Interaction between atoms

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Outline

- Scattering theory
  - slow particles / s-wave scattering

- Interaction in a dilute gas
  - Gross-Pitaevskii Equation
  - Bogoliubov Theory
  - Higher order approximation
  - quantum depletion

Scattering

- Ansatz for scattering:

$$\Psi = e^{ikz} + f \cdot \frac{e^{ikr}}{r}$$

$f:$ scattering amplitude

- Schrödinger's equation (spherical coordinates):

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

$l:$ angular momentum

$U(r):$ interaction potential

Asymptotic solution

- stationary wave

$$R_l \approx \frac{a_l \cdot \sin(kr - \frac{1}{2} l\pi + \delta_l)}{r}$$

δ_l: phase of R_l

- scattering amplitude:

$$f_l = \frac{1}{2ik}\left(e^{2i\delta_l} - 1\right)$$

- partial cross-section:

$$\sigma_l = 4\pi(2l+1)|f_l|^2$$

Slow particles scattering

- starting with (eq. from slide 3):

$$R_l'' + 2\frac{R_l'}{r} + k^2 R_l - \frac{l(l+1)}{r^2} R_l = \frac{2m}{\hbar^2}\, U(r) R_l$$

- derive: expression for phase δ_l

  to calculate f_l in the limit of

  slow particles $\rightarrow$ low energies $\rightarrow$ low temperatures

  $\Rightarrow$ ultra cold gases

- result: $f_l \sim k^{2l}$, and k is small
- $\Rightarrow$ neglect everything but $l = 0$ ($\Rightarrow$ s-wave scattering)

Assumption 1

- $R_l'' + 2\frac{R_l'}{r} + k^2 R_l - \frac{l(l+1)}{r^2} R_l = \frac{2m}{\hbar^2}\, U(r) R_l$

- slow particles:

  large wavelength $\rightarrow k = \frac{2\pi}{\lambda}$ small $\rightarrow k \cdot a \ll 1$

  a : radius of action of the field $U(r)$

- $a \ll r \ll 1/k$: neglect "k^2"- & "$U(r)$"-term

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

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

- with the general solution:

  $R_l = c_1 r^l + c_2 r^{-(l+1)}$

Assumption 2

- $R_l'' + 2\frac{R_l'}{r} + k^2 R_l - \frac{l(l+1)}{r^2} R_l = \frac{2m}{\hbar^2}\, U(r) R_l$

- $r \sim 1/k$: neglect "$U(r)$"-term

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

- equation of free motion with the solution:

$$R_l = c_1(-1)^l \frac{(2l+1)!!}{k^{2l+1}} r^l \left(\frac{1}{r}\frac{d}{dr}\right)^l \frac{sin(kr)}{r} +$$
$$+c_2(-1)^l \frac{1}{(2l-1)!!} r^l \left(\frac{1}{r}\frac{d}{dr}\right)^l \frac{cos(kr)}{r} +$$

S-wave scattering

In the limit of slow particles,

- scattering amplitude:

$$f \cong f_0 = \frac{\delta_0}{k} = \frac{c_2}{c_1} \equiv -\alpha$$

- total cross section:

$$\sigma = 4\pi\alpha^2$$

- replace full potential with effective potential, having the same s-wave scattering length a_s

