_0 - \epsilon_k)\,,$$
with the excitation spectrum $\epsilon_k = \sqrt{2n_0U_0\epsilon_0 + \epsilon_0^2}$.
- It describes quasi-particle excitations with the given dispersion relation above the ground state.

The total particle operator

$$\begin{aligned}\hat{N} &= N_0 + \sum_{\mathbf{k}\neq 0}\hat{a}_\mathbf{k}^\dagger \hat{a}_\mathbf{k} \\ &= N_0 + \sum_{\mathbf{k}\neq 0}|v_k|^2 + \sum_{\mathbf{k}\neq 0}(|u_k|^2 + |v_k|^2)\hat{\alpha}_\mathbf{k}^\dagger \hat{\alpha}_\mathbf{k} \\ &\quad - \sum_{\mathbf{k}\neq 0} u_k v_k\left(\hat{\alpha}_\mathbf{k}^\dagger \hat{\alpha}_{-\mathbf{k}}^\dagger + \hat{\alpha}_{-\mathbf{k}}\hat{\alpha}_\mathbf{k}\right)\end{aligned}$$

At finite temperature, on the mean field level, we may assume

- $\left\langle \hat{\alpha}_\mathbf{k}^\dagger \hat{\alpha}_{-\mathbf{k}}^\dagger \right\rangle = \langle \hat{\alpha}_{-\mathbf{k}}\hat{\alpha}_\mathbf{k}\rangle = 0$
- $\left\langle \hat{\alpha}_\mathbf{k}^\dagger \hat{\alpha}_\mathbf{k} \right\rangle = f(\epsilon_k)$, where $f(x) = \frac{1}{e^{\beta x}-1}$ is the Bose distribution function
- Non-interacting quasi-particles: $f(\epsilon_k)$ rather than $f(\epsilon_k - \mu_{\rm qp})$

Therefore

$$\begin{aligned}N &= N_0 + \sum_{\mathbf{k}\neq 0}|v_k|^2 + \sum_{\mathbf{k}\neq 0}\left(|u_k|^2 + |v_k|^2\right) f(\epsilon_k) \\ &= N_0 + \sum_{\mathbf{k}\neq 0}\left(\frac{\epsilon_0 + n_0U_0}{\epsilon_k}\frac{1}{e^{\epsilon_k}-1} + \frac{\epsilon_0 + n_0U_0 - \epsilon_k}{2\epsilon_k}\right)\end{aligned}$$

- This description works at low temperature when the quasi-particle density is low such that their interactions can be neglected
- To include these contributions, one can invoke the Hartree-Fock-Bogoliubov approximation
  - Consider the case of excitations with large momenta, so that $\epsilon_k \approx \epsilon_0 + n_0U_0$
  - The corresponding number equation
$$N = N_0 + \sum_{\mathbf{k}\neq 0}\frac{1}{e^{\beta(\epsilon_0 + n_0U_0)} - 1}$$

- Recall the effective Hamiltonian
$$\hat{H} = \frac{N_0^2U_0}{2V} + \sum_{\mathbf{k}\neq 0}(\epsilon_0 + 2n_0U_0)\hat{a}_\mathbf{k}^\dagger \hat{a}_\mathbf{k} + \frac{n_0U_0}{2}\sum_{\mathbf{k}\neq 0}(\hat{a}_\mathbf{k}^\dagger \hat{a}_{-\mathbf{k}}^\dagger + \hat{a}_\mathbf{k}\hat{a}_{-\mathbf{k}})\,,$$
- In addition to the above, HFB takes into account of the Hartree-Fock mean fields of the excited states, i.e. keeping terms like $\sum_{\mathbf{k}\neq 0}\langle \hat{a}_\mathbf{k}^\dagger \hat{a}_\mathbf{k}\rangle\langle \hat{a}_{\mathbf{k}'}^\dagger \hat{a}_{\mathbf{k}'}\rangle$
- Also, for HFB, one neglects anomalous pairing terms $\hat{a}_\mathbf{k}^\dagger \hat{a}_{-\mathbf{k}}^\dagger$ and $\hat{a}_\mathbf{k}\hat{a}_{-\mathbf{k}}$
- This gives
$$\hat{H} = \frac{N_0^2U_0}{2V} + \sum_{\mathbf{k}\neq 0}(\epsilon_0 + 2nU_0)\hat{a}_\mathbf{k}^\dagger \hat{a}_\mathbf{k} - \frac{U_0}{V}\sum_{\mathbf{k},\mathbf{k}'\neq 0} f(\epsilon_k)f(\epsilon_{k'})$$
- Self-consistent condensate chemical potential $\mu = (\epsilon_0 + 2nU_0) - (\epsilon_0 + n_0U_0) = (2n - n_0)U_0$

- Dispersion of the excitations, $\epsilon_0 + 2nU_0$, i.e. $2nU_0$ as $\mathbf{k}\to 0$
- This is due to the incorrect assumptions at small momenta
- Need both quasi-particles and Hartree-Fock mean field of excited states for more consistent finite temperature theory

Popov approximation (HFBP)

$$\begin{aligned}\hat{H} &= \frac{N_0^2U_0}{2V} + \sum_{\mathbf{k}\neq 0}(\epsilon_0 + 2nU_0)\hat{a}_\mathbf{k}^\dagger \hat{a}_\mathbf{k} + \frac{n_0U_0}{2}\sum_{\mathbf{k}\neq 0}(\hat{a}_\mathbf{k}^\dagger \hat{a}_{-\mathbf{k}}^\dagger + \hat{a}_\mathbf{k}\hat{a}_{-\mathbf{k}}) \\ &\quad - \frac{U_0}{V}\sum_{\mathbf{k},\mathbf{k}'\neq 0} f(\epsilon_k)f(\epsilon_{k'})\,,\end{aligned}$$

with the chemical potential $\mu = (2n - n_0)U_0$.

Consider a system with fixed particle number

$$\hat{H} - \mu\hat{N} = -\frac{N_0^2 U_0}{2V} - \frac{2N_0 N_{ex} U_0}{V} - \frac{N_{ex}^2 U_0}{V} + \sum_{\mathbf{k}\neq 0}\left[(\epsilon_0 + n_0 U_0)\,\hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}} + \frac{n_0 U_0}{2}\left(\hat{a}_{\mathbf{k}}^\dagger \hat{a}_{-\mathbf{k}}^\dagger + \hat{a}_{\mathbf{k}}\hat{a}_{-\mathbf{k}}\right)\right],$$

with $N_{ex} = \sum_{\mathbf{k}\neq 0}\left\langle \hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}}\right\rangle$.

- Same quadratic form as the Hamiltonian in the Bogoliubov theory, except for the zeroth order terms.
- Low energy dispersion is gapless, similar to the Bogoliubov phonons.
- Chemical potential, ground state energy and eventually the condensate fraction are affected by the Hartree-Fock mean field of the excited states.
- The condensate density is solved self-consistently.

General recipe

- Start with the Hamiltonian

$$\hat{H} - \mu\hat{N} = \sum_{\mathbf{k}}(E_k - \mu)\hat{a}_{\mathbf{k}}^\dagger a_{\mathbf{k}} + \frac{U_0}{2V}\sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} \hat{a}_{\mathbf{k}+\mathbf{q}}^\dagger \hat{a}_{\mathbf{k}'-\mathbf{q}}^\dagger \hat{a}_{\mathbf{k}'}\hat{a}_{\mathbf{k}}$$

- Make the following expansion around the Bogoliubov mean field

$$\hat{a}_0 = \langle \hat{a}_0\rangle + \hat{\tilde{a}}_0$$

- Expand the Hamiltonian to 1st order in $\{\hat{\tilde{a}}_0, \hat{\tilde{a}}_0^\dagger\}$
- Apply Wick's theorem for bosons

$$\hat{a}^\dagger\hat{a}\hat{a} \approx 2\langle \hat{a}^\dagger\hat{a}\rangle\hat{a} + \langle\hat{a}\hat{a}\rangle\hat{a}^\dagger$$
$$\hat{a}^\dagger\hat{a}^\dagger\hat{a}\hat{a} \approx 4\langle \hat{a}^\dagger\hat{a}\rangle\hat{a}^\dagger\hat{a} + \langle\hat{a}^\dagger\hat{a}^\dagger\rangle\hat{a}\hat{a} + \langle\hat{a}\hat{a}\rangle\hat{a}^\dagger\hat{a}^\dagger$$

- Bogoliubov theory: setting $\langle \hat{a}_{\mathbf{k}}^\dagger\hat{a}_{\mathbf{k}}\rangle = 0$, $\langle \hat{a}_{\mathbf{k}}\hat{a}_{-\mathbf{k}}\rangle \neq 0$ (for $\mathbf{k}\neq 0$)
- HFB: setting $\langle \hat{a}_{\mathbf{k}}^\dagger\hat{a}_{\mathbf{k}}\rangle \neq 0$, $\langle \hat{a}_{\mathbf{k}}\hat{a}_{-\mathbf{k}}\rangle = 0$, and neglecting $\hat{a}_{\mathbf{k}}\hat{a}_{-\mathbf{k}}$, $\hat{a}_{-\mathbf{k}}^\dagger\hat{a}_{\mathbf{k}}^\dagger$ (for $\mathbf{k}\neq 0$)
- HFBP: setting $\langle \hat{a}_{\mathbf{k}}^\dagger\hat{a}_{\mathbf{k}}\rangle \neq 0$, $\langle \hat{a}_{\mathbf{k}}\hat{a}_{-\mathbf{k}}\rangle \neq 0$
- Requires the coefficient of $\hat{\tilde{a}}_0$ and $\hat{\tilde{a}}_0^\dagger$ to vanish: chemical potential

$$\mu = n_0 U_0\,, \quad \text{Bogoliubov}$$
$$\mu = 2nU_0 - n_0 U_0\,, \quad \text{HFB, HFBP}$$

- Diagonalize the quadratic effective Hamiltonian, write down expressions for energy and number density

References:

Rev. Mod. Phys. 76, 599 (2004)
Phys. Rev. A 63, 053601 (2001)

Next Lecture

We have discussed the characterization of interacting BEC on the mean field level. As experimentally available dilute gases mostly feature weakly interacting BECs, the models given here may be applied to many experimentally relevant systems. Strongly interacting bosonic systems may be achieved via resonant scattering processes like Feshbach resonance, or by strong confinement like an optical lattice, which we will discuss later. Next, we will examine some exemplary topics in which the mean field description is valid.

Quantum Degenerate Gases

Lecture 7: BEC Topics

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Spring 2022

中国科学技术大学

Contents

Review of condensate velocity

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

Compare with the continuity equation

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

We may define the condensate velocity

$$\mathbf{v} = \frac{\hbar}{2mi}\frac{\psi^*\nabla\psi - \psi\nabla\psi^*}{|\psi|^2}$$

Arrange the condensate wavefunction as

$$\psi(\mathbf{r}) = \sqrt{n(\mathbf{r})}e^{i\varphi(\mathbf{r})}$$

The condensate velocity is then the phase gradient

$$\mathbf{v} = \frac{\hbar}{m}\nabla\varphi(\mathbf{r})$$

- A normal fluid can have either rotational or irrotational flow
- Classically, rotational flow has lower energy
- As $\nabla\times(\nabla\varphi) = 0$, the superfluid flow is irrotational, unless the phase (velocity) field has a singularity

- Following a closed contour, the phase of the wavefunction changes by integer multiples of 2π

$$\Delta\varphi = \oint \nabla\varphi \cdot d\mathbf{l} = 2\pi l\,, \quad \text{where } l \text{ is an integer}$$

Compare with the Stoke's theorem

$$\int_{\mathbf{S}} (\nabla \times \mathbf{v}) \cdot d\mathbf{S} = \oint \mathbf{v} \cdot d\mathbf{l}$$

- Superfluid can therefore carry angular momentum via these singularities, i.e. vortices
- Quantization of circulation

$$\Gamma = \oint \mathbf{v} \cdot d\mathbf{l} = \frac{\hbar}{m} 2\pi l$$

- Near the singularity, or the center of a vortex, the velocity field diverges, whereas density goes to zero

- As a simple example, consider a vortex with purely azimuthal flow that is rotationally invariant around the z-axis.
- The wavefunction should be proportional to $e^{il\varphi}$, where φ is the azimuthal angle.
- The gradient in polar coordinate

$$\nabla = \frac{\partial}{\partial\rho}\mathbf{e}_\rho + \frac{1}{\rho}\frac{\partial}{\partial\varphi}\mathbf{e}_\varphi$$

- Easy to see the velocity is

$$\mathbf{v} = l\frac{\hbar}{m\rho}\mathbf{e}_\varphi$$

- Hence for $l \neq 0$, the velocity field has a singularity at $\rho = 0$, the circulation is $2\pi l \frac{\hbar}{m}$ around the axis
- For $\rho \to \infty$, $|\mathbf{v}| \to 0$

GPE for a Single Vortex

For a single vortex located at the origin, we may write the wavefunction in cylindrical coordinate

$$\psi(\rho, \varphi, z) = f(\rho, z)e^{il\varphi}$$

Substitute the wavefunction into GPE, we have

$$-\frac{\hbar^2}{2m}\left[\frac{1}{\rho}\frac{d}{d\rho}\left(\rho\frac{df}{d\rho}\right) + \frac{d^2 f}{dz^2}\right] + \frac{\hbar^2}{2m\rho^2}l^2 f + V(\rho, z)f + U_0 f^3 = \mu f$$

Note in cylindrical coordinate, $\nabla^2 = \frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial}{\partial\rho}\right) + \frac{1}{\rho^2}\frac{\partial^2}{\partial\varphi^2} + \frac{\partial^2}{\partial z^2}$

- The term $\frac{\hbar^2 l^2}{2m\rho^2} = \frac{1}{2}mv^2$ gives the kinetic energy due to rotation
- f describes the core structure of the vortex

Asymptotic behavior in the absence of trapping potential

- At large distance, the dominant term is the interaction. Therefore

$$f_0 = \sqrt{\frac{\mu}{U_0}}$$

- Close to the axis, $\rho \sim 0$, the equation becomes

$$-\frac{1}{\rho}\frac{d}{d\rho}\left(\rho\frac{df}{d\rho}\right) + \frac{l^2}{\rho^2}f = 0$$

Therefore $f \propto \rho^l$.

- The crossover occurs roughly at $\frac{\hbar^2}{2m\rho^2}l^2 f = U_0 f^3$
- We will focus on the case of $l = 1$ first, for which at small distance, f is linear in ρ, and the crossover occurs at the length scale on order of the healing length ξ

To cast the GPE into dimensionless form, define

$$x = \frac{\rho}{\xi}, \quad \chi = \frac{f}{f_0}, \quad \text{where } \xi = \sqrt{\frac{\hbar^2}{2mU_0 f_0^2}}\,,$$

where f_0 is the asymptotic wavefunction at large distance. The dimensionless GPE in the absence of trap becomes

$$-\frac{1}{x}\frac{d}{dx}\left(x\frac{d\chi}{dx}\right) + \frac{\chi}{x^2} + \chi^3 - \chi = 0$$

One may then solve this equation numerically for the core structure.

GPE in the Rotating Frame

To describe a rotating BEC, it is more convenient to adopt the frame that is co-rotating. Suppose the rotation is about the z-axis with frequency ω. The transformation to the rotating frame is given as

$$x' = \cos(\omega t)x + \sin(\omega t)y$$
$$y' = -\sin(\omega t)x + \cos(\omega t)y$$

- Jacobian determinant of the transformation is unity, spatial derivatives are not changed
- Interaction not affected by change of frame
- Assuming external potential is a function of $\rho = \sqrt{x^2 + y^2}$, i.e. it is not affected either
- Only need to consider the time derivative term

We have

$$i\hbar\frac{\partial}{\partial t}\psi(x, y, z, t) = i\hbar\frac{\partial}{\partial t}\bar{\psi}(x', y', z, t) + i\hbar\left(\frac{\partial\bar{\psi}}{\partial x'}\frac{\partial x'}{\partial t} + \frac{\partial\bar{\psi}}{\partial y'}\frac{\partial y'}{\partial t}\right)$$

From the transformation

$$\frac{\partial x'}{\partial t} = \omega\left[-x\sin(\omega t) + y\cos(\omega t)\right] = \omega y'$$
$$\frac{\partial y'}{\partial t} = \omega\left[-x\cos(\omega t) - y\sin(\omega t)\right] = -\omega x'$$

Therefore

$$i\hbar\frac{\partial}{\partial t}\psi = i\hbar\frac{\partial}{\partial t}\bar{\psi} - i\hbar\omega\left(x'\frac{\partial}{\partial y'} - y'\frac{\partial}{\partial x'}\right)\bar{\psi}$$

The TDGPE then becomes

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}\bar{\psi} &= \left[-\frac{\hbar^2}{2m}\nabla^2 + V + U_0|\bar{\psi}|^2\right]\bar{\psi} + i\hbar\omega\left(x'\frac{\partial}{\partial y'} - y'\frac{\partial}{\partial x'}\right)\bar{\psi} \\ &= \left[-\frac{\hbar^2}{2m}\nabla^2 - \omega L_z + V + U_0|\bar{\psi}|^2\right]\bar{\psi}\,, \end{aligned}$$

where $L_z = -i\hbar\left(x'\frac{\partial}{\partial y'} - y'\frac{\partial}{\partial x'}\right)$. The GPE is therefore

$$\left[-\frac{\hbar^2}{2m}\nabla^2 - \omega L_z + V + U_0|\bar{\psi}|^2\right]\bar{\psi} = \mu\bar{\psi}\,,$$

which is consistent with the result that energies in the rotating frame

$$E' = E - \boldsymbol{\omega} \cdot \mathbf{L}$$

The GPE in the rotating frame can be rearranged into the following form

$$\left\{\frac{(\mathbf{p}'-m\boldsymbol{\omega}\times\mathbf{r}')^2}{2m}+V-\frac{1}{2}m\omega^2\rho'^2+U_0|\bar{\psi}|^2\right\}\bar{\psi}=\mu\bar{\psi}$$

Note $\mathbf{L}=\mathbf{r}\times\mathbf{p}$ and $\boldsymbol{\omega}\cdot(\mathbf{r}'\times\mathbf{p}')=\mathbf{p}'\cdot(\boldsymbol{\omega}\times\mathbf{r}')$.

