Manipulation of Ultracold Atoms near semiconductor surfaces

Workshop "Introduction to Solitary Waves: Mathematical & Physical Perspectives"

26th February 2018 (Monday)

SEMINAR ROOM
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Session 1: 9.00am - 12.00pm

- Basic Concept & Theoretical aspect of Bose-Einstein Condensate (BEC)
- Gross-Piteavskii Equation
- Significant Research in BEC

Session 2: 2.00pm - 4.00pm

Manipulating BEC near semiconductor surfaces:
- Modeling of Quantum Reflection
- Modeling of atom-surface Casimir-Polder
My campus is near to the hottest place in Malaysia (highest temperature ever recorded) ~ 41°C
Bose-Einstein Condensate (BEC)

* Fifth (5th) Element of Matter (Theory: at 0 Kelvin (~ 273.15 Celsius), Exp: at nano/pico Kelvin)

* Coldest place in the universe! (~ nano Kelvin)

Quantum Physics (Theoretical & Applied Science & Tech, Quantum Sensors, Atomic Clock, Foundation of Quantum fluid systems, Quantum Engineering, etc.)
Wave-particle duality

\[ \Delta x \Delta p \geq \frac{\hbar}{2} \]

Wave dominant

s-wave scattering

Few billionth of degree above absolute zero

Pico, Nano Kelvins

\( \approx 0 \text{ K} \)

Solid, Liquid, Gas

Room temperature 300K

\[ \lambda_{dB} = \sqrt{\frac{2\pi^2\hbar^2}{mk_B T}} \]

Speed of atoms are slowing down

PLASMA

\( \approx > 6000 \text{ K} \)

5th state of matter: ULTRACOLD ATOMS
(Bose-Einstein Condensates)

Fragile

0 K = 0 K.E (Classical)
0 K \( \neq \) 0 K.E (Quantum)

Quantum world, view in macroscopic level

Maxwell-Boltzmann Distribution

Kinetic Energy (K.E) ==> Temperature
What is Bose-Einstein condensation (BEC)?

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

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

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

$T = 0$:
- Pure Bose condensate
  - "Giant matter wave"
Two classes of Elementary Particles

- **Boson**
  - Bose-Einstein Statistics
  - E.g. Photons
  - Energy levels: $n=0, 1, 2, 3, \ldots$

- **Fermion**
  - Pauli’s principle
  - Fermi-Dirac Statistics
  - E.g. Electrons
  - Energy levels: $n=0, 1, 2, 3, \ldots$

$n=N$
Gross-Pitaevskii Equation

\[ i\hbar \frac{\partial}{\partial t} \psi (\vec{r}, t) = \left[ -\frac{\hbar^2}{2m} \nabla^2 + U_{\text{trap}} (\vec{r}) + g |\psi (\vec{r}, t)|^2 \right] \psi (\vec{r}, t) \]

- **Kinetic Energy**
- **Potential Energy**
- **Harmonic trap**
- **Nonlinear**
- **Mean-field energy of BEC**
- **Two-body interaction, depends on species of atom, where \( a \) is s-wave scattering length.**

\[ U_{\text{trap}} (\vec{r}) = \frac{1}{2} m (\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2). \]

\[ g = \frac{4\pi \hbar^2 aN}{m} \]

Total number of atoms trapped, \( N \)
$^{87}\text{Rb}$

T $\sim$ 313 nK  
Finer temperature condensate  
Nearly pure condensate


**JILA BEC & Ultracold Atoms** ([http://jilawww.colorado.edu/bec/](http://jilawww.colorado.edu/bec/)).

**Atomic Quantum Gases @ MIT** ([http://www.cua.mit/ketterle_group/](http://www.cua.mit/ketterle_group/)).
Bose-Einstein CONDENSATES

deep scientific interrelationship in Physics

This phenomenon to

(a) Thermodynamics
(b) Degeneracy
(c) Statistical mechanics
(d) Field Theory: Relativity
(e) Nuclear Physics:
(f) Condensed Matter Physics

has opened up a new arena of Quantum Engineering

Large variety of features to be explored in BECs:
Shape, stability, manipulation, dynamics like superfluids, excitations, etc...
Session II:
Quantum Reflection of BECs from semiconductor surfaces
Summary of van der Waals (vdW) Casimir effects between atoms and solid bodies.