Effective potential

- Pseudo potential: $V_{\text{eff}}(r) = g \cdot \delta(r)(\partial_r\ r)$

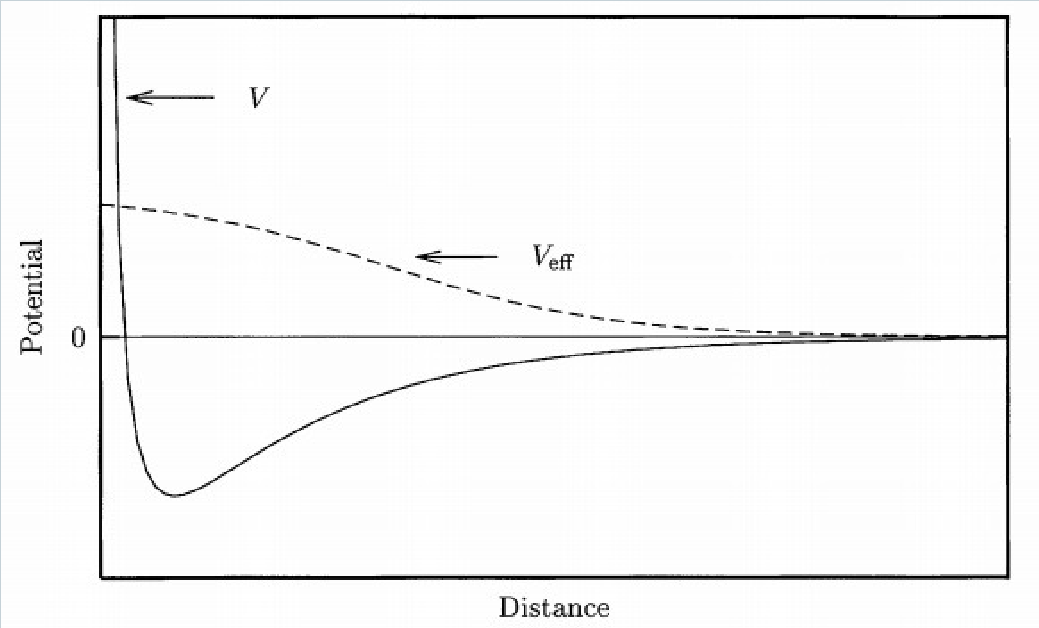

figure: schematic representation of the interatomic potential and the effective potential;
from L.Pitaevskii, S. Stringari: Bose-Einstein Condensation, p.28

Scattering length of the effective potential

- pseudo potential gives scattering length a_s:

$$g = \int dr V_{\text{eff}}(r)$$

- first order (Born approximation):

$$a_s = \frac{1}{4\pi}\frac{m}{\hbar^2} g$$

- higher order:

$$= \int dr dr' V_{\text{eff}}(r)\ G(r - r')\ V_{\text{eff}}(r')$$

$$= \int dr dr'\ g\ \delta(r)\ (\partial_r r)\ G(r - r')\ g\ \delta(r')\ (\partial_{r'} r')$$

$$= \int dr\ g\ \delta(r)\ (\partial_r r)\ G(r)\ V_0$$

$= 0$, because $G(r) \sim 1/r$

Microscopic Lennard-Jones

- microscopic: L.J. potential has positive scattering length
- $\frac{C_6}{r^6} \simeq \frac{\hbar^2}{m r_0^2}$ $\quad\quad\quad\quad \rightarrow r_0^4 = \frac{C_6 m}{\hbar^2}$
- for most gases: $r_0 \simeq 5nm$

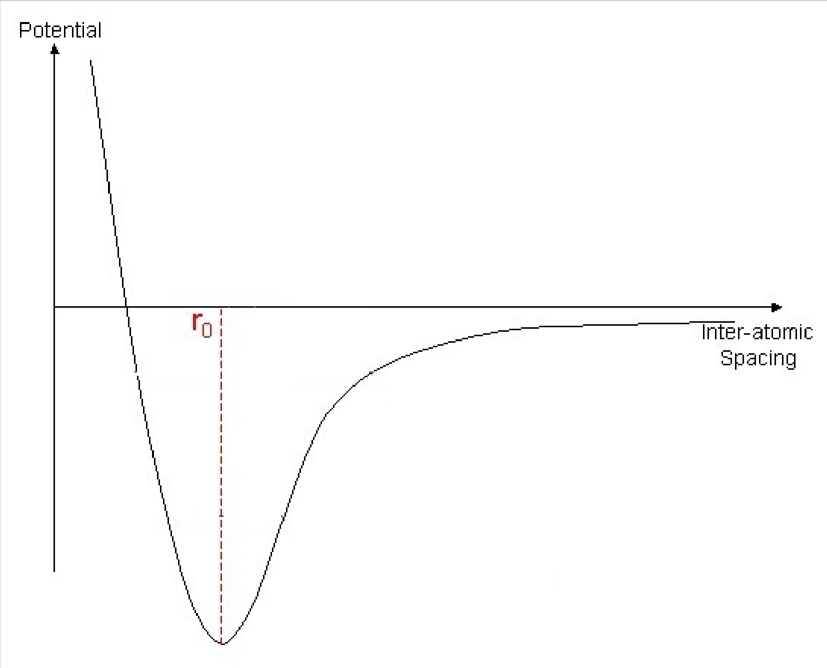

figure: Lennard-Jones potential
from: University of Cambridge webside

Interaction in a dilute gas

- slow particles $\rightarrow$ low energy particles $\rightarrow$ low temperatures
- dilute gas: $|r_0| \ll d = n^{-1/3}$
  - in BEC: $n \approx 10^{14} cm^{-3}$
  - $r_0 \sim 5nm$
- replace interaction potential by pseudo potential
- valid for all scattering lengths a_s
- here: $a_s \sim r_0, \rightarrow$ weak interactions
- use perturbation theory for interaction potential