- A centrifugal term countering the trapping potential
- For a charged particle moving in a magnetic field

$$H=\frac{1}{2m}\left(\mathbf{p}-\frac{e}{c}\mathbf{A}\right)^2,$$

  where $\mathbf{A}$ is the vector potential of the magnetic field $\mathbf{B}=\nabla\times\mathbf{A}$.
- We may identify a pseudo vector potential $\mathbf{A}=\frac{cm}{e}\omega\times\mathbf{r}$, so that rotating cold atoms can be used to simulate physics of charged particles in a magnetic field

As a simple example, let us consider a 3-d harmonic trap in the rotating frame (assuming ideal BEC)

$$\left[-\frac{\hbar^2}{2m}\nabla^2-\Omega\hat{L}_z+\frac{1}{2}m\omega^2r^2\right]\psi=\mu\psi$$

As the eigenfunctions of the 3-d harmonic potential are also eigenfunctions of $\hat{L}_z$, we have

$$\mu=E_{n,l,m}=(2n_r+l+\frac{3}{2})\hbar\omega-m\hbar\Omega$$

- For $\Omega<\omega$, the ground state is $|n_r=0,l=0,m=0\rangle$, $\mu=\frac{3}{2}\hbar\omega$
- For $\Omega>\omega$, the ground state is $|n_r=0,l=1,m=1\rangle$, $\mu=\frac{5}{2}\hbar\omega-\hbar\Omega$
- In the latter case, $\psi\propto e^{i\varphi}$, therefore the condensate velocity

$$\mathbf{v}=\frac{\hbar}{m}\nabla\varphi=\frac{\hbar}{mr\sin\theta}\mathbf{e}_\varphi$$

Critical rotation frequency

- For slow rotating frequencies the energy of the condensate is smaller without vortices, the ground state of the trapped BEC is close to the non-rotating ground state.
- Above a certain critical rotating frequency, the vortex state becomes energetically more favorable, and angular momentum are carried by both vortices and elementary excitations.
- Critical rotation frequency (estimation)

$$\Omega_c=\frac{E_v}{L}=\frac{5}{2}\frac{\hbar}{mR^2}\ln\left(0.671\frac{R}{\xi}\right)$$

- As the cloud becomes bigger or the healing length becomes larger, the critical rotation frequency decreases
- In practice, the critical frequency at which the vortex appears can be quite different from the equation above here

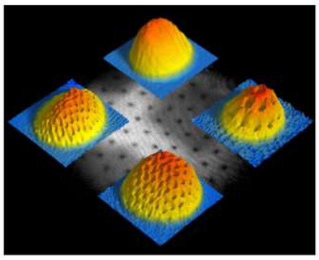
For multi-quantized vortices, the energy of the vortex is

$$E_v=\frac{\pi\hbar^2}{m}n_0\int_0^{R/\xi}xdx\left[\left(\frac{d\chi}{dx}\right)^2+\frac{l^2\rho^2}{x^2}+\frac{1}{2}(1-x^2)^2\right]$$
$$\approx l^2\pi n_0\frac{\hbar^2}{m}\ln\left(\frac{CR}{\xi}\right)$$

- The constant C is determined by the detailed structure of the vortex core
- A vortex with $l>1$ is less stable energetically than a collection of $l=1$ vortices
- One may define the inter-vortex interaction by evaluating this difference in energy. The effective interaction is repulsive.

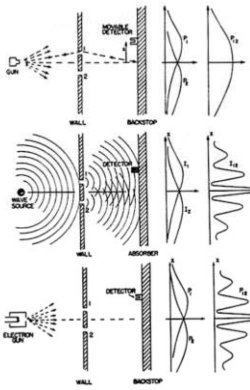
Vortex lattice

- Potentially many configurations of vortices. Eventually, the nature selects the one with the lowest energy
- For homogeneous systems, vortices form a hexgonal lattice (Abrikosov lattice)
- Existence of quantized vortices is direct evidence of superfluidity



Matter Wave Interference

- Superposition principle for waves: the net amplitude at a given point is the algebraic sum of amplitude of all contributing waves
- An important measurable quantity is intensity, square of the amplitude
- Classically, intensity is proportional to energy flow
- Quantum mechanically, it is proportional to probability

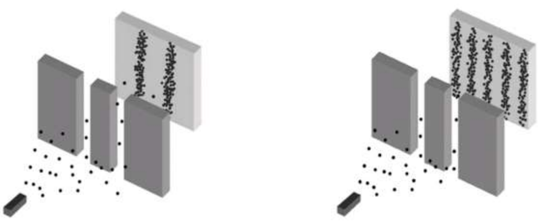


Superposition of states

$$|\psi\rangle\propto|1\rangle+|2\rangle$$

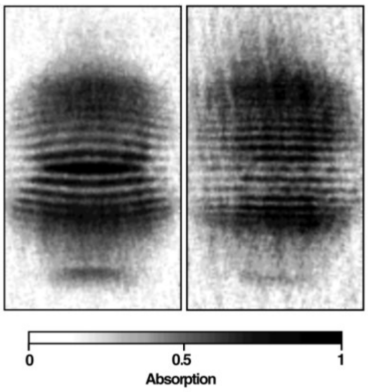
Probability measurement

$$I\propto|\psi|^2=|\langle1|1\rangle|^2+|\langle2|2\rangle|^2+2\mathrm{Re}\left(\langle1|2\rangle\right)$$



- Double-slit experiment for a single particle; measurement theory
  - Interference pattern for large number of single particle event, i.e. interference on a single particle level
  - Interference terms disappear with detectors introduced
  - Single particle source must be phase coherent
  - The matter wave of the particles should have the same wavelength (same velocity for identical particles)
- In a condensate, all atoms are in the same state, we therefore expect strong interference effects for a double-slit setup
- Interference of BEC:
  - Create two BECs' with/without phase coherence
  - Release them from the trap and let them overlap
  - Measure the density distribution

Result from Ketterle's group



Interference between coherent condensates

$$\psi(\mathbf{r},t) = \sqrt{N_1}\psi_1(\mathbf{r},t) + \sqrt{N_2}\psi_2(\mathbf{r},t)$$

The interference effect is given by the density expectation value

$$n(\mathbf{r},t) = |\psi(\mathbf{r},t)|^2 = N_1|\psi_1|^2 + N_2|\psi_2|^2 + 2\sqrt{N_1N_2}\text{Re}\left(\psi_1(\mathbf{r},t)\psi_2(\mathbf{r},t)\right)$$

- Interference effect is given by the $2\sqrt{N_1N_2}\text{Re}\left(\psi_1(\mathbf{r},t)\psi_2(\mathbf{r},t)\right)$ part
- In principle, the time evolution of the density distribution can be solved from the TDGPE.
- As a simplification, one may neglect two-body interactions and solve the problem of free expanding condensates

Starting from condensates with Gaussian distribution and with global phases ϕ_1 and ϕ_2

$$\psi_1 = \frac{e^{i\phi_1}}{(\pi a^2)^{3/4}} \exp\left[-\frac{(\mathbf{r}-\frac{\mathbf{d}}{2})^2}{2a^2}\right]$$
$$\psi_2 = \frac{e^{i\phi_2}}{(\pi a^2)^{3/4}} \exp\left[-\frac{(\mathbf{r}+\frac{\mathbf{d}}{2})^2}{2a^2}\right]$$

Making use of translational symmetry, Fourier transform $\psi = \frac{1}{(\pi a^2)^{3/4}} \exp\left(-\frac{r^2}{2a^2}\right)$ to momentum space and perform the time evolution there

$$\psi(\mathbf{k},t) = \left(\frac{a^2}{\pi}\right)^{3/4} \exp\left[-\frac{a^2k^2}{2}\right] \exp\left[-i\frac{\hbar k^2}{2m}t\right]$$

Fourier transform back to real space

$$\psi(\mathbf{r},t) = \frac{1}{(2\pi)^{3/2}} \int d^3\mathbf{k}\psi(\mathbf{k},t)e^{i\mathbf{r}\cdot\mathbf{k}}$$
$$\propto \prod_{i=x,y,z} \int d^3\mathbf{k} \exp\left[-\left(\frac{a^2}{2} + i\frac{\hbar}{2m}t\right)\left(k_i - \frac{ir_i}{a^2 + i\frac{\hbar}{m}t}\right)^2\right]$$
$$\times \exp\left[-\frac{r_i^2}{2(a^2 + i\frac{\hbar}{m}t)}\right]$$
$$\propto \exp\left[-\frac{r^2}{2a(t)^2}\left(1 - \frac{i\hbar}{ma^2}t\right)\right],$$

where $a(t)^2 = a^2 + \frac{\hbar^2 t^2}{m^2 a^2}$. Therefore the time dependent wavefunctions are

$$\psi_i(\mathbf{r},t) \propto \exp(i\phi_i) \exp\left[-\frac{(\mathbf{r}\mp\frac{\mathbf{d}}{2})^2}{2a(t)^2}\left(1 - \frac{i\hbar}{ma^2}t\right)\right]$$

The interference term is then

$$2\sqrt{N_1N_2}\text{Re}\left[\psi_1(\mathbf{r},t)\psi_2^*(\mathbf{r},t)\right]$$
$$= 2\sqrt{N_1N_2}\exp\left[-\frac{\left(\mathbf{r}-\frac{\mathbf{d}}{2}\right)^2 + \left(\mathbf{r}+\frac{\mathbf{d}}{2}\right)^2}{2a(t)^2}\right]$$
$$\times \text{Re}\left[\exp i\left(\phi_1 - \phi_2 - \frac{\hbar t}{ma^2a(t)^2}\mathbf{r}\cdot\mathbf{d}\right)\right]$$
$$\propto \cos\left[\phi_1 - \phi_2 - \frac{\hbar t}{ma^2a(t)^2}\mathbf{r}\cdot\mathbf{d}\right]$$

- Equi-phase lines (at a fixed time) satisfy $\mathbf{r}\cdot\mathbf{d} = \text{constant}$
- Positions of maxima/minima depend on the relative phase
- Distance between adjacent maxima/minima depends on the coefficient of $\mathbf{r}\cdot\mathbf{d}$

$$\Delta = \frac{2\pi m a(t)^2 a^2}{\hbar t d} \approx \frac{2\pi\hbar t}{md}$$

Interference between condensates with fixed particle number
Define number states

$$|N_1, N_2\rangle = \frac{1}{\sqrt{N_1!N_2!}}\left(a_1^\dagger\right)^{N_1}\left(a_2^\dagger\right)^{N_2}|0\rangle$$

In the single mode approximation, the field operator satisfies

$$\hat{\Psi}(\mathbf{r}) = \psi_1(\mathbf{r})a_1 + \psi_2(\mathbf{r})a_2$$

Therefore

$$\hat{\Psi}(\mathbf{r})|N_1, N_2\rangle = \sqrt{N_1}\psi_1(\mathbf{r})|N_1 - 1, N_2\rangle + \sqrt{N_2}\psi_2(\mathbf{r})|N_1, N_2 - 1\rangle$$

Expectation value of the single-body density operator

$$\langle N_1, N_2|\hat{\Psi}^\dagger(\mathbf{r})\hat{\Psi}(\mathbf{r})|N_1, N_2\rangle = N_1|\psi_1|^2 + N_2|\psi_2|^2$$

- It appears that there are no interference effects for isolated condensates with fixed particle number
- However, it does not agree with experimental observation
- What have we missed?

- It appears that there are no interference effects for isolated condensates with fixed particle number
- However, it does not agree with experimental observation
- What have we missed?
  - Experiment features a single-shot measurement of many particles, while our previous calculation is only for the multi-shot averages
  - Phase coherence and hence interference may be established dynamically in the measurement process
  - When a particle is annihilated, we cannot be certain which condensate it belonged to. Therefore the relative particle number difference becomes more and more uncertain as more and more particles are measured
  - The uncertainty in the relative particle number implies the establishment of relative phase, as they are conjugate variables

To formulate what we have learned, define the relative-phase state with a fixed total particle number

$$|\phi, N\rangle = \frac{1}{\sqrt{N!}}\left[\int d^3\mathbf{r}\psi_\phi(\mathbf{r})\hat{\Psi}^\dagger(\mathbf{r})\right]^N|0\rangle$$
$$= \frac{1}{\sqrt{N!2^N}}\left(a_1^\dagger e^{i\phi/2} + a_2^\dagger e^{-i\phi/2}\right)^N|0\rangle$$

The single body wave function of the phase state (free atoms)

$$\psi_\phi(\mathbf{r}) = \frac{1}{\sqrt{2}}\left[\psi_1(\mathbf{r})e^{i\phi/2} + \psi_2(\mathbf{r})e^{-i\phi/2}\right]$$

We have the following property

$$\hat{\Psi}|\phi, N\rangle = \hat{\Psi}\frac{1}{\sqrt{N!}}A^N|0\rangle$$
$$= \frac{1}{\sqrt{N!}}\left(A\hat{\Psi} + \psi_\phi\right)A^{N-1}|0\rangle$$
$$= \sqrt{N}\psi_\phi|\phi, N-1\rangle$$

Note the phase state is a superposition of states with different relative particle number

$$|\phi, N\rangle = \frac{1}{(2^N N!)^{1/2}}\sum_{N_1} C_N^{N_1}\left(a_1^\dagger\right)^{N_1}\left(a_2^\dagger\right)^{N_2} e^{i(N_1-N_2)\phi/2}|0\rangle$$

where $N_2 = N - N_1$. Extracting the $\left(a_1^\dagger\right)^{N_1}\left(a_2^\dagger\right)^{N_2}$ part relates the phase state to the number state,

$$\int\frac{d\phi}{2\pi}e^{-i(N_1-N_2)\phi/2}|\phi, N\rangle \propto |N_1, N_2\rangle$$

Actually, applying the Stirling relation $n! \sim \sqrt{2\pi n}\left(\frac{n}{e}\right)^n$ for large n, we have

$$|N/2, N/2\rangle \approx \left(\frac{\pi N}{2}\right)^{1/4}\int_0^{2\pi}\frac{d\phi}{2\pi}|\phi, N\rangle$$

It is apparent that relative phase and relative particle number are conjugate variables. Therefore, as the uncertainty in the relative number increases, the uncertainty in the relative phase decreases.

More specifically

- Single shot measurement

$$\prod_{i=1}^{k}\left[\frac{1}{\sqrt{2}}(a_1 e^{-i\phi_i/2} + a_2 e^{i\phi_i/2})\right]|N/2, N/2\rangle$$

- After two clicks: probability peaking at $\phi_1 = \phi_2$

$$\sqrt{N/2(N/2-1)}\Big(e^{-i(\phi_1+\phi_2)}|N/2-2, N/2\rangle$$
$$+ e^{i(\phi_1+\phi_2)}|N/2, N/2-2\rangle\Big) + N\cos(\phi_1-\phi_2)|N/2-1, N/2-1\rangle$$

- After k clicks peaked at φ: $\int d\phi[\cos(\phi/2-\varphi/2)]^k|\phi, N-k\rangle$
- The density distribution of a phase state

$$n(\mathbf{r}) = \langle\phi, N|\hat{\Psi}^\dagger(\mathbf{r})\hat{\Psi}(\mathbf{r})|\phi, N\rangle = \frac{N}{2}\left|\psi_1(\mathbf{r})e^{i\phi/2} + \psi_2(\mathbf{r})e^{-i\phi/2}\right|^2$$

where the cross term gives interference pattern

Spinor BEC

- We have considered so far cold atoms of the same species and with the same internal state.
- It is possible to prepare ensemble with different isotopes
- In an optical dipole trap, atoms with different hyperfine states can be trapped simultaneously
- In general there will be inter- and intra- species collisions
- What is the ground state in such systems? Is it dependent on system parameter? (Quantum phase transition?)

At the mean field level, a two-component BEC can be described by the TDGPE

$$i\hbar\dot{\psi}_1 = \left(-\frac{\hbar^2}{2m}\nabla^2 + V_1 + U_{11}|\psi_1|^2 + U_{12}|\psi_2|^2\right)\psi_1$$
$$i\hbar\dot{\psi}_2 = \left(-\frac{\hbar^2}{2m}\nabla^2 + V_2 + V_{hf} + U_{22}|\psi_2|^2 + U_{21}|\psi_1|^2\right)\psi_2$$

where V_{hf} is the energy offset of different hyperfine spins due to Zeeman shift, and U_{ij} are the collision rates

$$U_{ij} = \frac{2\pi\hbar^2 a_{ij}}{m_{ij}},$$

where m_{ij} is the reduced massed.

For a uniform gas in the steady state, $\psi_i = \sqrt{n_i}\exp(-i\mu_i t/\hbar)$

$$\mu_1 = U_{11}n_1 + U_{12}n_2$$
$$\mu_2 = U_{21}n_1 + U_{22}n_2$$

Stability analysis

- Study fluctuations in energy functional and require $\delta^2 E > 0$
- Alternatively, derive eigen energy equations for fluctuations and require the eigen energies for fluctuations be real
- Neglecting kinetic energy contribution

Energy functional

$$E = \int d^3\mathbf{r}\left\{\frac{\hbar^2}{2m_1}|\nabla\psi_1|^2 + \frac{\hbar^2}{2m_2}|\nabla\psi_2|^2 + V_1|\psi_1|^2 + V_2|\psi_2|^2\right.$$
$$\left. + \frac{1}{2}U_{11}|\psi_1|^4 + \frac{1}{2}U_{22}|\psi_2|^4 + U_{12}|\psi_1|^2|\psi_2|^2\right\}$$

The first order variation δE vanishes (GPE). Neglecting kinetic energy and requiring the second order variation be positive definite

$$\delta^2 E = \frac{1}{2}\int d^3\mathbf{r}\left[\frac{\partial^2\varepsilon}{\partial n_1^2}(\delta n_1)^2 + \frac{\partial^2\varepsilon}{\partial n_2^2}(\delta n_2)^2 + 2\frac{\partial^2\varepsilon}{\partial n_1\partial n_2}\delta n_1\delta n_2\right],$$

where

$$\varepsilon = \frac{1}{2}n_1^2 U_{11} + \frac{1}{2}n_2^2 U_{22} + n_1 n_2 U_{12}$$

Therefore the stability condition gives

$$U_{11} > 0, \quad U_{22} > 0, \quad U_{11}U_{22} > U_{12}^2 \text{ or } U_{12} > 0$$

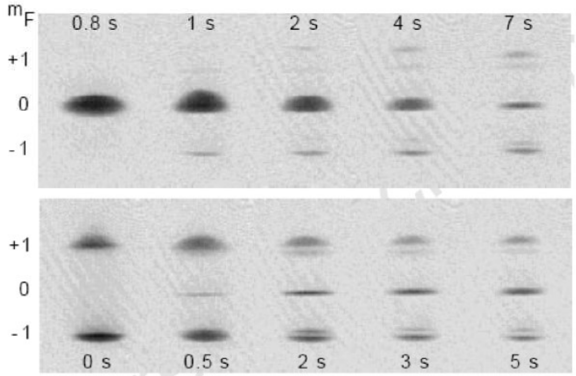
For $U_{11} > 0$, $U_{22} > 0$, $U_{11}U_{22} < U_{12}^2$ and $U_{12} < 0$, collapse! (Quantum droplet...)

Theory

- T.-L. Ho et al. (OSU), Existence of spin domains (1996)
- C.K. Law et al. (Rochester), Single mode approximation (1998)
- More ...

Experiment

- C.J. Myatt et al. (JILA), Overlapping condensates in two magnetic traps (1997)
- D.M. Stamper-Kurn et al. (MIT), Transfer BEC to optical traps (1998)
- J. Stenger et al. (MIT), Spin domains in Spinor BEC (1998)
- M.D. Barrett et al. (GIT), All optical Spinor BEC (2001)
- More ...