Zero-point energy (ZPE): at 0 Kelvin, $|0\rangle$
Casimir-Polder (CP) Interaction

Geometry: (Planar & Non-planar)

Pairwise-Summation method (PWS):

\[ V_{CP} = -C_m \bar{n} \int_{\Omega} \frac{d\Omega}{R^m} \]

van der Waals (vdW) atom-atom interaction, where \( m = 6 \) (non-retarded, NRt) and \( m = 7 \) (retarded, Rt) regimes (interaction strength). Integration over volume of surface \( \Omega \) (GEOMETRY). \( \bar{n} \) is volume density of atoms in the surface.

Clausius-Mossotti

\[ \frac{\bar{n} \alpha}{3\varepsilon_0} = \frac{\varepsilon - 1}{\varepsilon + 2} \]
Micro-engineered Surface: Fresnel Zone Plate
Half-plate Cylinder vs Planar Film

Fresnel Zone Plate

Total $V_{cp}$ (Joule)

$r$ (μm)

Si

Au

Perf. cond.
Stability & Lifetime of trapped atoms

\[ U_{\text{trap}} \]

energetic atoms escape from trap (Evaporating)

BEC

trapping instability (overwhelms)

\[ U_{\text{CP}} \]

Attractive Casimir-Polder

SURFACE
Quantum Reflection of BECs

1D model

\[ | \psi(x, 0) |^2 \]

\[ U_{\text{trap}} \]

\[ \Delta x \]

\[ V_{\text{CP; total}} \]

\[ V_{\text{total}} = \begin{cases} U_{\text{trap}}(x) + V_{\text{CP; total}}(x) & \text{for } x < \delta \\ U_{\text{CP; total}}(\delta) - i(x + \delta)V_{\text{IM}} & \text{for } x \geq \delta \end{cases} \]

BEC oscillate inside harmonic trap (SHO)

Potential

\[ x \]

\[ \Delta V \]

\[ \delta \]

(absorbed/scattered)

(SURFACE)

small offset
Quantum Reflection of BECs

This effect in contrast with the theory of QR for a single atom (non-interacting BEC), as $v_x \to 0$, will enhance $R$ ($R \to 1$).
Quantum Reflection of BECs
(Experimental works: MIT group)

T.A. Pasquini et al., PRL, 97, 093201 (2006)
Non-interacting 1D $^{87}\text{Rb}$ BECs quantum reflects from different Si slab thickness, $w$. 

The ground state BECs computed using imaginary time $4\text{RK}$ method to solve the time-dependent Gross-Pitaevskii (GP) equation.
Quantum Reflection of BECs

QR of the BECs from a hard wall Si surface with $v_x = 1.2$ mm/s at $t = 90$ ms (black = high density)
Quantum Reflection of BECs

BEC B: QR from hard wall

Low incident speed \( v_x = 1.2 \text{ mm/s} \)

High incident speed \( v_x = 2.1 \text{ mm/s} \)

\( t = 0 \)

\( t = 75 \text{ ms} \)

\( t = 144 \text{ ms} \)

Reflected cloud less excitations (more smooth density) at high incident speed due to \( E_k \gg E_g \)
Quantum Reflection of BECs from cylindrical (curved) surface

**BEC C**

$v_x = 1.2\text{mm/s}$

- $R_c = 60\mu\text{m}$
- $R_c = 120\mu\text{m}$
- $R_c = 300\mu\text{m}$
- $R_c = 600\mu\text{m}$

Half plate
Current & Future works

Flexibility of PWS-CP method from film, cylinder & sphere (finite curved) surfaces, and, extended for surface temperature effect (attractive to repulsive) – MSc (on-going)
Study the formation of vortex & soliton
(PhD project)

BEC A at $v_x = 1.2$ mm/s

$R_B = 12\mu m$

$R_C = 48\mu m$
Anisotropic 2D BEC (N = 20,000 $^{87}$Rb atoms)

<table>
<thead>
<tr>
<th>BEC D</th>
<th>Hard wall</th>
<th>-ve step</th>
<th>CP</th>
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<tbody>
<tr>
<td>$v_x = 1.2$ mm/s</td>
<td>![Image]</td>
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<tr>
<td>$v_x = 2.1$ mm/s</td>
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72 $\mu$m

$|v_x| = 1.2$ mm/s

$|v_x| = 2.1$ mm/s

FLAT SURFACE

CURVED SURFACE
(Solid cylinder $R = 30\mu$m)
Thank You for your attention
The Gross-Pitaevskii Equation
a nonlinear Schrödinger Equation

and
Bose-Einstein Condensates (BEC)
Low Temperature, atom & waves

• At very low temperature the de Broglie wavelengths of the atoms are very large compared to the range of the interatomic potential.