Equation of motion

- Hamiltonian for interaction: (2nd quantization)

$$\hat{H} = \int dx \hat{\Psi}^\dagger(x) \left(-\frac{\hbar^2}{2m}\nabla^2\right) \hat{\Psi}(x)$$
$$+\frac{1}{2}\int \hat{\Psi}^\dagger(x)\hat{\Psi}^\dagger(x')\, V(x'-x)\hat{\Psi}(x)\hat{\Psi}(x')dxdx'$$

- Heisenberg representation

$\rightarrow$ time dependence of the field operators $\hat{\Psi}(x,t)$

- equation of motion:

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

Gross-Pitaevskii equation

- macroscopic occupation of one specific mode (BEC)

  $\Rightarrow$ replace $\hat{\Psi}(\mathbf{r},t)$ with order parameter $\Psi_0(\mathbf{r},t)$
- replace potential by pseudo potential: $V_{\text{eff}}(r) = g \cdot \delta(r)\cancel{(\partial_r\, r)}$
- $\Psi_0(\mathbf{r},t)$ varies slowly in the range of interaction

  $\Rightarrow r' = r$ in the arguments of Ψ_0

- **Gross-Pitaevskii equation:**

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

- with $g = V_0 = \int V_{\text{eff}}(\mathbf{r})d\mathbf{r} = \frac{4\pi\hbar^2\, a}{m}$

  $n = |\Psi_0(\mathbf{r},t)|^2 =$ density of the gas

Application of G.P.equation

- non-uniform gases in external fields
- BEC trapped in magnetic field
- describing vortices
- similar to theory of superfluidity (Ginzburg & Pitaevskii)

Bogoliubov theory

- again Hamiltonian for interaction:

$$\hat{H} = \int \left(\frac{\hbar^2}{2m} \nabla \hat{\Psi}^\dagger \nabla \hat{\Psi} \right) d\mathbf{r}$$
$$+ \frac{1}{2} \int \hat{\Psi}^\dagger \hat{\Psi}^{\dagger\prime} \, V(\mathbf{r}' - \mathbf{r}) \hat{\Psi} \hat{\Psi}' d\mathbf{r}' d\mathbf{r}$$

- transformation:

$$\hat{\Psi}(\mathbf{r}) = \sum_{\mathbf{p}} \hat{a}_{\mathbf{p}} \frac{1}{\sqrt{V}} e^{i\mathbf{p}\cdot\mathbf{r}/\hbar}$$

Bogoliubov Hamiltonian

- $$\hat{H} = \sum_{\mathbf{p}} \frac{p^2}{2m} \hat{a}^\dagger_{\mathbf{p}} \hat{a}_{\mathbf{p}} + \frac{1}{2V} \sum_{\mathbf{p_1},\mathbf{p_2},\mathbf{q}} V_{\mathbf{q}} \hat{a}^\dagger_{\mathbf{p_1}+\mathbf{q}} \hat{a}^\dagger_{\mathbf{p_2}-\mathbf{q}} \hat{a}_{\mathbf{p_1}} \hat{a}_{\mathbf{p_2}}$$

with interaction potential:

$$V_{\mathbf{q}} = \int V(\mathbf{r}) e^{-i\mathbf{q}\cdot\mathbf{r}/\hbar} d\mathbf{r}$$

Lowest order approximation

- replace: $\hat{a}_0 = \sqrt{N_0}\,, \quad \rightarrow \quad \hat{a}_0^\dagger \hat{a}_0 = N_0$
- neglect: $\hat{a}_\mathbf{p}$ & $\hat{a}_\mathbf{p}^\dagger$ with $\mathbf{p} \neq 0$

  and therefore: $N_0 \sim N$
- lowest order Born approximation:

$$V_0 = g = \frac{4\pi\hbar^2 a}{m}$$

- $$\hat{H} = \sum_\mathbf{p} \frac{p^2}{2m} \hat{a}_\mathbf{p}^\dagger \hat{a}_\mathbf{p} + \frac{1}{2V} \sum_{\mathbf{p_1},\mathbf{p_2},\mathbf{q}} V_\mathbf{q} \hat{a}_{\mathbf{p_1}+\mathbf{q}}^\dagger \hat{a}_{\mathbf{p_2}-\mathbf{q}}^\dagger \hat{a}_{\mathbf{p_1}} \hat{a}_{\mathbf{p_2}}$$