J. Stenger et al. Nature 396, 345 (1998)

Spinor condensate

- For two component condensate, particle number for each species is conserved
- For spinor condensate, the simplest of which is composed of atoms with three internal states $|F=1, m_F=\pm 1, 0\rangle$, this is no longer so
- Interaction observes rotational symmetry and thus conserves the total angular momentum of the colliding atoms
- For two bosonic atoms each with $F=1$ and interacting via s-wave scattering, the total angular momentum must be even (0 or 2)
- We denote the s-wave scattering lengths in the two (0 or 2) scattering channels as a_0 and a_2

- The interaction can be written as

$$U(\mathbf{r}) = \delta(\mathbf{r})\left(c_0 + c_2 \mathbf{S}_1 \cdot \mathbf{S}_2\right) \ ,$$

where $c_0 = \frac{4\pi\hbar^2}{m}\frac{(a_0+2a_2)}{3}$, $c_2 = \frac{4\pi\hbar^2}{m}\frac{(a_2-a_0)}{3}$. Note we have used the relation

$$2\mathbf{S}_1 \cdot \mathbf{S}_2 = (\mathbf{S}_1 + \mathbf{S}_2)^2 - \mathbf{S}_1^2 - \mathbf{S}_2^2$$

So that for 0 total angular momentum, $\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle = -2$; while for total angular momentum of 2, $\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle = 1$.

We may then write the Hamiltonian

$$H = \int d^3\mathbf{r} \left(\frac{\hbar^2}{2m} \nabla \hat{\Psi}_\alpha^\dagger \cdot \nabla \hat{\Psi}_\alpha + (V + E_\alpha)\hat{\Psi}_\alpha^\dagger \hat{\Psi}_\alpha + \frac{1}{2} c_0 \hat{\Psi}_\alpha^\dagger \hat{\Psi}_{\alpha'}^\dagger \hat{\Psi}_{\alpha'} \hat{\Psi}_\alpha + \frac{1}{2} c_2 \hat{\Psi}_\alpha^\dagger \hat{\Psi}_{\alpha'}^\dagger \mathbf{S}_{\alpha\beta} \cdot \mathbf{S}_{\alpha'\beta'} \hat{\Psi}_{\beta'} \hat{\Psi}_\beta \right)$$

where E_α are the Zeeman shifts.

The TDGPE for different components is then

$$i\hbar \frac{\partial \psi_\alpha}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2 \psi_\alpha + V\psi_\alpha + c_0 \psi_{\alpha'}^* \psi_{\alpha'} \psi_\alpha + c_2 \psi_{\alpha'}^* \mathbf{S}_{\alpha'\beta} \cdot \mathbf{S}_{\alpha\beta'} \psi_{\beta'} \psi_\beta \ ,$$

where repeated indices are to be summed over.
The matrices for the angular momentum $S=1$ is

$$S_x = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} S_y = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix} S_z = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

- In principle, one may solve the GPE numerically to get the ground state configuration, dynamics, etc.
- Alternatively, one may assume that the three components have similar spatial wavefunctions and adopt the single mode approximation

$$\psi_\alpha(\mathbf{r}) \approx \sqrt{N}\phi(\mathbf{r})\xi_\alpha e^{-i\mu t/\hbar}$$

Ground state of spinor condensate under mean field

- For $c_2 < 0$, ground state has spinor configuration (100), i.e. it is 'ferromagnetic'
- For $c_2 > 0$, ground state has spinor configuration (010), i.e. it is 'anti-ferromagnetic' or 'polar'
- These are in the absence of magnetic fields
- In the absence of magnetic fields, there exists rotational symmetry in addition to the $U(1)$ gauge symmetry (global phase)
- We may define the rotation operator

$$\hat{U}(\alpha, \beta, \gamma) = e^{-i\hat{F}_z\alpha} e^{-i\hat{F}_y\beta} e^{-i\hat{F}_z\gamma}$$

- The degeneracy of the ground state is characterized by

$$\xi' = e^{i\theta}\hat{U}(\alpha, \beta, \gamma)\xi$$

Rotation for polar state

$$\xi = e^{i\theta}\begin{bmatrix} -\frac{1}{\sqrt{2}}e^{-i\alpha}\sin\beta \\ \cos\beta \\ \frac{1}{\sqrt{2}}e^{i\alpha}\sin\beta \end{bmatrix}$$

Rotation for ferromagnetic state

$$\xi = e^{i(\theta-\gamma)}\begin{bmatrix} e^{-i\alpha}\cos^2\beta/2 \\ \sqrt{2}\cos\beta/2\sin\beta/2 \\ e^{i\alpha}\sin^2\beta/2 \end{bmatrix}$$

- For local rotations, α, β, γ together with the global phase θ can all be spatially varying
- This may lead to interesting properties such as coreless vortices for ferromagetic state $c_2 < 0$

Single mode approximation in magnetic field

$$i\hbar\dot{\xi}_\pm = E_\pm\xi_\pm + c\left[(\rho_\pm + \rho_0 - \rho_\mp)\xi_\pm + \xi_0^2\xi_\mp^*\right]$$
$$i\hbar\dot{\xi}_0 = E_0\xi_0 + c\left[(\rho_+ + \rho_-)\xi_0 + 2\xi_+\xi_-\xi_0^*\right] \ ,$$

where $c = c_2 N \int d^3\mathbf{r}|\phi|^4$ and $\rho_\alpha = |\xi_\alpha|^2$. Making the transformation

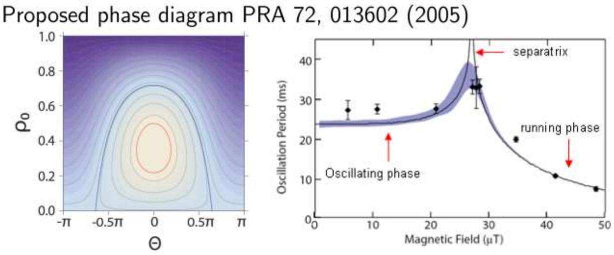
$$\xi_\pm = \sqrt{\rho_\pm}e^{-i\theta_{pm}}e^{-i(E_0\mp\eta)t/\hbar}$$
$$\xi_0 = \sqrt{\rho_0}e^{-i\theta_0}e^{-iE_0 t/\hbar} \ ,$$

with $\eta = (E_- - E_+)/2$. Also define $\delta = (E_+ + E_- - 2E_0)/2$, $m = \rho_+ - \rho_-$, $\theta = \theta_+ + \theta_- - 2\theta_0$, we have

$$\dot{\rho}_0 = \frac{2c}{\hbar}\rho_0\sqrt{(1-\rho_0)^2 - m^2}\sin\theta$$
$$\dot{\theta} = -\frac{2\delta}{\hbar} + \frac{2c}{\hbar}(1-2\rho_0) + \frac{2c}{\hbar}\frac{(1-\rho_0)(1-2\rho_0) - m^2}{\sqrt{(1-\rho_0)^2 - m^2}}\cos\theta$$

For anti-ferromagnetic spinor BEC ($c_2 > 0$)

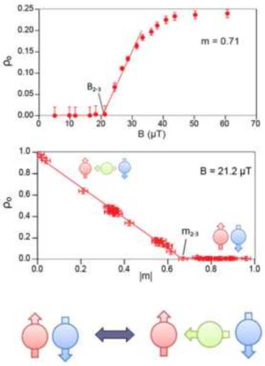
- Analogous to non-rigid pendulum
- Three different regions: running phase, separatrix, oscillating phase
- Proposed phase diagram PRA 72, 013602 (2005)



- Experimental observation PRL 102, 125301 (2009)

Phase transition in the mean-field ground state

- At zero magnetic field, the ground state of an anti-ferromagnetic spinor condensate has the spinor configuration $\left[\sqrt{(1+m)/2}, 0, \sqrt{(1-m)/2}\right]$
- At very large magnetic field, due to quadratic Zeeman shift, the ground state configuration becomes $\left[\sqrt{\frac{1-n_0+m}{2}}, \sqrt{n_0}, \sqrt{\frac{1-n_0-m}{2}}\right]$
- Thus there should be a phase transition inbetween



Next Lecture

- We have been dealing with bosons mostly. What about cold fermions?
- From another perspective, atoms are composed of neutrons, protons, electrons, etc.
- This means we have been dealing with composite bosons all the time
- What about bosons composed of fermionic atoms? Is it possible to create condensate of composite bosons from a Fermi sea?
- We will discuss degenerate Fermi gas and Feshbach resonance in the next lecture

Quantum Degenerate Gases

Lecture 8: Degenerate Fermi Gas

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Spring 2022

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Contents

Degenerate Fermi Gas

What about ultracold fermions?

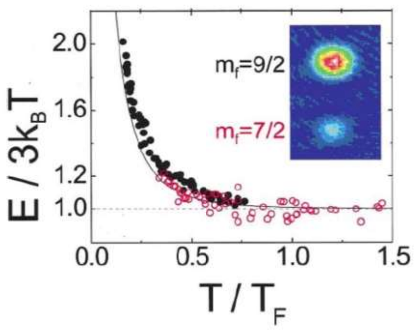
- Laser cooling schemes can be applied to fermionic species
- Evaporative cooling becomes problematic for single species fermions due to Pauli blocking
- Sympathetic cooling, either simultaneously cool atoms of different species or cool the same isotope with different hyperfine spins
- Typical fermionic atoms: ^{6}Li, ^{40}K, ^{171}Yb, ^{87}Sr, etc.
- Degenerate Fermi gas: phase space density approaching unity

$$n(\lambda_{dB})^3 = n\left(\frac{2\pi\hbar^2}{mk_BT}\right)^{\frac{3}{2}} \approx 1$$

- Alternatively,

$$T \approx T_F = \frac{(6\pi^2)^{\frac{2}{3}}\hbar^2 n^{\frac{2}{3}}}{2mk_B}$$

JILA group data (D.S. Jin et al.)
Thermodynamics from density profile



Ideal Fermi gas at zero temperature with a single internal state

$$\frac{V}{(2\pi)^3}\frac{4\pi}{3}k_F^3 = N$$

Therefore the Fermi energy (or chemical potential) in the homogeneous case

$$\epsilon_F = \frac{\hbar^2 k_F^2}{2m} = \frac{(6\pi^2 n)^{\frac{2}{3}}\hbar^2}{2m} = k_B T_F$$

For an ideal Fermi gas in a harmonic trap

$$G(\epsilon) = \frac{1}{6}\left(\frac{\epsilon}{\hbar\bar{\omega}}\right)^3, \quad \text{where } \bar{\omega} = (\omega_x\omega_y\omega_z)^{\frac{1}{3}}$$

$$G(\mu) = N \quad \rightarrow \mu = (6N)^{\frac{1}{3}}\hbar\bar{\omega}$$

Note the chemical potential is defined as the energy it takes to put an atom into the gas.

Energy of an ideal Fermi gas at zero temperature

- Homogeneous Fermi gas

$$\begin{aligned} E &= \frac{V}{(2\pi)^3}\int_0^{k_F} 4\pi k^2 dk \frac{\hbar^2 k^2}{2m} \\ &= \frac{V}{(2\pi)^3}4\pi\frac{\hbar^2}{2m}\frac{k_F^5}{5} \qquad \text{note } k_F^3 = 6\pi^2 n \\ &= \frac{3}{5}\epsilon_F N \end{aligned}$$

- Fermi gas in a harmonic trap

$$\begin{aligned} E &= \int_0^{\mu} g(\epsilon)\epsilon d\epsilon = \int_0^{\mu}\frac{1}{2}\frac{\epsilon^2}{\hbar^3\bar{\omega}^3}\epsilon d\epsilon \\ &= \frac{1}{8}\mu^4\frac{1}{\hbar^3\bar{\omega}^3} \qquad \text{note } \mu = (6N)^{\frac{1}{3}}\hbar\bar{\omega} \\ &= \frac{3}{4}N\mu \end{aligned}$$

- We applied the Thomas-Fermi approximation to interacting Bose gases to calculate density distribution in a trap

$$n(\mathbf{r}) = \frac{1}{U}\left[\mu - V(\mathbf{r})\right]$$

- For Fermions in a trap, we may assume that the density profile varies sufficiently slowly in space so that we may treat each point $\mathbf{r}$ as a homogeneous system. This is called the Local Density Approximation (LDA). This is valid when cloud size is much larger than the Fermi wavelength at trap center ($k_F(0)\bar{R} \sim N^{\frac{1}{3}} \gg 1$): kinetic vs. trapping.

Under LDA,

$$n(\mathbf{r}) = \frac{k_F^3}{6\pi^2} \quad \epsilon_F(\mathbf{r}) = \frac{\hbar^2 k_F^2}{2m} = \mu - V(\mathbf{r})$$

$$n(\mathbf{r}) = \frac{1}{6\pi^2}\left\{\frac{2m}{\hbar^2}\left[\mu - V(\mathbf{r})\right]\right\}^{\frac{3}{2}}$$

Range of the cloud

$$R_i^2 = \frac{2\mu}{m\omega_i^2}, \quad i = x, y, z$$
$$= \frac{2(6N)^{\frac{1}{3}}\hbar\bar{\omega}}{m\omega_i^2}$$

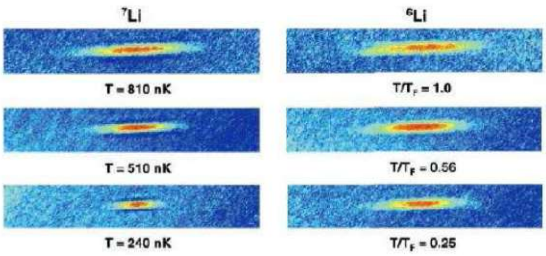
$$\bar{R} = (R_x R_y R_z)^{\frac{1}{3}} = (48N)^{\frac{1}{6}}\sqrt{\frac{\hbar}{m\bar{\omega}}} = (48N)^{\frac{1}{6}}\bar{a}$$

Recall the range of cloud for bosons under TFA

$$\bar{R} = 15^{\frac{1}{5}}\left(\frac{Na}{\bar{a}}\right)^{\frac{1}{5}}\bar{a}$$

For typical experimental parameters, $N = 10^5$, $\omega = 2\pi \times 200$Hz, $a = 100a_0$, $\bar{R}_F \approx 1.5 \times 10^{-5}$m, and $\bar{R}_B \approx 6.5 \times 10^{-6}$m. Thus the size of a Fermi gas is in general larger than that of a Bose gas given the same particle number.

Rice group data (R. G. Hulet et al.)
Mixture of ^{6}Li and ^{7}Li at various temperatures



Fermi gas with interactions

- Due to Fermi-Dirac statistics, s-wave scattering for identical Fermions vanishes
- The interaction Hamiltonian for a two-component Fermi gas

$$H = U\int d^3\mathbf{r}\hat{\Psi}_\uparrow^\dagger(\mathbf{r})\hat{\Psi}_\downarrow^\dagger(\mathbf{r})\hat{\Psi}_\downarrow(\mathbf{r})\hat{\Psi}_\uparrow(\mathbf{r})$$

  Note the absence of $1/2$ factor. The interaction energy per particle is therefore of the order $nU = \frac{4\pi\hbar^2 an}{m}$.
- We have seen before that the kinetic energy per particle is of the order ϵ_F
- The ratio between interaction and kinetic energy

$$\frac{nU}{\epsilon_F} = \frac{4}{3\pi}k_F a$$

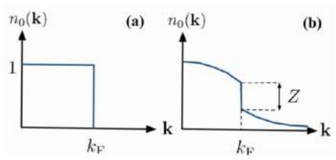
  In a harmonic trap, the ratio $\sim N^{\frac{1}{6}}a/\bar{a} \sim 10^{-2}$ for typical parameters.

Fate of interacting Fermi gases

- Fermi liquid: polaron, etc.
  - Gapless quasiparticles carrying the same quantum numbers

$$\epsilon_p \approx \epsilon_F + \left.\frac{\partial\epsilon_p}{\partial p}\right|_{p=p_F}(p - p_F)$$

  - Residue Fermi surface with discontinuous density



- Symmetry-broken phases: BCS state, etc.
- Non-Fermi liquid: Luttinger liquid, etc.

Cooper instability (under attractive interaction)

- Cooper pointed out in 1956 that the ground state of a normal metal should be unstable at zero temperature
- Electrons near the Fermi surface interact with those on the opposite side of the Fermi sea, and thus develops a bound state
- More on that in the section of BCS theory

Simple description

- Study the interaction of two fermions above a Fermi sea (at zero T)
- Solve the two-body Schrödinger's equation for eigen-energy
- Bound state exists if $E < 2\epsilon_F$

The Schrödinger's equation for wavefunction of the relative motion

$$-\frac{\hbar^2}{m}\nabla^2\psi(\mathbf{r}) + V(\mathbf{r})\psi(\mathbf{r}) = E\psi(\mathbf{r})$$

In momentum space $\psi(\mathbf{r}) = \sum_{k>k_F} f_k e^{i\mathbf{k}\cdot r}$

$$2\epsilon_k f_k + \sum_{k'>k_F} V_{-k'}f_{k'} = Ef_k$$

Naive assumption: $V_k = -U$ in the energy range $(\epsilon_F, \epsilon_F + \hbar\omega_c)$

$$(2\epsilon_k - E)f_k = U{\sum_{k'}}' f_{k'}$$

$${\sum_k}' f_k = {\sum_k}'\frac{U}{2\epsilon_k - E}{\sum_{k'}}' f_{k'}$$

Thus

$$\frac{1}{U} = {\sum_k}'\frac{1}{2\epsilon_k - E}$$

Convert to integral of energy

$$\frac{1}{U} = N_F\int_{\epsilon_F}^{\epsilon_F+\hbar\omega_c}\frac{d\epsilon}{2\epsilon - E}$$
$$= \frac{N_F}{2}\ln\frac{2\epsilon_F - E + 2\hbar\omega_c}{2\epsilon_F - E}$$

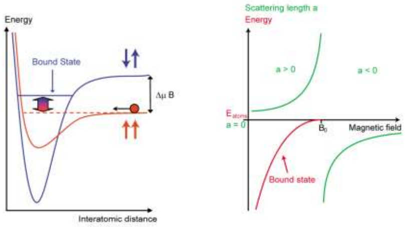
With N_F the density of state at Fermi surface. For $N_F U \ll 1$

$$E \approx 2\epsilon_F - 2\hbar\omega_c\exp\left(-\frac{2}{N_F U}\right)$$

Bound state.