• This, together with the fact that the density and energy of the atoms are so low that they rarely approach each other very closely, means that atom–atom interactions are effectively weak and dominated by (elastic) $s$-wave scattering.

• The $s$-wave scattering length $”a”$ the sign of which depends sensitively on the precise details of the interatomic potential.

  * $a > 0$ for repulsive interactions.
  * $a < 0$ for attractive interactions.

• In the Bose-Einstein Condensation, the majority of the atoms condense into the same single particle quantum state and lose their individuality (identity crisis).
Low Temperature, atom & waves

• Since any given atom is not aware of the individual behaviour of its neighbouring atoms in the condensate, the interaction of the cloud with any single atom can be approximated by the cloud's mean field, and the whole ensemble can be described by the same single particle wavefunction.

• In $|g\rangle$, each of the $N$ particles occupies a definite single-particle state, so that its motion is independent of the presence of the other particles.

• Hence, a natural approach is to assume that each particle moves in a single-particle potential that comes from its average interaction with all the other particles.

• This is the definition of the self-consistent mean-field approximation.
Mean-field theory (concept)

- Decompose wave function into two parts:
  1) The **condensate wave function**, which is the expectation value of wave function.
  2) The **non-condensate wave function**, which describes quantum and thermal fluctuations around this mean value but can be ignored due to ultra-cold temperature.
The Mean-Field Approximation

- The many-body Hamiltonian describing $N$ interacting bosons confined by an external potential $V_{\text{trap}}$ is given, in second quantization, by

\[
\hat{H} = \int d^3 r \hat{\Psi}^\dagger(r, t) \left[ -\frac{\hbar^2 \nabla^2}{2m} + V_{\text{trap}}(r, t) \right] \hat{\Psi}(r, t)
\]

\[
+ \frac{1}{2} \int \int d^3 r d^3 r' \hat{\Psi}^\dagger(r, t) \hat{\Psi}^\dagger(r', t) V(r - r') \hat{\Psi}(r', t) \hat{\Psi}(r, t)
\]

boson field operators that create and annihilate particle at the position $r$, respectively.

$V(r-r')$ is the two body interatomic potential (interaction potential) related to the s-wave scattering length $a$.
The Mean-Field Approximation

The boson field operators $\hat{\Psi}(\mathbf{r}, t)$ satisfy the following commutation relations:

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

• The field operators can in general be written as a sum over all participating single-particle wave functions and the corresponding boson creation and annihilation operators.

$$\hat{\Psi}(\mathbf{\bar{r}}, t) = \sum_i \Psi_i(\mathbf{\bar{r}}, t) \hat{a}_i$$
Gross-Piteavskii Equation (GPE)

\[
\frac{i\hbar}{\partial t}\psi (\vec{r}, t) = -\frac{\hbar^2}{2m} \nabla^2 \psi (\vec{r}, t) + V_{\text{ext}} \psi (\vec{r}, t) + g \left| \psi (\vec{r}, t) \right|^2 \psi (\vec{r}, t)
\]

- Schrödinger equation with nonlinear term caused by atom-atom interaction. The interaction constant given by

\[
g = \frac{4\pi \hbar^2 aN}{m}
\]

- The order parameter, \( \psi \), is normalized to the total number of atom, \( N \), as follows:

\[
\int \left| \psi (\vec{r}, t) \right|^2 d\vec{r} = N
\]

- The external trap potential \( V_{\text{ext}} \) often represented as a harmonic 3D:

\[
V_{\text{ext}} (\vec{r}) = \frac{m}{2} \left( \omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2 \right)
\]
Gross-Piteavskii Equation (GPE)

- BEC in dependence of mean field: \( g = \frac{4\pi \hbar^2 aN}{m} \)

- At very low temperature, one parameter sufficient to describe interaction is scattering length, \( a \), where:

  (i) Ideal gas, \( a = 0 \) (linear case)

  (ii) Repulsive, \( a > 0 \) (nonlinear case)

  (iii) Attractive, \( a < 0 \) (nonlinear case)

(ii) & (iii) \( a \neq 0 \) (non-spreading wave-packet (solition) are possible)

3D Collapse for \( N > N_{\text{crit}} \)

\( ^{87}\text{Rb}, ^{23}\text{Na} \) Dark soliton

\( ^{7}\text{Li} \) Bright soliton

Non-interacting BEC (Gaussian)

Interacting BEC (Parabola)
The famous experimental picture of the density distribution in a \textit{chain of 7 solitons} in Li-7 (produced by the group of \textit{R. Hulet}):
Gross-Piteavskiiii Equation (GPE)

Matter-Wave Soliton BEC:
- Better understanding of the stability, as well as the static and dynamical properties of matter-wave dark soliton.
- In experiments (not directly related to dark solitons) – reported observation of these structure (i.e, manipulation of BEC near dielectric surfaces – Quantum Reflection of BEC)
1D and 2D Condensates (harmonic trap)

1D cigar-shaped
\[ \omega_z \approx \omega_y >> \omega_x \]

1D elongated BEC

2D disc-shaped (isotropic/anisotropic)
\[ \omega_x \approx \omega_y ; \omega_z >> \omega_x \]

2D disc-shaped BEC

\[ U_{\text{trap}}(x, y, z) = \frac{1}{2}m\left(\omega_x^2x^2 + \omega_y^2y^2 + \omega_z^2z^2\right) \]

\[ \sim 2\pi \times 3.3\text{Hz} \]

Using imaginary-time method to simulate GPE – ground state BEC (Number of atoms, \( N \), and types of atom (mass))
Ground state BEC

\[ i\hbar \frac{\partial}{\partial t} \psi (\vec{r}, t) = -\frac{\hbar^2}{2m} \nabla^2 \psi (\vec{r}, t) + V_{\text{ext}} \psi (\vec{r}, t) + g|\psi (\vec{r}, t)|^2 \psi (\vec{r}, t) \]

\[ g_j = \begin{cases} 
2aN \hbar \omega_{\perp} \\
\sqrt{8\pi \hbar^2 aN} \\
\sqrt{m\omega_z} \\
4\pi \hbar^2 aN \\
m \\
\end{cases} \quad ; \quad V_j = \begin{cases} 
\frac{1}{2} m \omega_x^2 x^2 \\
\frac{1}{2} m \left( \omega_x^2 x^2 + \omega_y^2 y^2 \right) \\
\frac{1}{2} m \left( \omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2 \right) \\
\end{cases} \quad j = 1, 2, 3
\]

Dimensionless GPE, using scaling parameters:

\[ \omega_x = 2\pi \times 3.3 \text{ Hz} \]

\[ a_x = \sqrt{\frac{\hbar}{m\omega_x}} \quad t = \frac{\tau}{\omega_x} \]

Ground State: The Imaginary Time Method (\( \Delta t \rightarrow -i\Delta t \))
Ground state BEC

Density profile:
Black = high density
Manipulating BECs

\[ i\hbar \frac{\partial}{\partial t} \psi(\vec{r}, t) = -\frac{\hbar^2}{2m} \nabla^2 \psi(\vec{r}, t) + V_{\text{ext}} \psi(\vec{r}, t) + g |\psi(\vec{r}, t)|^2 \psi(\vec{r}, t) \]

- Species of atom
- Modified mean-field energy
- Many-body interaction with surface

Harmonic Trap + Potential barrier *
* Atom-surface interaction (Casimir-Polder theory)
* Gaussian barrier

Off harmonic trap (expansion of BEC)
Soliton in BEC

- Dark soliton in BEC (theoretical) started as early as 1971 (T. Tsuzuki, J. Low Temp. Phys. 4, 441 (1971)) and a new era for dark solitons started shortly after the realization of atomic BECs in 1995.
- See: D. J. Frantzeskakis “Dark solitons in atomic Bose-Einstein condensates: from theory to experiments” arXiv:1004.4071v1

- One of the example of manipulating BEC to create solition: Quantum Reflection of BEC from dielectric surfaces (semiconductor surfaces)