- ground state energy

$$E_0 = \cancel{\sum \frac{p^2}{2m}} N_0 + \frac{N^2}{2V} g$$

Sound velocity of the BEC

- ground state energy: $E_0 = \frac{1}{2} N n g \,,$ with $n = \frac{N}{V}$
- pressure: $P = -\frac{\partial E_0}{\partial V} = \frac{g n^2}{2}$
- compressibility: $\frac{\partial n}{\partial P} = \frac{1}{g n} = \frac{1}{m c^2}$
- sound velocity: $c = \sqrt{\frac{g n}{m}}$

Higher order approximation

lowest order	higher order
neglect $\hat{a}_{\mathbf{p}}^{(\dagger)}, \mathbf{p} \neq 0$	just neglect quadratic terms of $\hat{a}_{\mathbf{p}}^{(\dagger)}, \mathbf{p} \neq 0$
replace $\hat{a}_0^\dagger \hat{a}_0 = N_0 \approx N$	replace $\hat{a}_0^\dagger \hat{a}_0^\dagger \hat{a}_0 \hat{a}_0 = N^2 - 2N \sum_{\mathbf{p}\neq 0} \hat{a}_{\mathbf{p}}^\dagger \hat{a}_{\mathbf{p}}$
$V_0 = g = \frac{4\pi\hbar^2 a}{m}$	$V_0 = g\left(1 + \frac{g}{V} \sum_{\mathbf{p}\neq 0} \frac{m}{p^2}\right)$

- new Hamiltonian:

$$\hat{H} = g\frac{N^2}{2V} + \sum \frac{p^2}{2m}\hat{a}_{\mathbf{p}}^\dagger \hat{a}_{\mathbf{p}} + \frac{1}{2}gn \sum_{\mathbf{p}\neq 0}\left(2\hat{a}_{\mathbf{p}}^\dagger \hat{a}_{\mathbf{p}} + \hat{a}_{\mathbf{p}}^\dagger \hat{a}_{-\mathbf{p}}^\dagger + \hat{a}_{\mathbf{p}}\hat{a}_{-\mathbf{p}} + \frac{mgn}{p^2}\right)$$

Bogoliubov transformation

- linear transformation:

$$\hat{a}_{\mathbf{p}} = u_{\mathbf{p}}\hat{b}_{\mathbf{p}} + v^*_{-\mathbf{p}}\hat{b}^\dagger_{-\mathbf{p}} \qquad \hat{a}^\dagger_{\mathbf{p}} = u^*_{\mathbf{p}}\hat{b}^\dagger_{\mathbf{p}} + v_{-\mathbf{p}}\hat{b}_{-\mathbf{p}}$$

- with: $|u_{\mathbf{p}}|^2 - |v_{-\mathbf{p}}|^2 = 1$

$$\hat{H} = g\frac{N^2}{2V} + \sum \frac{p^2}{2m}\hat{a}^\dagger_{\mathbf{p}}\hat{a}_{\mathbf{p}} + \frac{1}{2}gn\sum_{\mathbf{p}\neq 0}\left(2\hat{a}^\dagger_{\mathbf{p}}\hat{a}_{\mathbf{p}} + \hat{a}^\dagger_{\mathbf{p}}\hat{a}^\dagger_{-\mathbf{p}} + \hat{a}_{\mathbf{p}}\hat{a}_{-\mathbf{p}} + \frac{mgn}{p^2}\right)$$

$$\Downarrow$$

$$\hat{H} = E_0 + \sum \epsilon(p)\hat{b}^\dagger_{\mathbf{p}}\hat{b}_{\mathbf{p}}$$

Dispersion law & ground state

- excited states of interacting Bose gas

  $\widehat{=}$ gas of non-interacting quasi-particles

- $$\hat{H} = E_0 + \sum \epsilon(p)\hat{b}^\dagger_{\mathbf{p}}\hat{b}_{\mathbf{p}}$$

- ground state with higher order approximation:

$$E_0 = g\frac{N^2}{2V} + \frac{1}{2}\sum_{\mathbf{p}\neq 0}\left[\epsilon(p) - gn - \frac{p^2}{2m} + \frac{m(gn)^2}{p^2}\right]$$

- replace $\sum$ with $\int$ in momentum space: (Lee and Young, 1957)

$$E_0 = g\frac{N^2}{2V}\left[1 + \frac{128}{15\sqrt{\pi}}(na^3)^{1/2}\right]$$

Elementary excitations

- **Bogoliubov dispersion law** for elementary excitations:

$$\epsilon(p) = \left[\frac{gn}{m}p^2 + \left(\frac{p^2}{2m}\right)^2\right]^{1/2}$$