Feshbach Resonance

- First investigated by H. Feshbach in 1962 in the context of nuclear physics (also known as Fano-Feshbach resonance)
- Nowadays it has found applications mostly in tuning the two-body interaction strengths between cold atoms
- The scattering length diverges as the threshold of an 'open' channel coincides with a bound state energy of a 'closed' channel



- In shape resonance, the relative position of the bound state and the threshold is tuned by varying the shape of the scattering potential
- In multi-channel scattering process, this can be done by changing the relative positions of the scattering potentials. But how?
- For a two-body scattering process, the interaction potential is affected by the internal states of the atoms. For instance, a singlet pair has a deeper potential than a triplet pair at intermediate range. The scattering channels are thus characterized by the internal states.
- Different internal states are affected differently by the magnetic field due to different Zeeman shifts.
- The resonance scattering condition can thus be achieved by tuning the magnetic field.
- Note that the coupling between the scattering channels is typically provided by the hyperfine interaction $V = A\mathbf{I}\cdot\mathbf{S} = A(I_+S_- + I_-S_+) + AI_zS_z$

Formal scattering description of Feshbach resonnance

- Consider a two-channel problem, with open channel (triplet state) P, and closed channel (singlet state) Q
- Define projection operator $\hat{P}$ and $\hat{Q}$ which project the state vector into the open and closed channel respetively

$$|\Psi\rangle = \hat{P}|\Psi\rangle + \hat{Q}|\Psi\rangle = |\Psi_P\rangle + |\Psi_Q\rangle \,,$$

where $\hat{P}^2 = \hat{P}$, $\hat{Q}^2 = \hat{Q}$, $\hat{P} + \hat{Q} = 1$, $\hat{P}\hat{Q} = 0$

- Apply the projection operator to the left of $H|\Psi\rangle = E|\Psi\rangle$,

$$\hat{P}H|\Psi\rangle = \hat{P}H(\hat{P}\hat{P} + \hat{Q}\hat{Q})|\Psi\rangle = H_{PP}|\Psi_P\rangle + H_{PQ}|\Psi_Q\rangle$$
$$\hat{P}E|\Psi\rangle = E|\Psi_P\rangle$$
$$(E - H_{PP})|\Psi_P\rangle = H_{PQ}|\Psi_Q\rangle$$

Similarly,

$$(E - H_{QQ})|\Psi_Q\rangle = H_{QP}|\Psi_P\rangle$$

- Formal solution

$$|\Psi_Q\rangle = (E - H_{QQ} + i\delta)^{-1} H_{QP}|\Psi_P\rangle$$
$$\left[E - H_{PP} - H_{PQ}\left(E - H_{QQ} + i\delta\right)^{-1} H_{QP}\right]|\Psi_P\rangle = 0$$

The effective interaction in the open channel $H'_{PP} = H_{PQ}\left(E - H_{QQ} + i\delta\right)^{-1} H_{QP}$ describes the tunneling to and back from the closed channel, which naturally takes the form of second-order perturbation.

- Our goal is to understand the dependence of the effective scattering length with respect to the energy differences. In particular, we wish to establish a relation between the effective scattering length close to resonance with the background scattering length away from the resonance which can be measured with ease.
- It is convenient then to separate the background interaction term from the Hamiltonian in the open channel $H_{PP} = H_0 + U_1$, $U_2 = H'_{PP}$

- Recall the Lippmann-Schwinger equation

$$T = U + UG_0T \,,$$

where $U = U_1 + U_2$ and $G_0 = (E - H_0 + i\delta)^{-1}$.

- Formal solution

$$\begin{aligned} T &= (1 - UG_0)^{-1}U \\ &= G_0^{-1}G_0(1 - UG_0)^{-1}U \\ &= G_0^{-1}\left[(1 - UG_0)G_0^{-1}\right]^{-1}U \\ &= G_0^{-1}(G_0^{-1} - U_1 - U_2)^{-1}U \end{aligned}$$

- Note the matrix identity

$$\begin{aligned} & A^{-1}\left[1 + B(A-B)^{-1}\right] \\ &= A^{-1}\left[1 + B(A-B)^{-1}\right](A-B)(A-B)^{-1} \\ &= A^{-1}\left[(A-B) + B\right](A-B)^{-1} = (A-B)^{-1} \end{aligned}$$

- Let $A = G_0^{-1} - U_1$, $B = U_2$.

- We have

$$\begin{aligned} T &= G_0^{-1}(G_0^{-1} - U_1 - U_2)^{-1}U \\ &= G_0^{-1}\left(G_0^{-1} - U_1\right)^{-1}\left[1 + U_2(G_0^{-1} - U)^{-1}\right]U \\ &= \left[(G_0^{-1} - U_1)G_0\right]^{-1}\left[1 + U_2(G_0^{-1} - U)^{-1}\right](U_1 + U_2) \\ &= (1 - U_1G_0)^{-1}U_1 + (1 - U_1G_0)^{-1}U_2\left[1 + (G_0^{-1} - U)^{-1}U\right] \\ &= T_1 + (1 - U_1G_0)^{-1}U_2\left\{1 + G_0U\left[U^{-1}G_0^{-1}(G_0^{-1} - U)^{-1}U\right]\right\} \\ &= T_1 + (1 - U_1G_0)^{-1}U_2\left\{1 + G_0U\left[U^{-1}(G_0^{-1} - U)G_0U\right]^{-1}\right\} \\ &= T_1 + (1 - U_1G_0)^{-1}U_2\left\{1 + G_0U\left[1 - G_0U\right]^{-1}\right\} \\ &= T_1 + (1 - U_1G_0)^{-1}U_2(1 - G_0U)^{-1} \end{aligned}$$

- Note $T_1 = (1 - U_1G_0)^{-1}U_1$ is the T-matrix in the open channel with the background scattering only; and we have used the matrix identity by setting $A = 1$, $B = G_0U$ in the last step.

- In momentum space, we have

$$\langle\mathbf{k}'|T|\mathbf{k}\rangle = \langle\mathbf{k}'|T_1|\mathbf{k}\rangle + \langle\mathbf{k}'|(1 - U_1G_0)^{-1}U_2(1 - G_0U)^{-1}|\mathbf{k}\rangle$$

- Recall definition of T-matrix $T|\varphi\rangle = U|\Psi\rangle$, where $|\varphi\rangle$ is eigenstate of H_0 and $|\Psi\rangle$ is the eigenstate of $H_0 + U$ (scattering state)
- Keep terms of first order in U_2

$$\begin{aligned} \langle\mathbf{k}'|T|\mathbf{k}\rangle &\approx \langle\mathbf{k}'|T_1|\mathbf{k}\rangle + \langle\mathbf{k}'|(1 - U_1G_0)^{-1}U_2(1 - G_0U_1)^{-1}|\mathbf{k}\rangle \\ &= \langle\mathbf{k}'|T_1|\mathbf{k}\rangle + \langle\mathbf{k}'; U_1, -|U_2|\mathbf{k}; U_1, +\rangle \,, \end{aligned}$$

with $-$ and $+$ specifying the sign of the infinitesimal identity $i\delta$, which implies incoming and outgoing wave respectively.

- Neglect coupling between open channels and take the low energy scattering limit, under which the difference in the incoming wave and the outgoing wave at large distances can be neglected.

- We then have

$$\frac{4\pi\hbar^2}{m}a = \frac{4\pi\hbar^2}{m}a_P + \sum_n \frac{|\langle\Psi_n|H_{QP}|\Psi_0\rangle|^2}{E - E_n}$$

The summation over n is in the closed channel.

- Near resonance, only one bound state in the closed channel is important, the contribution from the rest can be absorbed into the background scattering length

$$\frac{4\pi\hbar^2}{m}a = \frac{4\pi\hbar^2}{m}a_{bg} + \frac{|\langle\Psi_b|H_{QP}|\Psi_0\rangle|^2}{E - E_b}$$

- The energy difference $E - E_b$ can be tuned by external parameters. In particular, if it is sensitive to magnetic field, we may expand the energy difference to lowest order in magnetic field

$$E - E_b \approx \alpha(B - B_0) \,,$$

where B_0 is the magnetic field where the bound state energy exactly matches the threshold of the open channel.

- We then have the important relation characterizing the scattering length near a Feshbach resonance

$$a = a_{bg}\left(1 + \frac{\Delta B}{B - B_0}\right) ,$$

where the resonance width $\Delta B = \frac{m}{4\pi\hbar^2 a_{bg}} \frac{|\langle\Psi_b|H_{QP}|\Psi_0\rangle|^2}{\alpha}$.
- When higher order contributions of U_2 are considered, the bound state energy has an additional shift and a finite width, which is typically small for cold atoms.
- Note that these bound states in the closed channel are typically high-lying quasi-bound states. To get to the ground state of the two-body Hamiltonian (molecular ground state), further cooling is needed.

Next Lecture

- Cooper instability revisited, BCS theory
- Application of Feshbach resonance: BCS-BEC crossover
- Crossover theory, mean field and beyond

Quantum Degenerate Gases

Lecture 9: Fermi Condensate

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Contents

BCS theory

- Proposed in 1957, Bardeen-Cooper-Schrieffer (BCS) theory was the first microscopic theory of superconductivity since its discovery in 1911
- The superconductivity is described as the condensation of Cooper pairs
- BCS theory is one of the most successful theories of physics, with which many experimental observations of superconductors can be explained
- Also important for the understanding of superconductivity is the Landau-Ginzburg theory and Bogoliubov theory
- BCS theory cannot explain high-Tc superconductivity discovered in 1986

Cooper instability

- Cooper pointed out in 1956 that the ground state of a normal metal should be unstable at zero temperature
- Electrons near the Fermi surface interact with those on the opposite side of the Fermi sea, and thus develops a pole (divergence) in the T-matrix
- Poles of T-matrix suggests bound state. However, these electrons cannot really bind together, as they have positive total energy and are spatially far apart
- These correlated electron pairs are called Cooper pairs
- Note the interaction needs to be attractive in nature (electron-phonon interaction induced in reality)
- Cooper pairs stabilize the ground state (at zero temperature) by smoothing out the sharp Fermi distribution at Fermi surface

Cooper instability: formal description
Lipmann-Schwinger equation

$$\begin{aligned} T &= V + VG_0T \\ &= V + VG_0V + VG_0VG_0V + \cdots \\ &= V + V\chi T \end{aligned}$$

Therefore

$$\begin{aligned} \chi(\mathbf{k}, \mathbf{k}') &\approx \frac{1}{\mathcal{V}} \sum_{\mathbf{k}_1} \frac{V(\mathbf{k}, \mathbf{k}_1)V(\mathbf{k}_1, \mathbf{k}')}{2\xi_{\mathbf{k}} - 2\xi_{\mathbf{k}_1}} \\ &\quad \times \left\{ [1 - n(\xi_{\mathbf{k}_1})][1 - n(\xi_{-\mathbf{k}_1})] - n_{\xi_{\mathbf{k}_1}} n_{\xi_{-\mathbf{k}_1}} \right\} \\ V_{\text{eff}} &\approx -\frac{V_0}{1 + N_F V_0 \ln(\xi/\omega_D)} \end{aligned}$$

The pole in the T-matrix (effective interaction potential) suggests bound state and instability. (cf. G. D. Mahan, *Many-particle physics*)

BCS Hamiltonian (free space)

$$H - \mu N = \sum_{\mathbf{k},\sigma} (\epsilon_{\mathbf{k}} - \mu)\, a^\dagger_{\mathbf{k},\sigma} a_{\mathbf{k},\sigma} + \frac{1}{\mathcal{V}} \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} U_{\mathbf{k},\mathbf{k}',\mathbf{q}}\, a^\dagger_{\mathbf{k}+\mathbf{q},\uparrow} a^\dagger_{-\mathbf{k},\downarrow} a_{-\mathbf{k}',\downarrow} a_{\mathbf{k}'+\mathbf{q},\uparrow}$$

Several simplifications

- Cooper pairs with zero center of mass momentum condense: take $\mathbf{q} = 0$
- The electron-electron coupling rate $U_{\mathbf{k},\mathbf{k}'}$ is considered to be negative and arbitrarily small
- As the electron-electron coupling is mediated by phonons in the solids, BCS theory assumes constant $U_{\mathbf{k},\mathbf{k}'}$ for electrons near the Fermi surface, within the range of approximately the Debye energy, and zero otherwise

BCS wavefunction

$$|\Psi\rangle = \prod_{\mathbf{k}} \left(u_{\mathbf{k}} + v_{\mathbf{k}} a^\dagger_{\mathbf{k},\uparrow} a^\dagger_{-\mathbf{k},\downarrow} \right) |\text{vac}\rangle$$

- Normalization condition, $|u_{\mathbf{k}}|^2 + |v_{\mathbf{k}}|^2 = 1$
- Pairing of fermions with zero center of mass momentum
- Equivalent to coherent state of fermion pairs

$$|\Psi\rangle = \mathcal{N} \exp \left[\sum_{\mathbf{k}} f_{\mathbf{k}} a^\dagger_{\mathbf{k},\uparrow} a^\dagger_{-\mathbf{k},\downarrow} \right] |\text{vac}\rangle$$
$$= \mathcal{N} \prod_{\mathbf{k}} \left(1 + f_{\mathbf{k}} a^\dagger_{\mathbf{k},\uparrow} a^\dagger_{-\mathbf{k},\downarrow} \right) |\text{vac}\rangle$$

- We can identify the pairing wavefunction $f_{\mathbf{k}} = v_{\mathbf{k}}/u_{\mathbf{k}}$
- As with typical variational approaches, need to minimize $\langle H - \mu N \rangle$. Alternatively, diagonalize it.

Expand around the mean fields of the pairing operators

$$a^\dagger_{\mathbf{k},\uparrow} a^\dagger_{-\mathbf{k},\downarrow} = \left\langle a^\dagger_{\mathbf{k},\uparrow} a^\dagger_{-\mathbf{k},\downarrow} \right\rangle + \left(a^\dagger_{\mathbf{k},\uparrow} a^\dagger_{-\mathbf{k},\downarrow} - \left\langle a^\dagger_{\mathbf{k},\uparrow} a^\dagger_{-\mathbf{k},\downarrow} \right\rangle \right)$$

Retain up to first order fluctuation $\left(a^\dagger_{\mathbf{k},\uparrow} a^\dagger_{-\mathbf{k},\downarrow} - \left\langle a^\dagger_{\mathbf{k},\uparrow} a^\dagger_{-\mathbf{k},\downarrow} \right\rangle \right)$.
And define the pairing order parameter

$$\Delta = -\frac{U}{\mathcal{V}} \sum_{\mathbf{k}} \langle a_{-\mathbf{k},\downarrow} a_{\mathbf{k},\uparrow} \rangle$$

The effective BCS Hamiltonian becomes

$$H - \mu N = \sum_{\mathbf{k},\sigma} (\epsilon_{\mathbf{k}} - \mu)\, a^\dagger_{\mathbf{k},\sigma} a_{\mathbf{k},\sigma}$$
$$- \sum_{\mathbf{k}} \left(\Delta a^\dagger_{\mathbf{k},\uparrow} a^\dagger_{-\mathbf{k},\downarrow} + \Delta^* a_{-\mathbf{k},\downarrow} a_{\mathbf{k},\uparrow} \right) - \frac{|\Delta|^2}{U}$$

Note the effective Hamiltonian is quadratic. To diagonalize the Hamiltonian, we may apply the Bogoliubov transformation

$$\alpha_{\mathbf{k},\uparrow} = u_{\mathbf{k}} a_{\mathbf{k},\uparrow} - v_{\mathbf{k}} a^\dagger_{-\mathbf{k},\downarrow}$$
$$\alpha^\dagger_{\mathbf{k},\downarrow} = v^*_{\mathbf{k}} a_{\mathbf{k},\uparrow} + u^*_{\mathbf{k}} a^\dagger_{-\mathbf{k},\downarrow}$$

The quasi-particle operators satisfy the Fermi-Dirac commutation relations

$$\left\{ \alpha_{\mathbf{k},\sigma}, \alpha^\dagger_{\mathbf{k}',\sigma'} \right\} = \delta_{\sigma,\sigma'} \delta_{\mathbf{k},\mathbf{k}'}$$

- Plug these into the effective Hamiltonian
- Require that the final Hamiltonian be diagonal in the basis of quasi-particle operators
- This is equivalent to requiring that the Hamiltonian describe non-interacting quasi-particles

We have

$$H - \mu N = \sum_{\mathbf{k}} E_{\mathbf{k},\sigma} \alpha^\dagger_{\mathbf{k},\sigma} \alpha_{\mathbf{k},\sigma} + \sum_{\mathbf{k}} (\epsilon_{\mathbf{k}} - \mu - E_{\mathbf{k}}) - \frac{|\Delta|^2}{U},$$

where the dispersion for the quasi-particle is gapped, $E_{\mathbf{k}} = \sqrt{|\Delta|^2 + (\epsilon_{\mathbf{k}} - \mu)^2}$. The coefficients in the Bogoliubov expansion are

$$|u_{\mathbf{k}}|^2 = \frac{E_{\mathbf{k}} + (\epsilon_{\mathbf{k}} - \mu)}{2E_{\mathbf{k}}}$$
$$|v_{\mathbf{k}}|^2 = \frac{E_{\mathbf{k}} - (\epsilon_{\mathbf{k}} - \mu)}{2E_{\mathbf{k}}}$$

- Identify the ground state as the vacuum state of the quasi-particles
- Take the chemical potential to be the Fermi energy

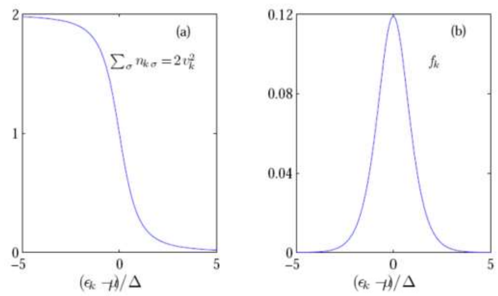
From the definition $\Delta = -\frac{U}{\mathcal{V}} \sum_{\mathbf{k}} \langle a_{-\mathbf{k},\downarrow} a_{\mathbf{k},\uparrow} \rangle$

$$\Delta = -\frac{U}{\mathcal{V}} \sum_{\mathbf{k}} \left\langle \left(u^*_{\mathbf{k}} \alpha_{\mathbf{k},\downarrow} - v_{\mathbf{k}} \alpha^\dagger_{\mathbf{k},\uparrow} \right) \left(u^*_{\mathbf{k}} \alpha_{\mathbf{k},\uparrow} + v_{\mathbf{k}} \alpha^\dagger_{\mathbf{k},\downarrow} \right) \right\rangle$$
$$= -\frac{U}{\mathcal{V}} \sum_{\mathbf{k}} \left(u^*_{\mathbf{k}} v_{\mathbf{k}} \left\langle \alpha_{\mathbf{k},\downarrow} \alpha^\dagger_{\mathbf{k},\downarrow} \right\rangle - v_{\mathbf{k}} u^*_{\mathbf{k}} \left\langle \alpha^\dagger_{\mathbf{k},\uparrow} \alpha_{\mathbf{k},\uparrow} \right\rangle \right)$$
$$= -\Delta \frac{U}{\mathcal{V}} \sum_{\mathbf{k}} \frac{1}{2E_k} [1 - 2f(E_k)]$$

And we have the gap equation

$$-\frac{1}{U} = \frac{1}{\mathcal{V}} \sum_{\mathbf{k}} \frac{1 - 2f(E_k)}{2E_k}$$

- Summation over states with energy close to the Fermi surface (in range of Debye energy)
- In the weak coupling limit of the standard BCS theory, the gap is exponentially small, the Fermi surface is only slightly perturbed in the BCS ground state.



- Momentum space density distribution is reminiscent of a Fermi surface at zero temperature
- At finite temperature, the quasi-particle excitation is centered around the Fermi surface

Energy gap at zero temperature

$$1 = \frac{|U|}{\mathcal{V}} \sum_{\mathbf{k}} \frac{1}{2E_k}$$
$$= \int_{\epsilon_F - \hbar\omega}^{\epsilon_F + \hbar\omega} d\epsilon \frac{g(\epsilon)}{2} \frac{|U|}{2\sqrt{(\epsilon - \epsilon_F)^2 + |\Delta|^2}}$$
$$\approx |U| \int_0^{\hbar\omega/\Delta} dx \frac{g(\epsilon_F)}{2\sqrt{x^2+1}} \qquad x = \epsilon - \epsilon_F$$
$$= \frac{|U| g(\epsilon_F)}{2} \sinh^{-1} \frac{\hbar\omega}{\Delta}$$

Therefore

$$\Delta = 2\hbar\omega \exp\left[-\frac{2}{g(\epsilon_F)|U|} \right]$$

Critical temperature

$$1 = \frac{|U|}{\mathcal{V}} \sum_{\mathbf{k}} \frac{1 - 2f(E_k)}{2E_k} \Bigg|_{T = T_c, \Delta = 0}$$
$$\approx \int_0^{\beta_c \hbar\omega} |U| \frac{g(\epsilon_F)}{2} \frac{dx}{x} \left[1 - \frac{2}{e^x + 1} \right], \qquad x = \beta_c(\epsilon_k - \mu)$$
$$\approx \frac{|U| g(\epsilon_F)}{2} \left\{ \ln \beta_c \hbar\omega \left[1 - \frac{2}{e^{\beta_c \hbar\omega} + 1} \right] + 2 \int_0^\infty \ln x \frac{\partial}{\partial x} \frac{1}{e^x + 1} \right\}$$
$$= \frac{|U| g(\epsilon_F)}{2} \left\{ \ln \beta_c \hbar\omega + \ln \left(\frac{2\gamma_E}{\pi} \right) \right\}$$

Therefore

$$k_B T_c \approx \hbar\omega \frac{2\gamma_E}{\pi} \exp\left[-\frac{2}{|U| g(\epsilon_F)} \right],$$

with the ratio

$$\frac{2\Delta(T=0)}{k_B T_c} \approx 3.53$$

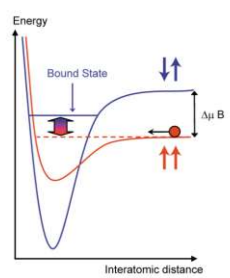
BCS-BEC Crossover

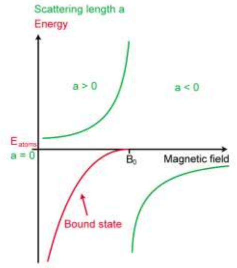
D.M. Eagles (1969) and A.J. Leggett (1980) pointed out that the BCS wavefunction has wider applications

$$|\Psi\rangle_{BCS} = \mathcal{N}\prod_{\mathbf{k}}(u_{\mathbf{k}} + v_{\mathbf{k}} a^\dagger_{\mathbf{k}\uparrow} a^\dagger_{-\mathbf{k}\downarrow})|\text{vac}\rangle$$

- The wavefunction should be able to describe pairing from weak to strong interaction limit
- Need to relax the condition that $\mu \approx E_F$, instead, the chemical potential can be determined self consistently from the number equation
- To solve for physical parameters, one needs to solve the gap equation and the number equation simultaneously
- Only a theory before the advent of cold atoms etc. as it is very hard to tune the interaction with solid materials

Feshbach resonance and crossover picture

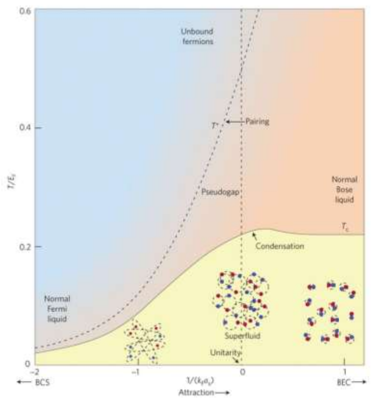


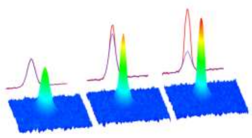


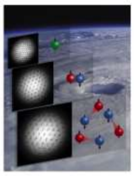
s-wave scattering length tunable via magnetic field

$$a_s = a_{bg}\left(1 - \frac{W}{B - B_0}\right)$$

BCS-BEC crossover in ultracold fermions







Two channel model

$$\begin{aligned} H - \mu N = &\sum_{\sigma,\mathbf{k}}(\epsilon_{\mathbf{k}} - \mu)a^\dagger_{\mathbf{k},\sigma}a_{\mathbf{k},\sigma} + \sum_{\mathbf{q}}(\gamma + \epsilon_{\mathbf{q}}/2 - 2\mu)b^\dagger_{\mathbf{q}}b_{\mathbf{q}} \\ &+ \left(g/\sqrt{\mathcal{V}}\right)\sum_{\mathbf{k},\mathbf{q}}\left(b^\dagger_{\mathbf{q}}a_{-\mathbf{k}+\mathbf{q}/2,\downarrow}a_{\mathbf{k}+\mathbf{q}/2,\uparrow} + h.c.\right) \\ &+ (U/\mathcal{V})\sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} a^\dagger_{\mathbf{k}+\mathbf{q}/2,\uparrow}a^\dagger_{-\mathbf{k}+\mathbf{q}/2,\downarrow}a_{-\mathbf{k}'+\mathbf{q}/2,\downarrow}a_{\mathbf{k}'+\mathbf{q}/2,\uparrow}, \end{aligned}$$

where $a^\dagger_{\mathbf{k},\sigma}$ and $b^\dagger_{\mathbf{q}}$ are the creation operators for the open channel fermions and the closed channel bosons; μ is the atom chemical potential; $N = \sum_{\mathbf{k}\sigma} a^\dagger_{\mathbf{k}}a_{\mathbf{k}} + 2\sum_{\mathbf{q}} b^\dagger_{\mathbf{q}}b_{\mathbf{q}}$ is the total particle number; $\epsilon_{\mathbf{k}} = \hbar^2k^2/(2m)$; $\mathcal{V}$ is the quantization volume; $\sigma = \uparrow,\downarrow$ denotes the different hyperfine states of the atoms; γ is the bare detuning.

Single channel model

$$\begin{aligned} H - \mu N = &\sum_{\sigma,\mathbf{k}}(\epsilon_{\mathbf{k}} - \mu)a^\dagger_{\mathbf{k},\sigma}a_{\mathbf{k},\sigma} \\ &+ (U/\mathcal{V})\sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} a^\dagger_{\mathbf{k}+\mathbf{q}/2,\uparrow}a^\dagger_{-\mathbf{k}+\mathbf{q}/2,\downarrow}a_{-\mathbf{k}'+\mathbf{q}/2,\downarrow}a_{\mathbf{k}'+\mathbf{q}/2,\uparrow} \end{aligned}$$

- U is the bare interaction rate, which needs to be renormalized in order to be connected with the experimental parameters
- For most experiments with ^{6}Li and ^{40}K, the resonance is 'wide', i.e. population of the closed channel is negligible, which means single channel model is sufficient
- There are 'narrow' Feshbach resonances that need to be modeled with two channel Hamiltonian
- We will focus on the single channel model henceforth

Effective single channel Hamiltonian

$$\begin{aligned} H - \mu N = &\sum_{\mathbf{k},\sigma}(\epsilon_{\mathbf{k}} - \mu)\,a^\dagger_{\mathbf{k},\sigma}a_{\mathbf{k},\sigma} \\ &- \sum_{\mathbf{k}}\left(\Delta a^\dagger_{\mathbf{k},\uparrow}a^\dagger_{-\mathbf{k},\downarrow} + \Delta^* a_{-\mathbf{k},\downarrow}a_{\mathbf{k},\uparrow}\right) - \frac{|\Delta|^2}{U} \end{aligned}$$

With the order parameter

$$\Delta = -\frac{U}{\mathcal{V}}\sum_{\mathbf{k}}\langle a_{-\mathbf{k},\downarrow}a_{\mathbf{k},\uparrow}\rangle$$

- Same in form as the effective BCS Hamiltonian
- It leads to the same form of gap equation as before
- In addition, from $N = -\frac{\partial\langle H - \mu N\rangle}{\partial\mu}$, we have the number equation (zero temperature)

Gap equation and number equation (zero temperature)

$$-\frac{1}{U} = \frac{1}{\mathcal{V}}\sum_{\mathbf{k}}\frac{1}{2E_k}$$

$$n = \frac{1}{\mathcal{V}}\sum_{\mathbf{k}}\left(1 - \frac{\epsilon_k - \mu}{E_k}\right)$$

- $E_k = \sqrt{|\Delta|^2 + (\epsilon_k - \mu)^2}$
- In the standard BCS theory, U is only non-vanishing within a small energy range around Fermi surface. This is no longer the case for cold atom scattering with psuedo-potential
- If we take the bare interaction rate to be the pseudo-potential $U = \frac{4\pi\hbar^2 a_s}{m}$, where $a_s = a_{\text{bg}}(1 - \frac{W}{B - B_0})$, the summation in the gap equation diverges: ultraviolet divergence
- As in the Bogoliubov theory for Bosons, we need to renormalize the bare interaction rate

Renormalization (review)

- We start from the formal Lippmann-Schwinger equation

$$T = U + U\frac{1}{E - H_0 + i\delta}T$$

- Project it into k-space, and taking the zero energy scattering limit (hence also neglecting $i\delta$)

$$U_p = U - \frac{UU_p}{\mathcal{V}}\sum_{\mathbf{k}}\frac{1}{2\epsilon_k}$$

- Therefore we have

$$\frac{1}{U} = \frac{1}{U_p} - \frac{1}{\mathcal{V}}\sum_{\mathbf{k}}\frac{1}{2\epsilon_k}$$

The renormalized gap equation and number equation

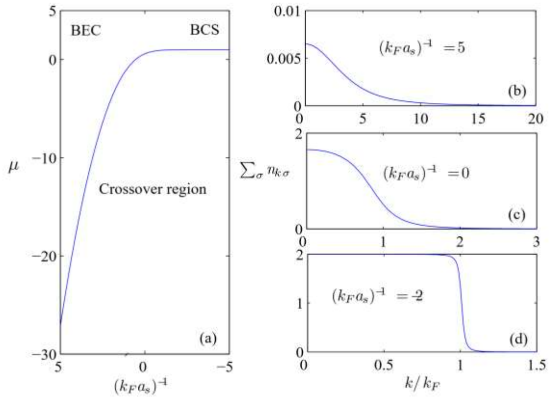
$$-\frac{1}{U_{\mathrm{p}}} = \frac{1}{\mathcal{V}}\sum_{\mathbf{k}}\left(\frac{1}{2E_k} - \frac{1}{2\epsilon_k}\right)$$
$$n = \frac{1}{\mathcal{V}}\sum_{\mathbf{k}}\left(1 - \frac{\epsilon_k - \mu}{E_k}\right)$$

With the physical interaction rate

$$U_{\mathrm{p}} = \frac{4\pi\hbar^2}{m}a_s = \frac{4\pi\hbar^2}{m}a_{\mathrm{bg}}\left(1 - \frac{W}{B - B_0}\right)$$

- These equations need to be solved simultaneously for μ and Δ, as a function of the external magnetic field, or equivalently, $(k_F a_s)^{-1}$
- The background scattering length is the scattering length in the open channel, far away from the resonant point

BCS-BEC crossover mean field results



Finite temperature mean field equations
We have already derived the gap equation

$$-\frac{1}{U} = \frac{1}{\mathcal{V}}\sum_{\mathbf{k}}\left(\frac{1-2f(E_k)}{2E_k}\right) = \frac{1}{\mathcal{V}}\sum_{\mathbf{k}}\frac{1}{2E_k}\tanh\left(\frac{\beta E_k}{2}\right)$$

For the number equation, note $N = \sum_{\mathbf{k},\sigma}\left\langle a^\dagger_{\mathbf{k},\sigma}a_{\mathbf{k},\sigma}\right\rangle$, we have

$$n = \frac{1}{\mathcal{V}}\sum_{\mathbf{k}}\left[1 - \frac{\epsilon_k - \mu}{E_k} + 2\frac{\epsilon_k - \mu}{E_k}f(E_k)\right]$$
$$= \frac{1}{\mathcal{V}}\sum_{\mathbf{k}}\left[1 - \frac{\epsilon_k - \mu}{E_k}\tanh\left(\frac{\beta E_k}{2}\right)\right]$$

Alternatively, one can first calculate the thermodynamic potential $\Omega = -\frac{1}{\beta}\ln\mathrm{tr}\left[e^{-\beta(H-\mu N)}\right]$ and derive the gap and number equations from the conditions: $\frac{\partial\Omega}{\partial|\Delta|^2} = 0$ and $N = -\frac{\partial\Omega}{\partial\mu}$.

Further discussions of mean field theory

- Very good approximation in the weak coupling BCS limit
- In the BEC limit, single channel model fails, as population in the closed channel becomes important
- However, on the BEC side, two channel model treats the closed channel molecules as structureless bosons. Hence, the two channel model cannot reproduce the experimental measurement on the scattering properties of the Feshbach molecules
- In the strongly interacting region, i.e. $-1 < (k_F a_s)^{-1} < 1$, single channel and two channel models yield similar results for wide resonance ($g\sqrt{n} \gg E_F$). Therefore, for these wide resonance, single channel model is sufficient
- Yet in the strongly interacting region, mean field theories in general become unreliable, as quantum depletion becomes important
- The strongly interacting region is physically the most interesting region

Experimental parameters

- ^{6}Li: (MIT, Innsbruck)
  $\{|F=\frac{1}{2}, m_F=\frac{1}{2}\rangle, |F=\frac{1}{2}, m_F=-\frac{1}{2}\rangle\}$,
  $B_0 \approx 834G$, $a_{\mathrm{bg}} \approx -1405a_0$, $W \approx 300G$,
  $\frac{g\sqrt{n}}{E_F} \sim 98$ for $n \sim 10^{13}cm^{-3}$
- ^{40}K: (JILA)
  $\{|F=\frac{9}{2}, m_F=-\frac{9}{2}\rangle, |F=\frac{9}{2}, m_F=-\frac{7}{2}\rangle\}$,
  $B_0 \approx 202G$, $a_{\mathrm{bg}} \approx 174a_0$, $W \approx 7.8G$,
  $\frac{g\sqrt{n}}{E_F} \sim 13$ for $n \sim 10^{13}cm^{-3}$
- For both species, $\frac{g\sqrt{n}}{E_F} \gg 1$, therefore both are wide resonance.
- Some literatures use the following parameter to characterize the type of resonance

$$\bar{\gamma} = \frac{m a_{\mathrm{bg}}^2 W^2 \mu_{\mathrm{co}}^2}{E_F} = \left[\frac{3\sqrt{2}}{16}\pi\frac{g^2 n}{E_F^2}\right]^2$$

Beyond Mean Field

Approaching BCS-BEC crossover region beyond mean field

- Self consistent many-body approaches: Saddle point expansion, self-consistent Green's function approach etc.
- Numerical simulations: Quantum Monte Carlo etc.
- Exact solution at unitary point $(k_F a_s)^{-1} = 0$

Path integral approach

$$H = \int dx\psi^\dagger_\sigma(x)\left(-\frac{\nabla^2}{2m}\right)\psi_\sigma(x) + U\int dx\psi^\dagger_\uparrow(x)\psi^\dagger_\downarrow(x)\psi_\downarrow(x)\psi_\uparrow(x)$$

The finite temperature grand canonical partition function Z in the form of path integrals

$$Z = \mathrm{Tr}e^{-\beta(H-\mu N)} = \int\mathcal{D}\left[\psi^\dagger,\psi\right]e^{-S[\psi^\dagger,\psi]},$$

where the action is

$$S\left[\psi^\dagger,\psi\right] = \int_0^\beta d\tau\left\{\int d^3\mathbf{r}\psi^\dagger(x)\left(\frac{\partial}{\partial\tau} - \mu\right)\psi(x) + H\right\}$$

Note $\beta = 1/T$, $x = (\mathbf{r},\tau)$.

see e.g. *Quantum Many-Particle Systems* by J. W. Negele and H. Orland

Hubbard-Stratonovich transformation: introduce an auxiliary boson field, which makes the action quadratic. Define

$$\xi(x) = \psi_\downarrow(x)\psi_\uparrow(x)$$

Then we have

$$e^{U\int x\psi^\dagger_\uparrow(x)\psi^\dagger_\downarrow(x)\psi_\downarrow(x)\psi_\uparrow(x)} = e^{\int dx\xi^\dagger(x)U\xi(x)}$$

Making use of the Gaussian integral

$$e^{\int dx\xi^*(x)\Lambda^{-1}(x)\xi(x)} = \left[\det\Lambda(x)\right]$$
$$\times\int\mathcal{D}\left[\eta^*,\eta\right]e^{-\int dx\eta^*(x)\Lambda(x)\eta(x)+\int dx\xi^*(x)\eta(x)+\int dx\xi(x)\eta^*(x)}$$

Setting $\Lambda^{-1}(x) = U$, $\Delta(x) = \eta(x)$, we have

$$e^{\int dx\xi^\dagger(x)U\xi(x)} = \int\mathcal{D}\left[\Delta^*,\Delta\right]e^{\int dx\left\{-\frac{|\Delta|^2}{U}+\psi^\dagger_\uparrow(x)\psi^\dagger_\downarrow(x)\Delta(x)+\psi_\downarrow(x)\psi(x)_\uparrow\Delta^*(x)\right\}}$$

The partition function now looks like

$$\begin{aligned} Z &= \int \mathcal{D}\left[\Delta^*, \Delta\right] e^{\int dx \frac{|\Delta|^2}{U}} \\ &\times \int \mathcal{D}\left[\psi^*, \psi\right] e^{-\int dx \left\{\psi_\sigma^\dagger\left(-\frac{\nabla^2}{2m}+\partial_\tau-\mu\right)\psi_\sigma+\psi_\uparrow^\dagger\psi_\downarrow^\dagger\Delta+\psi_\downarrow\psi_\uparrow\Delta^*\right\}} \\ &= \int \mathcal{D}\left[\Delta^*, \Delta\right] e^{\int dx \frac{|\Delta|^2}{U}+\mu} \int \mathcal{D}\left[\psi^*, \psi\right] e^{\int dx \psi^\dagger G^{-1}\psi}, \end{aligned}$$

where we identify the Green's function (Nambu)

$$G^{-1}(x) = \begin{pmatrix} -\partial_\tau + \frac{\nabla^2}{2m} + \mu & \Delta(x) \\ \Delta^*(x) & -\partial_\tau - \frac{\nabla^2}{2m} - \mu \end{pmatrix}$$

Now we may integrate out the fermion fields $\psi^\dagger, \psi$, which is again a Gaussian integral (but over fermion field).