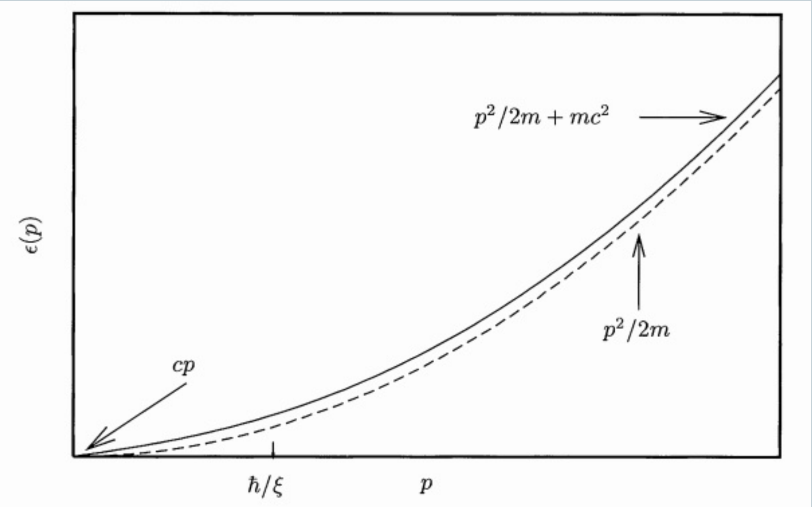

figure: Bogoliubov excitation spectrum: dispersion law for elementary excitations;
from L.Pitaevskii, S. Stringari: Bose-Einstein Condensation, p.34

- large momenta ($p \gg mc$):

$$\epsilon(p) \approx \frac{p^2}{2m} + gn$$

- small momenta ($p \ll mc$):

$$\epsilon(p) = \sqrt{\frac{gn}{m}}p = cp$$

- consistence: $\frac{p^2}{2m} \sim gn = mc^2$

Healing length

- setting: $\frac{p^2}{2m} = gn$ at $p = \frac{\hbar}{\xi}$

- characteristic interaction length:

$$\xi = \sqrt{\frac{\hbar}{2mgn}} = \frac{1}{\sqrt{2}} \frac{\hbar}{mc}$$

- ξ : thickness of the layer from a density of $n = 0$ to $n = \text{const.}$

Occupation numbers

- occupation number of the quasi-particles:

$$N_{\mathbf{p}} \equiv \langle \hat{b}^{\dagger}_{\mathbf{p}} \hat{b}_{\mathbf{p}} \rangle = \frac{1}{\exp[\beta \epsilon(p)] - 1}$$

- occupation number of the particles:

$$n_{\mathbf{p}} = \langle \hat{a}^{\dagger}_{\mathbf{p}} \hat{a}_{\mathbf{p}} \rangle = |v_{-\mathbf{p}}|^2 + |u_{\mathbf{p}}|^2 \langle \hat{b}^{\dagger}_{\mathbf{p}} \hat{b}_{\mathbf{p}} \rangle + |v_{-\mathbf{p}}|^2 \langle \hat{b}^{\dagger}_{-\mathbf{p}} \hat{b}_{-\mathbf{p}} \rangle$$

Quantum depletion

- number of atoms in the condensate:

$$N_0 = N - \sum_{\mathbf{p}\neq 0} n_{\mathbf{p}} = N - \frac{V}{(2\pi\hbar)^3} \int d\mathbf{p} \left[|v_{\mathbf{p}}|^2 + \frac{|u_{\mathbf{p}}|^2 + |v_{-\mathbf{p}}|^2}{\exp[\beta\epsilon(p)] - 1} \right]$$

- particle occupation number at $T = 0\,\mathrm{K}$:

$$n_{\mathbf{p}} = \frac{\frac{p^2}{2m} + mc^2}{2\epsilon(p)} - \frac{1}{2}$$

- integration at $T = 0\,\mathrm{K}$:

$$n_0 \equiv \frac{N_0}{V} = n \left[1 - \frac{8}{3\sqrt{\pi}} (na^3)^{1/2} \right]$$

- same parameter as corrections to the ground state energy

Conclusion

- scattering with low energy particles:
  - neglect everything but the s-wave scattering
  - use an effective soft potential instead of the real interaction-potential
- Gross-Pitaevskii equation:
  - describe a dilute gas in an external field at $T = 0$K
  - lowest order approximation
- Bogoliubov Theory:
  - lowest order approximation coincides with G.P.equation without external field
  - higher order approximation: excitations of the condensate
  - describes Quantum depletions

Thank you for your attention!

questions?