The final form of the partition function

$$Z = \int \mathcal{D}\left[\Delta^*, \Delta\right] e^{-S_{\text{eff}}[\Delta^*, \Delta]}$$

And the effective action

$$S_{\text{eff}}\left[\Delta^*, \Delta\right] = -\int dx \left\{\frac{|\Delta(x)|^2}{U} + \mu + \text{Tr}\left[\ln G^{-1}(x)\right]\right\}$$

Hence, one must find approximate ways to calculate $\text{Tr}\left[\ln G^{-1}(x)\right]$, which is equivalent to the Green's function approach. To proceed, we may rewrite the Green's function matrix

$$G^{-1} = G_0^{-1} + \Sigma = \begin{pmatrix} -\partial_\tau + \frac{\nabla^2}{2m} + \mu & \Delta_0 \\ \Delta_0^* & -\partial_\tau - \frac{\nabla^2}{2m} - \mu \end{pmatrix} + \begin{pmatrix} 0 & \varphi(x) \\ \varphi^*(x) & 0 \end{pmatrix}$$

With the expansion $\Delta(x) = \Delta_0 + \varphi(x)$, where Δ_0 is the stationary state solution (saddle point).

The saddle point equation and the number equation can be derived

$$\left.\frac{\delta S_{\text{eff}}\left[\Delta(x)\right]}{\delta \Delta^*(x)}\right|_{\Delta_0} = 0$$

$$N = \frac{1}{\beta}\frac{\partial}{\partial \mu}\ln Z_0 = -\frac{1}{\beta}\left.\frac{\partial S_{\text{eff}}}{\partial \mu}\right|_{\Delta_0}$$

After some manipulations,

$$-\frac{1}{U} = \frac{1}{\mathcal{V}}\sum_{\mathbf{k}} \frac{1}{2E_k}\tanh\left(\frac{\beta E_k}{2}\right)$$

$$n = \frac{1}{\mathcal{V}}\sum_{\mathbf{k}}\left\{1 - \frac{\epsilon_k - \mu}{E_k}\tanh\left(\frac{\beta E_k}{2}\right)\right\}$$

These are just the finite temperature BCS gap and number equations.

Gaussian fluctuations around the saddle point $\varphi(x)$

- Substitute the Hubbard-Stratonovich field expansion $\Delta(x) = \Delta_0 + \varphi(x)$ into the action, and expand to the second order in $\{\varphi, \varphi^*\}$

$$S_{\text{eff}}\left[\varphi\right] = S_0 + S_1\left[\varphi\right] + S_2\left[\varphi^2\right] + O(\varphi^3)$$

- S_0 is the saddle point action, first order expansion S_1 vanishes
- Fourier transform into momentum space to get

$$S_2\left[\varphi\right] = \frac{1}{2}\sum_k \begin{pmatrix} \varphi^*(k) & \varphi(-k) \end{pmatrix} M(k) \begin{pmatrix} \varphi(k) \\ \varphi^*(-k) \end{pmatrix}$$

- Modify the gap or the number equations or both

Some variations

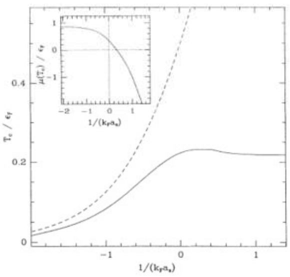
- Set $\Delta_0 = 0$, modify the number equation using the Gaussian fluctuations to solve for T_c. (Nosières, Schmitt-Rink scheme)
- For $T < T_c$, modify the number equation to solve for order parameter and other properties. (Broken symmetry scheme)
- Alternatively, T-matrix formalism

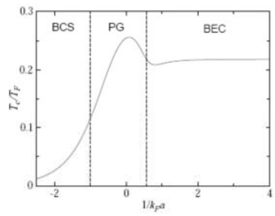
$$T = U + U\chi T$$

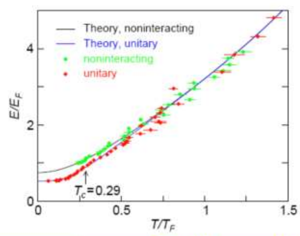
$$\chi = G_0 G_0$$

Let $G_{\text{free}} = G_0|_{\Delta_0=0}$, we have
  - NSR scheme: $\chi = G_{\text{free}}G_{\text{free}}$ (only above T_c)
  - Symmetric scheme: $\chi = GG$
  - Asymmetric scheme: $\chi = G_{\text{free}}G$

How do these theories behave?

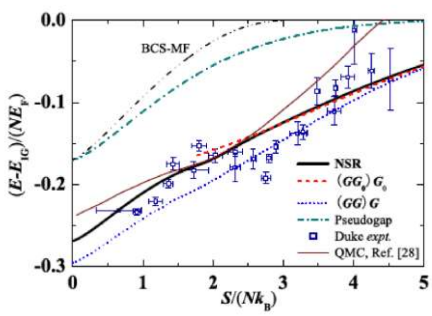






C.A.R. Sá de Melo et al., PRL 71, 3202 (1993)
Q.-J. Chen et al., Phys. Rep. 412, 1 (2005)
Q.-J. Chen et al., Low Temp. Phys. 32(4), 406 (2006)

More on the comparison with experiment



H. Hu et al., Phys. Rev. A 77, 0601605(R) (2008)

Next Lecture

Interesting topics

- Brief overview of ultracold atomic Fermi gases
- Topics of BCS-BEC crossover
  - Collective modes
  - Gap and pseudogap
  - Unitary gas
  - Polarized Fermi gas
  - Polaron/Itinerant Ferromagnetism

Quantum Degenerate Gases

Lecture 10: Topics in BCS-BEC Crossover

易为

University of Science and Technology of China

Spring 2022

中国科学技术大学

Contents

Reference:
S. Giorgini, L. P. Pitaevskii, S. Stringari, Rev. Mod. Phys. 80, 1215 (2008)
T. Köhler, K. Goral, and P. S. Julienne, Rev. Mod. Phys. 78, 1311 (2006)

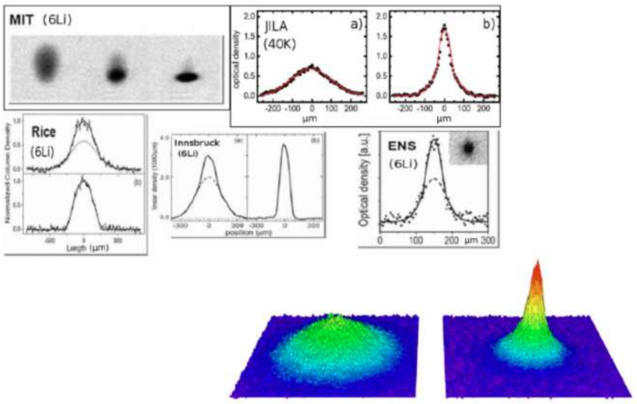
Brief Overview of Experiments

Degenerate Fermi gas

- Similar scaling of degenerate temperatures: $k_B T_d \sim \frac{\hbar^2 n^{2/3}}{m}$
- Phase transition vs. smooth crossover (non-interacting)
- Condensate of Cooper pairs only occurs due to interaction
- Effects of Pauli blocking

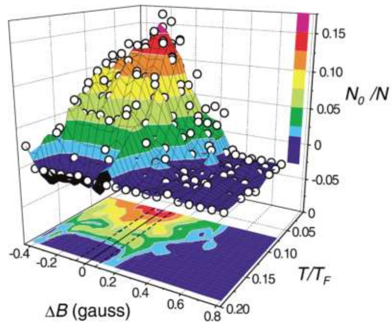
- De Marco et al. (JILA) quantum degeneracy of ^{40}K (1999)
- Schreck et al. (ENS), Truscott et al. (Rice) quantum degeneracy of ^{6}Li (2001); sympathetic cooling with ^{7}Li
- Courteille et al. (UT and EUT), Inouye et al. (MIT) Feshbach resonance in bosonic systems (1998)
  - For bosons, atom-dimer relaxation rate $\sim a$ $(a>0)$ E. Nielsen et al. (1999)
  - For fermions, atom-dimer relaxation rate $\sim a^{-3.33}$ $(a>0)$, dimer-dimer relaxation rate $\sim a^{-2.55}$ $(a>0)$ Petrov et al. (2004,2005)
  - Three body recombination rate increases with increasing $|a|$
- Greiner et al. (JILA), Jochim et al.(Innsbruck), Zwierlein et al.(MIT), molecular BEC from a Fermi sea (2003); Bourdel et al. (ENS, 2004), Partridge et al. (Rice, 2005)
- Regal et al. (JILA), Zwierlein et al. (MIT), condensation of pairs on the fermionic side (2004)

Molecular BEC from a Fermi sea



Greiner et al. Nature 426, 537 (2003)

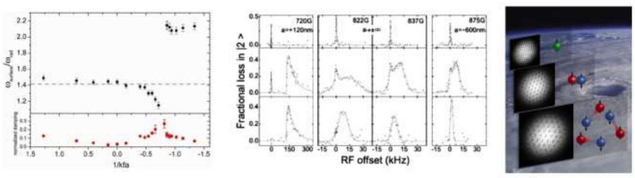
Pairwise projection and condensate fraction



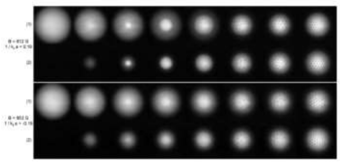
Regal et al. Phys. Rev. Lett. 92, 040403 (2004)

Other key measurements

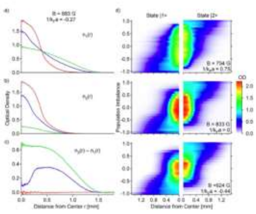
- Bartenstein et al. (Innsbruck), Kinast et al. (Duke), collective excitations of Fermi superfluid (2004)
- Chin et al. (Innsbruck), pairing gap measurement via rf excitation spectra(2004)
- Zwierlein et al. (MIT), observation of quantized vortices in Fermi condensate (2005)

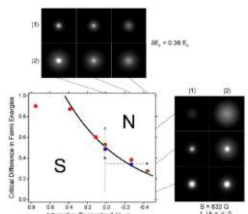


- Schunck et al. (MIT), Patridge et al. (Rice), Fermi condensate with spin imbalance (2006)



M.W. Zwierlein et al., Science 311, 492 (2006)

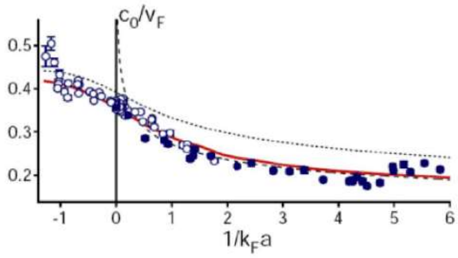




Collective excitations

- In the BEC limit, molecular BEC. The low energy excitations should be Bogoliubov phonons
- In the BCS limit, condensate of Cooper pairs. In addition to the quasi-particle excitations (pair breaking), there would be long wavelength Bogoliubov-Anderson excitations (up to frequency $\Delta/\hbar$), which are also gapless Goldstone modes.
- In the BCS limit, at low temperatures, the collective modes are characterized by that of a non-interacting Fermi liquid $c_s \approx \frac{v_F}{\sqrt{3}}$
- In the BEC limit, speed of sound following the Bosonic Bogoliubov theory
- Experimental signals: speed of sound and critical velocity in the crossover region

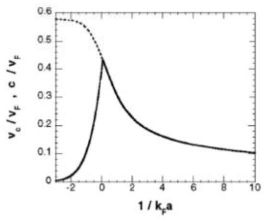
Speed of sound



J. Joseph et al. PRL 98, 170401 (2007)

- Mean field result with $a_{\text{mol}} = 0.6a_s$ agrees well with experimental result
- Mean field with BCS like state gives significantly higher sound speed

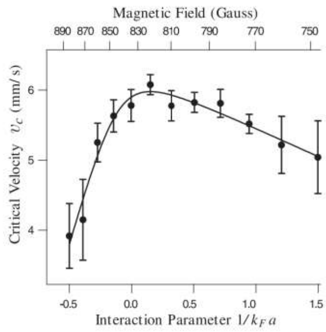
Landau's critical velocity vs. speed of sound throughout crossover region



R. Combescot et al. Phys. Rev. A 74, 042717 (2006)

- At low frequencies, the excitation is gapless and phonon like, characterized by a sound speed
- At high frequencies, the excitation is a gapped pair breaking process, which gives a critical velocity by Landau's criteria
- Landau critical velocity is the smaller of the two

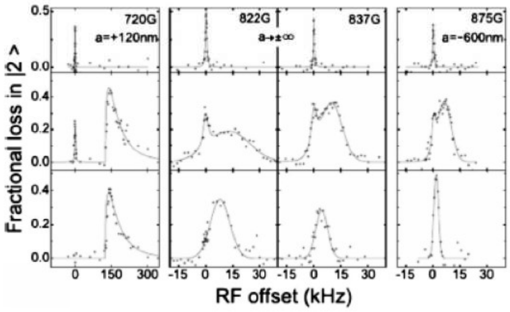
Critical velocity



D. E. Miller et al., Phys. Rev. Lett. 99, 070402 (2007)

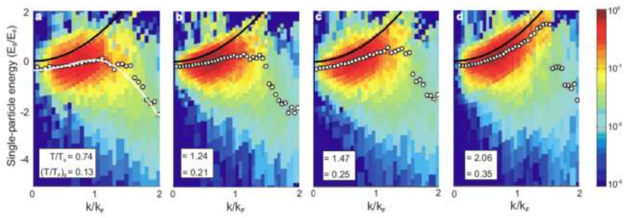
- Critical velocity peaking at the crossover region

Gap/Pseudogap measurement: r.f. spectroscopy



C. Chin et al. Science 05, 1128 (2004)

'ARPES' with ultracold atoms



J.T. Stewart et al. Nature 454, 744 (2008)

- Measurement of dispersion of single particle excitation via momentum resolved rf spectroscopy
- Pseudo-gap (pre-formed pairs) above T_c?

Unitary gas

- At resonance, $(k_F a_s)^{-1} = 0$, the only relevant length scale left is $(1/n)^{1/3}$
- Universality: properties of a degenerate Fermi gas near resonance are characterized by only a few universal numbers
- Universal relations

$$\mu = (1+\beta)E_F$$
$$c = (1+\beta)^{1/2} v_F/\sqrt{3}$$
$$T_c = \alpha T_F$$

QMC gives $\beta \approx 0.58$, lattice QMC gives $\alpha \approx 0.157$

- Exact results for short-range interactions, Tan's relations

Reference:
T.-L. Ho PRL 92, 090402 (2004)
S.-N. Tan Ann. Phys. 323, 2952; *ibid* 323, 2971; *ibid* 323, 2987 (2008)
E. Braaten et al. PRL 100, 205301 (2008)

Tan's relations

- Relates the asymptotic behavior of many-body systems at short-range to thermodynamic properties
- $1/k^4$ tail in momentum distribution $\lim_{k\to\infty} n(k) = C/k^4$
- $1/\omega^{5/2}$ tail in rf-spectroscopy
- Adiabatic sweep theorem

$$[dE/d(1/a)]_{S,N} = -\hbar^2 C/(4\pi m)$$

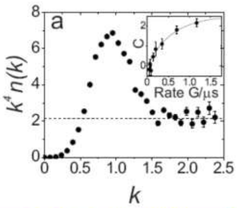
- Two-body interaction effects dominates at short-range

$$\psi(r) \propto (\frac{1}{r} - \frac{1}{a})$$

- Wide applicability
(zero/finite T, normal/superfluid, uniform/trapped...)

Experimental verifications

		β
Expt. ^{6}Li	ENS (1)	−0.59(15)
	Duke (2)	−0.49(4)
	Rice (3)	−0.54(5)
	Innsbruck (4)	$-0.73^{+0.12}_{-0.09}$
Expt. ^{40}K	JILA (5)	$-0.54^{+0.05}_{-0.12}$
Theory	BCS mean field	−0.41
	QMC (6,7,8)	−0.58(1)
	T-matrix (9)	−0.545

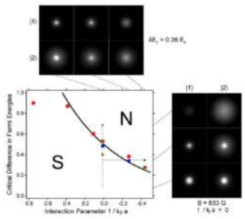


J. Stewart et al. PRL 104, 235301 (2010)
E. D. Kuhnle et al. PRL 105, 070402 (2010)

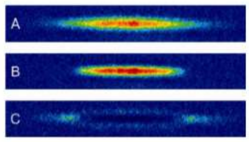
- $1/k^4$ tail in momentum distribution $\lim_{k\to\infty} n(k) = C/k^4$
- Can be extracted from structure factor measurement (Bragg spectroscopy)

Polarized Fermi gas

- Pairing superfluidity in the presence of chemical potential mismatch
- Quantum simulation of magnetized superconductor, cold dense quark matter, neutron stars, etc.



M.W. Zwierlein et al. Science 311, 492 (2006)

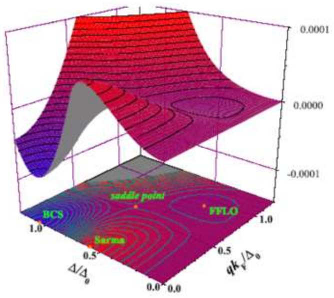


G.B. Partridge et al. Science 311, 503 (2006)

Mean field description

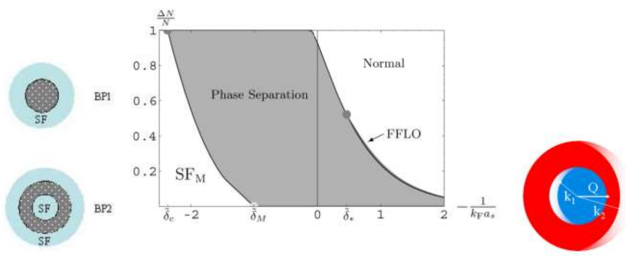
- Similar to the mean field theory of the BCS-BEC crossover, only need to introduce $\mu_\uparrow$ and $\mu_\downarrow$ separately
- Due to the existence of meta-stable and unstable states, need to be careful with the gap equation
- Minimize the thermodynamic potential while fixing the particle number of different spins
- In uniform system, also need to consider the possibility of phase separation
- Dispersion has the form $E_{k,\sigma} = \sqrt{(\epsilon_k - \bar{\mu})^2 + |\Delta|^2} \pm h$, where $\bar{\mu} = (\mu_\uparrow + \mu_\downarrow)/2$ and $h = \mu_\uparrow - \mu_\downarrow$
- There might be regions in the momentum space where one branch of the dispersion becomes negative. Fermions do not pair in these regions

Typical thermodynamic potential landscape



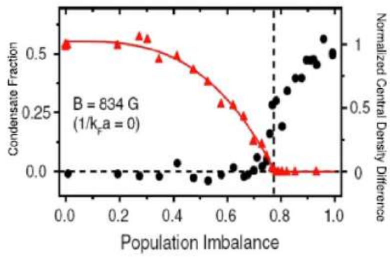
H. Hu et al. Phys. Rev. A 73, 051603(R) (2006)

What to expect



- Various exotic phases
- In trap, phase separation: SF core surrounded by polarized normal gas
- Experimentally, at critical population imbalance, gas undergoes SF-N phase transition at trap center

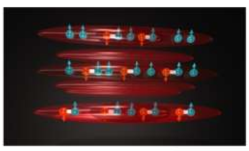
Phase separation

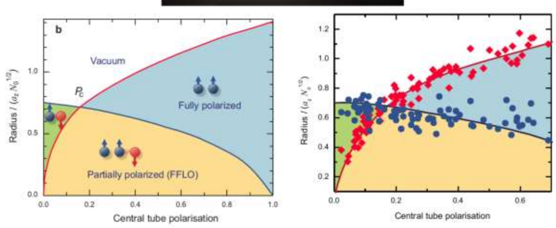


Y. Shin et al., PRL 97, 030401 (2006)

- Mean field not sufficient. Critical population imbalance ~ 0.75 at unitarity
- Influence of trap anisotropy

Rice Experiment





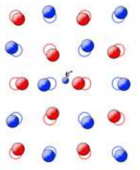
- Evidence of FFLO state (Rice, Nature)

Polaron physics

- Quasiparticle excitation describing a single impurity moving in its environment (in a general sense)

Polaron physics

- Quasiparticle excitation describing a single impurity moving in its environment (in a general sense)
- Landau (localized electrons) and Pekar (phonon clouds) (1933-1951)
- The Fröhlich polaron (1950s)



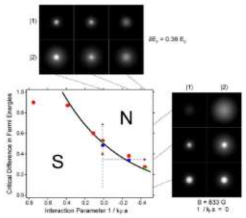
- Electron-phonon interaction in solids
- Phonons not affected by a single electron
- Brillouin-Wigner perturbation theory

$$E_p = E_0 + \frac{p^2}{2m^*} + O(p^4)$$

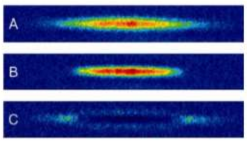
- Large (Fröhlich) vs. small polarons (Landau)

In cold atoms

- Pairing in polarized Fermi gases



M. W. Zwierlein et al. Science 311, 492 (2006)

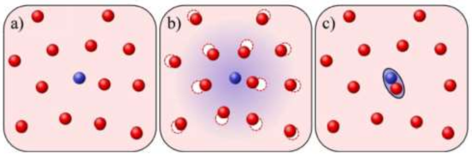


G. B. Partridge et al. Science 311, 503 (2006)

- Large-polarization limit: polaron physics
- Interaction tunable through Feshbach resonance

Fate of impurity: limiting cases and those in between

- Weak-interaction limit: free impurity
- Strong-interaction limit: impurity-atom dimer

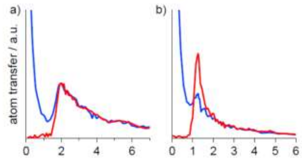


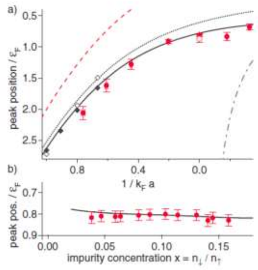
From Phys. Rev. Lett. 102, 230402 (2009)

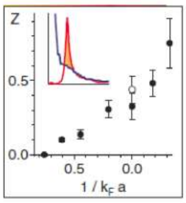
- Inbetween: polaronic branch and dimeronic branch
- Transition occurs between polaronic quasiparticles and many-body bound states
- Predicted by diagrammatic QMC calculations

N. Prokof'ev and B. Svistunov, Phys. Rev. B 77, 020408(R) (2008)

Early experiments on polaron-molecule transition I



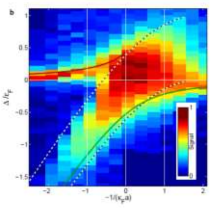




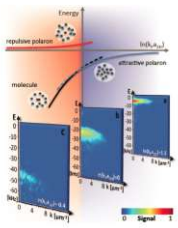
- rf-spectroscopy measurement
- Weakly interacting quasiparticle
- Polaron-molecule transition
- Consistent with QMC

A. Schirotzek, C.-H. Wu, A. Sommer, M. W. Zwierlein, Phys. Rev. Lett. 102, 230402 (2009)

Early experiments on polaron-molecule transition II



C. Kohstall, *et al.*, Nature 485, 615 (2012)

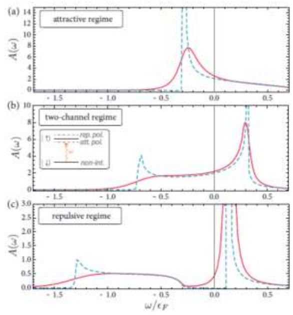


M. Koschorreck, *et al.*, Nature 485, 619 (2012)

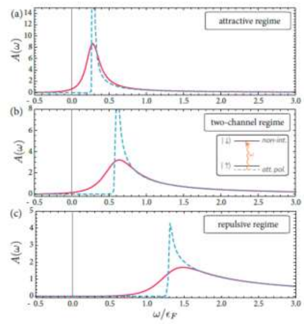
- Attractive and repulsive polarons in 3D and 2D
- Repulsive polaron: a metastable quasiparticle
- Molecule-hole continuum
- Consistent with calculations based on perturbation theory

Detection schemes

- Reverse rf spectroscopy



- Standard rf spectroscopy



R. Schimdt, M. Knap, D. A. Ivanov, J.-S. You, M. Cetina, E. Demler, Rep. Prog. Phys. 81, 024401 (2018)

How to characterize polarons theoretically?

- Variational approach: Chevy's ansatz
  F. Chevy, Phys. Rev. A 74, 063628 (2006)
- T-matrix approach
  R. Combescot, A. Recati, C. Lobo, F. Chevy, Phys. Rev. Lett. 98, 180402 (2007)
  M. Punk, W. Zwerger Phys. Rev. Lett. 99, 170404 (2007)
- $1/N$ expansion
  M. Veillette *e al.*, Phys. Rev. A 78, 033614 (2008)
- Fixed-node QMC
  C. Lobo, A. Recati, S. Giorgini, S. Stringari, Phys. Rev. Lett. 97, 200403 (2006)
- Diagrammatic QMC
  N. V. Prokof'ev, B. V. Svistunov, Phys. Rev. B 77, 020408(R) (2008)
- Other
  R. Schimdt, *et al.*, Rep. Prog. Phys. 81, 024401 (2018)

Chevy's ansatz (polarons in a polarized two-component Fermi gas)

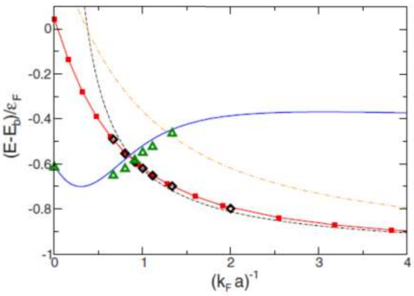
- Polaron ansatz wave function

$$|\Psi\rangle_{\mathbf{Q}} = \left(\psi_{\mathbf{Q}} b^\dagger_{\mathbf{Q}} + \sum_{q<k_F, k>k_F} \psi_{\mathbf{kq}} b^\dagger_{\mathbf{Q-k+q}} a^\dagger_{\mathbf{k}} a_{\mathbf{q}}\right) |\mathrm{FS}\rangle_N$$

- Minimize $\langle\Psi|H|\Psi\rangle_{\mathbf{Q}}$ or $H|\Psi\rangle_{\mathbf{Q}} = E_P|\Psi\rangle_{\mathbf{Q}}$ (truncation)
- More particle-hole excitations possible
- Competing state: the molecular state

$$|M\rangle_{\mathbf{Q}} = \sum_{k>k_F} \phi_{\mathbf{k}} b^\dagger_{\mathbf{Q-k}} a^\dagger_{\mathbf{k}} |\mathrm{FS}\rangle_{N-1} + \sum_{k,k'>k_F} \phi_{\mathbf{kk'q}} b^\dagger_{\mathbf{Q-k-k'+q}} a^\dagger_{\mathbf{k}} a^\dagger_{\mathbf{k'}} a_{\mathbf{q}} |\mathrm{FS}\rangle_{N-1}$$

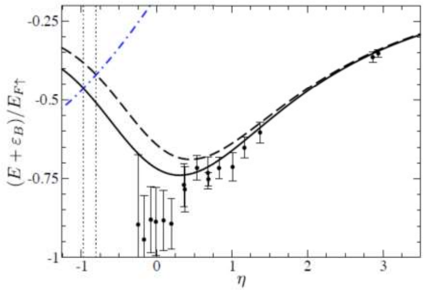
Comparison of results (3D)



- Compare $E_M - E_F$ with E_P ($E_b = -\hbar^2/ma_s^2$ subtracted)
- Crossing at $(k_F a_s)_c^{-1} = 0.84$ vs 0.90 (diagrammatic QMC)

M. Punk, P. T. Dumitrescu, W. Zwerger, Phys. Rev. A 80, 053605 (2009)

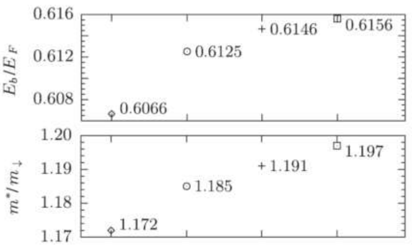
Comparison of results (2D)



- Polaron-molecule transition exists in 2D
- Polaron with single (two) particle-hole pair(s)

M. M. Parish, Phys. Rev. A 83, 051603(R) (2011)
M. M. Parish, J. Levinsen, Phys. Rev. A 87, 033616 (2013)
M. Koschorreck *et al.*, Nature 485, 619 (2012)

Convergence of results on the single particle-hole level

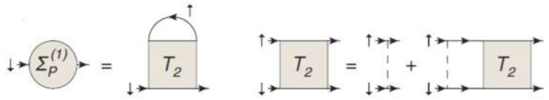


- Converge quickly at the lowest orders of particle-hole excitations
- Destructive interference between higher-order terms

R. Combescot, S. Giraud, Phys. Rev. Lett. 101, 050404 (2008)

T-matrix approach (polaron single-hole level)

$$G_\downarrow^{-1}(\mathbf{p},\omega) = \omega + i0^+ - \epsilon_{p\downarrow} - \Sigma(\mathbf{p},\omega)$$
$$\Sigma(\mathbf{p},\omega) = \Sigma^{(1)}(\mathbf{p},\omega) + \Sigma^{(2)}(\mathbf{p},\omega) + \ldots$$
$$E_P = \mathrm{Re}\left[\Sigma(\mathbf{p}=0, E_P)\right]$$

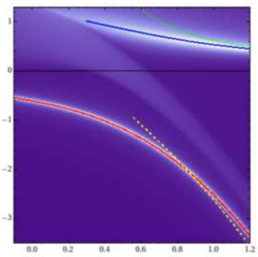


- Equivalent to the variational approach
- Better extendability, e.g., capable of analyzing losses

R. Combescot, A. Recati, C. Lobo, F. Chevy, Phys. Rev. Lett. 98, 180402 (2007)
G. M. Bruun and P. Massignan, Phys. Rev. Lett. 105, 020403 (2010)

General features in the spectral function

$$A_\downarrow(\mathbf{p},E) = -2\mathrm{Im}\frac{1}{E + i0^+ - \epsilon_{\mathbf{p}\downarrow} - \Sigma(\mathbf{p},E)}$$



- Attractive and repulsive polaron
- Broadening and decay channels
- Molecule-hole continuum

P. Massignan, G. Bruun, Eur. Phys. J. D 65, 83 (2011)

Polaron decay rate, impurity residue and effective mass

- Pole expansion (for well-defined quasiparticles)

$$G_\downarrow(\mathbf{p},\omega) \approx \frac{Z_P}{\omega - E_P - \frac{p^2}{2m^*} + i\frac{\Gamma_P}{2}}$$

- Impurity residue

$$Z_P = \{1 - \mathrm{Re}\left[\partial_\omega \Sigma(0, E_P)\right]\}^{-1}$$

- Effective mass

$$\frac{m}{m^*} = Z_P\left\{1 + \mathrm{Re}\left[\partial_{\epsilon_p}\Sigma(0,E_P)\right]\right\}$$

- Polaron decay rate

$$\Gamma_P = -2Z_P \mathrm{Im}\left[\Sigma(0,E_P)\right]$$

Outlook

Variants of the polaron problem

- Polaron in a Bose-Einstein condensate
- Polaron in a Fermi superfluid
- Polaron in spin-orbit coupled Fermi gas
- Rotating impurities: angulon

A probe to many-body system, a bridge between few and many...

Next Lecture: Optical Lattice

Quantum Degenerate Gases

Lecture 11: Cold Atoms in Optical Lattice Potentials

易为

University of Science and Technology of China

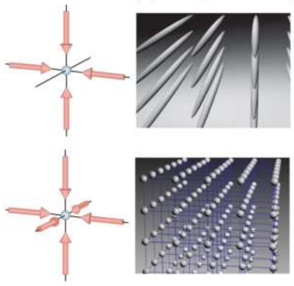
Spring 2022

中国科学技术大学

Contents

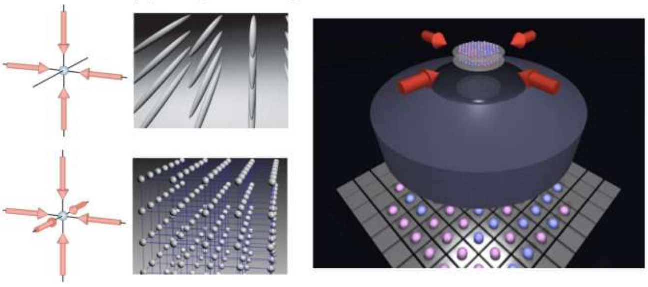
Optical Lattice

- Dipole trap: red-detuned (high-field seeking); blue-detuned (low-field seeking)
- Atoms trapped by standing-wave fields



Optical Lattice

- Dipole trap: red-detuned (high-field seeking); blue-detuned (low-field seeking)
- Atoms trapped by standing-wave fields



Optical Lattice

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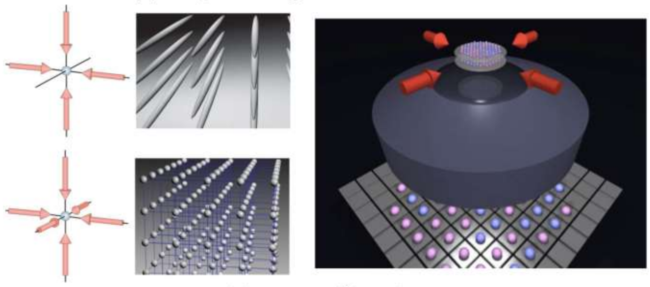
- Atoms trapped by standing-wave fields



- Lattice potential $V(\mathbf{r}) = V_0 \cos^2(\mathbf{k}\cdot\mathbf{r})$.

Wave function in a lattice potential

- Eigen problem under a periodic potential (one-dimensional for simplicity)

$$\begin{aligned} H &= -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial r^2} + V(r) \\ H\Psi &= E\Psi \\ V(r) &= V(r+R) \end{aligned}$$

- Define translation operator $T_R f(r) = f(r+R)$
- As $HT_R = T_R H$, we choose $\Psi(r)$ to be the mutual eigenstate of H and T_R
- Bloch's theorem (periodic boundary condition)

$$T_R\Psi(r) = C_R\Psi(r) = \Psi(r+R) = e^{ikR}\Psi(r)$$

- Assuming system size L, periodic boundary condition. k is then discretized.

Fourier transformation for periodic functions

- Normal Fourier transform

$$f(r) = \int e^{ikr} f(k) dk \qquad f(k) = \frac{1}{L}\int e^{-ikr} f(r) dr$$

- If $f(r) = f(r+R)$,

$$f(r+R) = \int e^{ikr} e^{ikR} f(k) dk$$

$$\Rightarrow \quad e^{ikR} = 1 \quad \text{for} \quad R = na \quad n \in \text{integer}$$

$$\Rightarrow \quad k \text{ is discretized as:} \quad K = m\frac{2\pi}{a} \quad m \in (0, \pm 1, \cdots)$$

- Fourier transformation for periodic functions

$$f(r) = \sum_K e^{iKr} f_K \qquad f_K = \frac{1}{a}\int_{\text{cell}} e^{-iKr} f(r) dr$$

Fourier transform the eigen problem

$$V(r) = \sum_K e^{iKr} V_K \qquad \text{this is periodical}$$

$$\Psi(r) = \sum_q c_q e^{iqr} \qquad \text{this is not}$$

K: reciprocal lattice vector
q: momentum space vector, discretized based on the system size L
Fourier transformed Schrödinger's equation:

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial r^2} + \sum_K e^{iKr} V_K\right)\sum_q c_q e^{iqr} = E\sum_q c_q e^{iqr}$$

$$\int e^{-iq'r} dr \times \Rightarrow \quad \frac{\hbar^2 q^2}{2m} c_q + \sum_K V_K c_{q-K} = E c_q$$

Importantly, coefficients in sectors $\{q, q-K, q-2K, \cdots\}$ are coupled.

Simplification:
We write $q = nG + k$, with $k \in (-\frac{\pi}{a}, \frac{\pi}{a})$, i.e. first Brillouin zone.

$$\frac{\hbar^2 k^2}{2m} c_k + \sum_n V_{nG} c_{k-nG} = E_k c_k,$$

where G is the unit vector of the reciprocal lattice, n is the band index.
Note:

- The number of coupled equations for each k is equal to the number of bands n, which depends on the $\max(q)$, or the inverse of the spatial resolution, which can be infinite. (matrix equation)
- The total number of eigen solutions for each k is then the number of bands. (matrix diagonalization)
- The number of independent sets of equations (different k) is equal to the number of discrete k in the 1BZ, which is the total number of sites N in the system. $(L = Na)$

In a more familiar form

- The Bloch function

$$\Psi_{nk}(r) = e^{ikr}u_{nk}(r) \qquad \text{with } u_{nk}(r) = \sum_n c_{k-nG}e^{-inGr}$$

- Eigen equations for $u_{nk}(r)$

$$\left[\frac{\hbar^2}{2m}\left(i\frac{\partial}{\partial r} + nG + k\right)^2 + V(r)\right]u_{nk}(r) = E_{nk}u_{nk}(r)$$

- Properties:

$$u_{n(k+G)}(r) = u_{nk}(r)e^{-iGr}$$
$$\Psi_{n(k+G)} = \Psi_{nk}$$
$$E_{n(k+G)} = E_{nk}$$

This is the translational symmetry of $\Psi_{nk}(r)$ in momentum space

Fourier transform of the Bloch function (Wannier function)

- Bloch function is periodic in momentum space
  $\Rightarrow$ Its Fourier components in real space is discrete
- Wannier function

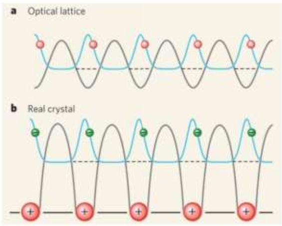
$$\Psi_{nk}(r) = \sum_R e^{ikR}\omega_{nR}(r)$$
$$\omega_{nR}(r) = \frac{a}{2\pi}\sum_{k\in 1BZ} e^{-ikR}\Psi_{nk}(r) = \frac{a}{2\pi}\sum_{k\in 1BZ}\Psi_{nk}(r-R)$$
$$= \omega_{n0}(r-R)$$

$\omega_{nR}(r)$ is only relevant with $r-R$, therefore sufficient to examine $\omega_{n0}(r) = \omega_n(r)$.

- Localized wavefunction in the tight-binding model (see later slides)

Bose-Hubbard model

Tight-binding in an optical lattice



- Consider the orthonormal bases: $\{\Psi_{nk}(r)\}$, and $\{\omega_{nR}(r)\}$:

$$\hat{\Psi}(r) = \sum_{nk\in 1BZ}\hat{C}_{nk}\Psi_{nk}(r), \qquad \hat{\Psi}(r) = \sum_{nR}\hat{C}_{nR}\omega_{nR}(r)$$
$$\hat{C}_{nR} = \sum_{k\in 1BZ} e^{ikR}\hat{C}_{nk}, \qquad \hat{C}_{nk} = \sum_R e^{-ikR}\hat{C}_{nR}$$

Tight-binding model in different forms

- Non-interacting Hamiltonian (single-band for simplicity)

$$H = \int \hat{\Psi}^\dagger(r)\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial r^2} + V(r)\right]\hat{\Psi}(r)dr$$

- Transform into the Wannier basis, and consider only overlap integrals between nearest neighbor sites

$$H = \sum_{RR'}\hat{C}_R^\dagger\hat{C}_{R'}\int \omega^*(r-R)\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial r^2} + V(r)\right]\omega(r-R')dr$$
$$= \epsilon(0)\sum_R \hat{C}_R^\dagger\hat{C}_R + \sum_{R,\rho}\epsilon(\rho)\hat{C}_R^\dagger\hat{C}_{R+\rho}$$

- Transform into the Bloch basis

$$H = \sum_{k\in 1BZ}\left[\epsilon(0) + \epsilon(\rho)\sum_\rho e^{ik\rho}\right]\hat{C}_k^\dagger\hat{C}_k$$
$$= \sum_{k\in 1BZ}\epsilon_k\hat{C}_k^\dagger\hat{C}_k$$

With interaction: Hubbard Model (Bose case here)

$$H_{int} = \int \hat{\Psi}^\dagger(r)\hat{\Psi}^\dagger(r')\frac{U(r-r')}{2}\hat{\Psi}(r')\hat{\Psi}(r)drdr'$$

In the Wannier basis

$$H_{int} = \sum_{R_1R_2R_3R_4}\int \omega^*_{R_1}(r)\omega^*_{R_2}(r')\frac{U(r-r')}{2}\omega_{R_3}(r)\omega_{R_4}(r')drdr'$$
$$\times \hat{C}_{R_1}^\dagger\hat{C}_{R_2}^\dagger\hat{C}_{R_3}\hat{C}_{R_4}$$
$$\approx \frac{U}{2}\sum_R \hat{C}_R^\dagger\hat{C}_R^\dagger\hat{C}_R\hat{C}_R = \frac{U}{2}\sum_R \hat{n}_R(\hat{n}_R - 1)$$

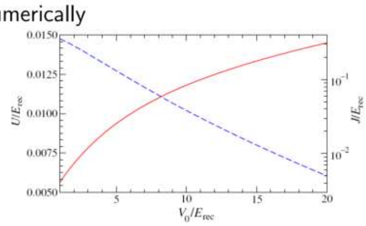
We have assumed short-range interaction and considered only on-site interactions in the overlap integral.

The Bose-Hubbard Model

$$H = -t\sum_{R,\rho}\hat{C}_R^\dagger\hat{C}_{R+\rho} + \frac{U}{2}\sum_R \hat{C}_R^\dagger\hat{C}_R^\dagger\hat{C}_R\hat{C}_R$$

Parameters of Bose-Hubbard model

- The hopping rate t and the on-site interaction U can be estimated numerically



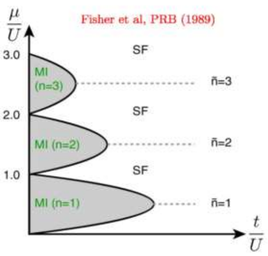
New J. Phys. 10, 053038 (2008).

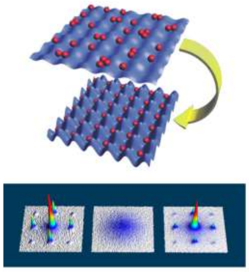
- Fitting in three-dimensions

$$t/E_r \approx \frac{3.5}{\sqrt{\pi}}(V_0/E_r)^{3/4}e^{-2\sqrt{V_0/E_r}}$$
$$U/E_r \approx 3.05(V_0/E_r)^{0.85}(a_s/a)$$

The recoil energy $E_r = \hbar^2/2ma^2$.

Phases of the Bose-Hubbard model





- Large t: superfluid
- Large U: Mott-insulator
- Phase transition inbetween

Properties of Mott-insulator and superfluid

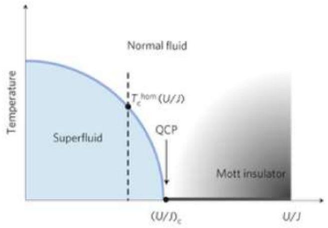
Mott-insulator

- Integer filling
- Finite gap, $\langle\hat{C}_i^\dagger\hat{C}_j\rangle$ with exponential decay
- Flat $n(q)$
- Not compressible ($\partial n/\partial\mu = 0$)

Superfluid

- Any filling
- Gapless, ODLRO in 3D, power-law decay in lower dimensions
- Peaked $n(q)$
- Compressible

Finite temperature phase diagram



- Superfluid to Mott-insulator (quantum phase transition) at zero temperature
- Superfluid to normal (thermal phase transition) at finite temperature
- Crossover between Mott-insulator and normal?
- Quantum critical region

Experimental signal of the superfluid state

- Momentum distribution

$$
\begin{aligned}
n(q) = \langle \hat{\Psi}_q^\dagger \hat{\Psi}_q \rangle &= \sum_{nkn'k'} \Psi_{nk}^*(q)\Psi_{n'k'}(q)\langle \hat{C}_{nk}^\dagger \hat{C}_{n'k'} \rangle \\
&\propto \sum_{nkn'k'} \langle \hat{C}_{nk}^\dagger \hat{C}_{n'k'} \rangle \omega_n(q)\omega_{n'}(q)\delta_{q-K-k,0}\delta_{q-K-k',0} \\
&= \sum_n \langle \hat{C}_{n(q-K)}^\dagger \hat{C}_{n(q-K)} \rangle |\omega_n(q)|^2,
\end{aligned}
$$

where we have used

$$
\hat{\Psi}(q) = \sum_{nk} \hat{C}_{nk}\Psi_{nk}(q) = \sum_{nR} \omega_{nR}(q)\hat{C}_R
$$

Fourier transform of Wannier function

$$
\begin{aligned}
\omega_n(q) &= \frac{1}{L}\int e^{-iqr}\omega_n(r)dr = \frac{1}{2\pi N}\int e^{-iqr}\sum_{k\in 1BZ} e^{ikr}u_{nk}(r)dr \\
&= \frac{1}{2\pi N}\int e^{-iqr}\sum_{k\in 1BZ} e^{ikr}\sum_K e^{iKr}u_{nk}(K)dr \\
&= \frac{1}{a}u_{nk}(K)\delta_{q-K-k,0}.
\end{aligned}
$$

Note $u_{nk}(r) = u_{nk}(r+R)$, hence its Fourier transform is discrete.

Fourier transform of Wannier function

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&= \frac{1}{a}u_{nk}(K)\delta_{q-K-k,0}.
\end{aligned}
$$

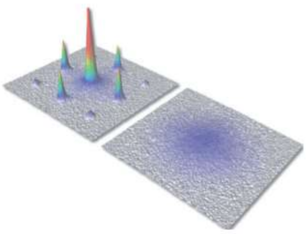
Note $u_{nk}(r) = u_{nk}(r+R)$, hence its Fourier transform is discrete.

Relation with Bloch function

$$
\begin{aligned}
\Psi_{nk}(q) &= \frac{1}{L}\int e^{-iqr}u_{nk}(r)e^{ikr}dr = \frac{1}{L}\int e^{-iqr}e^{ikr}\sum_K e^{iKr}u_{nk}(K)dr \\
&= u_{nk}(K)\delta_{q-K-k,0}.
\end{aligned}
$$

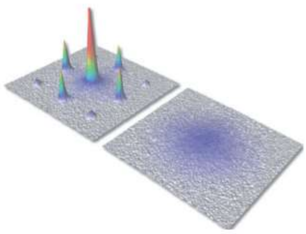
Hence $\omega_n(q) \propto \Psi_{n(q-K)}(q)$. Important for momentum distribution.

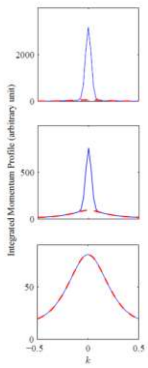
Structure of momentum distribution for a BEC in lattice potential



- Bimodal structure in each BZ
- Modulated by $|\omega_n(q)|^2$

Structure of momentum distribution for a BEC in lattice potential





- Bimodal structure in each BZ
- Modulated by $|\omega_n(q)|^2$

Characterizing SF-Mott transition (Mean-field approach)

$$
H - \mu N = -t\sum_{\langle i,j\rangle} \hat{C}_i^\dagger \hat{C}_j + \frac{U}{2}\sum_i \hat{C}_i^\dagger \hat{C}_i^\dagger \hat{C}_i \hat{C}_i - \mu\sum_i \hat{C}_i^\dagger \hat{C}_i
$$

- Decouple sites
- Mean field $\hat{C}_i = \langle \hat{C}_i \rangle + (\hat{C}_i - \langle \hat{C}_i \rangle)$, retain up to first order in fluctuation

$$
H_i - \mu\hat{n}_i = -t\left(\left\langle \hat{C}_i^\dagger \right\rangle \hat{C}_i + h.c.\right) + t|\langle \hat{C}_i \rangle|^2 + \frac{U}{2}\hat{n}_i(\hat{n}_i - 1) - \mu\hat{n}_i
$$

- Equivalently, Gutzwiller ansatz

$$
|G\rangle = \prod_i^N \left(\sum_{n=0}^\infty f_n^i |n_i\rangle\right)
$$

D. S. Rokhsar, B. G. Kotliar, Phys. Rev. B 44, 10328 (1991)
C. Schroll, F. Marquardt, C. Bruder, Phys. Rev. A 70, 053609 (2004)

Mean field recipe for numerical calculation (zero temperature)

- Mean field Hamiltonian (single-site)

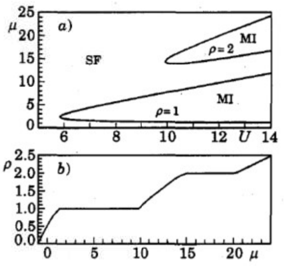
$$
H = -t(\hat{C} + \hat{C}^\dagger)\psi + \frac{U}{2}n(n-1) - \mu n + t\psi^2,
$$

where $\psi = \langle \hat{C} \rangle$.

- Fix U and μ.
- Truncate the Hilbert space $\{|n\rangle\}$ at a large n_c.
- Diagonalize the Hamiltonian, find E_g, which should converge for large enough n_c.
- Minimize E_g with respect to ψ. If $\psi > 0$: supefluid; if $\psi = 0$: Mott-insulator.
- Change U and μ, rinse and repeat.

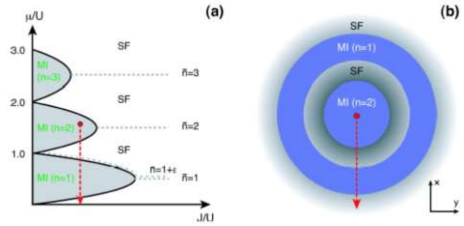
K. Sheshadri et al., EPL 22, 257 (1993).

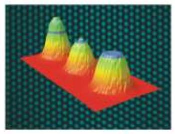
Mean field phase diagram



- Lobes of Mott-insulator region with integer filling.
- Vanishing compressibility $\partial n/\partial \mu$.

In the presence of a harmonic trap



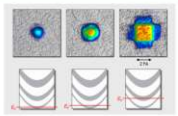


- Slow-varying global harmonic trapping potential
- Shell structure

Fermions in a lattice potential

Fermi-Hubbard Model

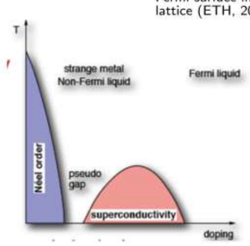
- SF phase transition for attractive interaction?
- Rich phases: d-wave SF, RVB, AF etc.
- Implications on high-T_c superconductors



Fermi surface in an optical lattice (ETH, 2005)

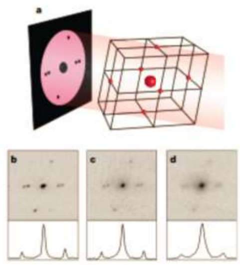
Questions

- How to measure temperature?
- Cooling?



Temperature measurement

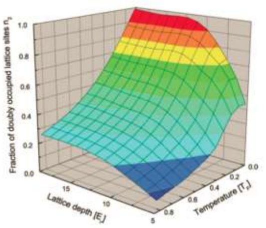
- Fitting TOF results in a superfluid state



2006 MIT

Temperature measurement

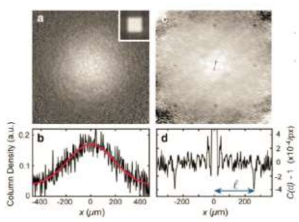
- Fitting TOF results in a superfluid state
- Measure double occupancy



2006 ETH

Temperature measurement

- Fitting TOF results in a superfluid state
- Measure double occupancy
- Noise correlation



2006 Mainz

Temperature measurement

- Fitting TOF results in a superfluid state
- Measure double occupancy
- Noise correlation
- More...

Cooling?

- General problem: Need lower temperature for interesting physics to emerge
- Hubbard model energy scales: t, U, t^2/U
- Current temperature $T \sim t$
- Desired temperature $T \sim t^2/U$
- At least 2-3 orders of magnitude away

Cooling schemes (remove entropy):

- Setup a reservoir (T.-L. Ho and Q. Zhou, arXiv:0911.5506)
- Shaping confinement (J.-S. Bernier et al. PRA 061601(R), (2009))
- Reservoir engineering (J. Catani et al. PRL 103, 140401 (2009))
- More...

Fermi-Hubbard Model

$$H = -t\sum_{\langle i,j\rangle,\sigma} c_{i\sigma}^\dagger c_{j\sigma} + U\sum_i n_{i\uparrow}n_{i\downarrow} - \sum_{i\sigma}\mu_\sigma n_{i\sigma}$$
$$= -t\sum_{\langle i,j\rangle,\sigma} c_{i\sigma}^\dagger c_{j\sigma} + U\sum_i (n_{i\uparrow}-\frac{1}{2})(n_{i\downarrow}-\frac{1}{2})$$
$$-\mu\sum_i(n_{i\uparrow}+n_{i\downarrow}) - h\sum_i(n_{i\uparrow}-n_{i\downarrow}) + \frac{U}{2}\sum_{i\sigma}n_{i\sigma} - \frac{U}{4}$$

- Particle-hole symmetry (at half filling with $\mu = h = 0$)

$$c_{i\downarrow}\to(-1)^i c_{i\downarrow}^\dagger,\quad c_{i\downarrow}^\dagger\to(-1)^i c_{i\downarrow}$$

- Mapping pairing ($U<0$) with anti-ferromagnetism ($U>0$)

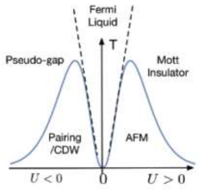
$$\sum_k\langle c_{-k\downarrow}c_{k\uparrow}\rangle\to\sum_k\langle c_{k+k_0\downarrow}^\dagger c_{k\uparrow}\rangle$$

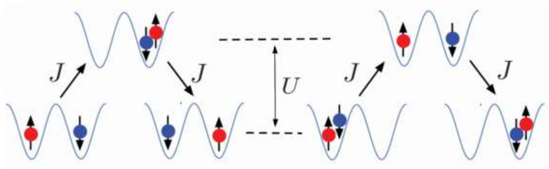
Phase diagram and excitations (at half filling)

- Excitations with energy scale t^2/U
- Heisenberg model ($U>0$)

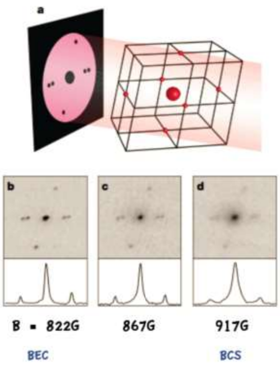
$$H_{\rm eff} = \frac{4t^2}{U}\sum_{\langle ij\rangle}\boldsymbol{S}_i\cdot\boldsymbol{S}_j,$$

where $\boldsymbol{S}_i = \frac{1}{2}\sum_{\alpha\beta}c_{i\alpha}^\dagger\boldsymbol{\sigma}_{\alpha\beta}c_{i\beta}$



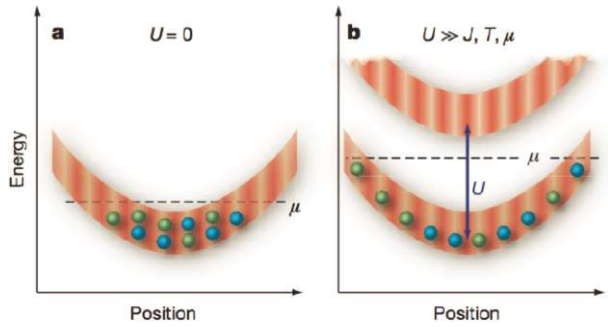


BCS-BEC crossover in lattice potential



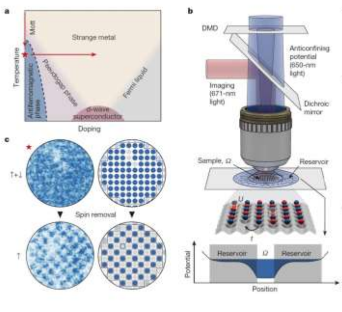
J. K. Chin et al., Nature 443, 961 (2006).

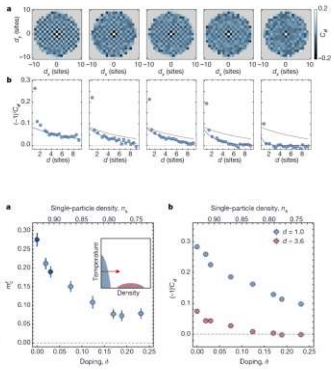
Band insulator to Mott insulator crossover (repulsive interaction)



R. Jordens et al., Nature 455, 204 (2008).

Observation of anti-ferromagnetic correlation





$T\sim0.25t$, $U\sim7.2t$, $T\sim1.8t^2/U$

A. Mazurenko et al., Nature 545, 462 (2017)

Quantum simulation

Quantum simulation with optical lattice

- Highly controllable geometry
- Clean environment
- Tunable parameters
- Optical lattice+Feshbach resonance: strongly correlated system in a dilute gas

Applications

- Floquet engineering
- Many-body localization
- Reservoir engineering (open system)
- Quantum magnetism
- Synthetic gauge field and topological order