P452 Lec. 3 10/2/2017

Summary of 2 approaches to Gross-Pitaevski Eqn

1. Compare Schroedinger's Eqn $H_N \varphi_N = E_N \varphi_N$ for $N+1$ & N particles:
2. Variational approach to the total free energy $\delta\langle H-\mu N\rangle = 0$

$$\langle H-\mu N\rangle = \langle \sum_i P_i^2/2m + \sum_i V(x_i) + g\sum_{i<j} \delta(|x_i - x_j|) - \mu N \rangle$$
$$\approx \int \frac{\hbar^2}{2m}|\nabla\psi|^2 + V|\psi|^2 - \mu|\psi|^2 + \frac{g}{2}|\psi|^4\,dx$$

$$\delta\langle H-\mu N\rangle = \ldots\ldots\delta\psi + \ldots\ldots\delta\psi^* = 0$$

Both approaches gives Gross-Pitaevskii Eqn:

$$\left[P^2/2m + V(x) + g|\psi(x)|^2 \right]\psi(x) = \mu\psi(x)$$

but based on different assumptions:

- $\Psi(x_1, x_2 \cdots) = \phi(x_1)\phi(x_2)\cdots$ $\quad \psi = \sqrt{N}\phi(x)$, $\int \psi^*\psi = N$ is assumed for both of them
- No ground state is assumed for 2.

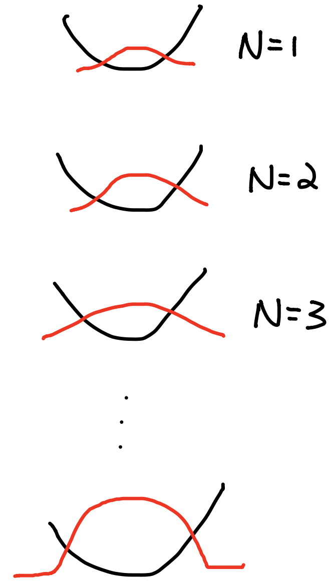
Using approach 1, we may further speculate a

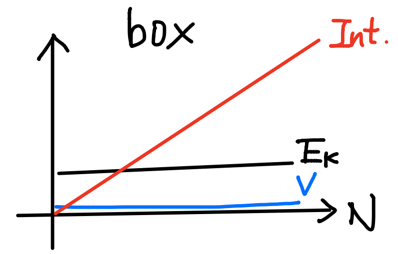
time-dependent GP Eqn: $i\hbar\partial_t\psi = [P^2/2m + V + g|\psi|^2]\psi$

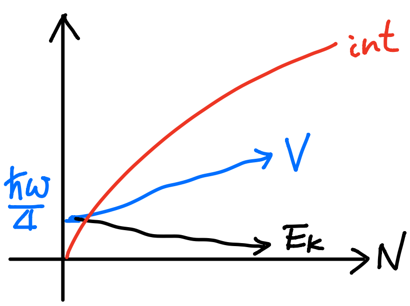
Large particle # limit $N \gg 1$

$$\Big[\frac{\hbar^2 k^2}{2m} + V + g|\psi|^2\Big]\psi = \mu\psi$$

$$\sim \frac{1}{L^2} \qquad \sim L^2 \qquad \sim \frac{N}{L}$$







in the large N limit, E_K is not important

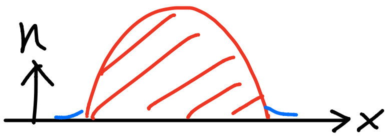
$\Rightarrow$ Thomas-Fermi approximation

$$(V(x) + g|\psi|^2)\psi = \mu\psi$$

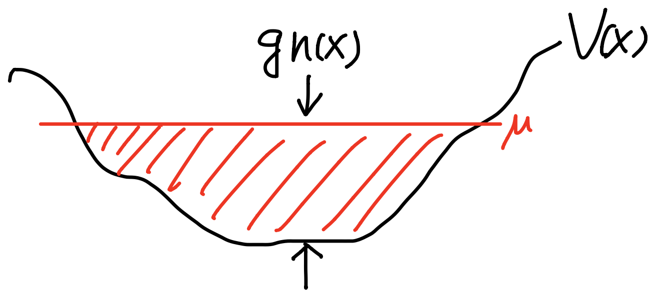
$$\Rightarrow n(x) = \frac{1}{g}[\mu - V(x)]$$

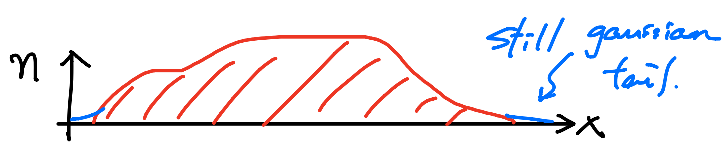
In a harmonic trap

$$n(x) = n_0\Big[1 - \Big(\frac{x}{x_{TF}}\Big)^2\Big]$$



$$\frac{1}{2}m\omega^2 x_{TF}^2 = \mu.$$





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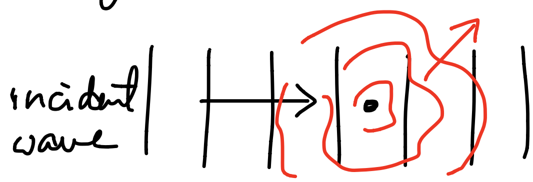
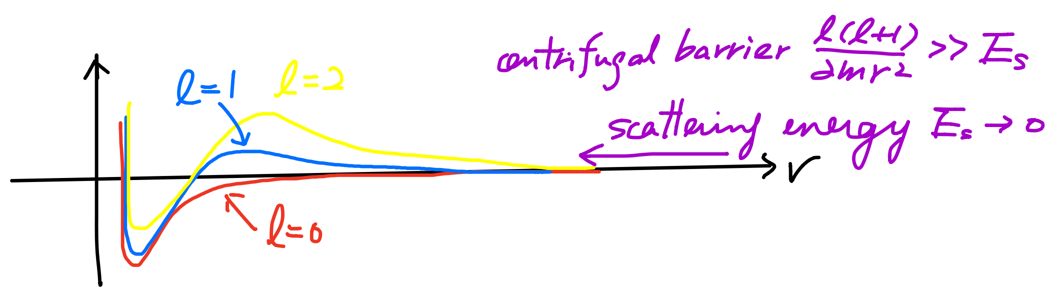
What determine the coupling constant g?

Scattering theory

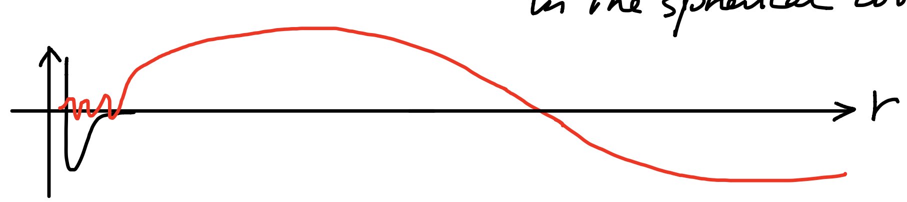


$$\text{wavefunction} = e^{ikz} + f(\theta,\varphi)\frac{e^{ikr}}{r}$$
$$= e^{ikz} + \sum_{lm} f_{lm} Y_l^m(\theta,\varphi)\frac{e^{ikr}}{r}$$

Low temperature limit: only f_{00} is non-zero (s-wave)



Only s-wave (head-on collisions) is left, we have in the spherical coordinate

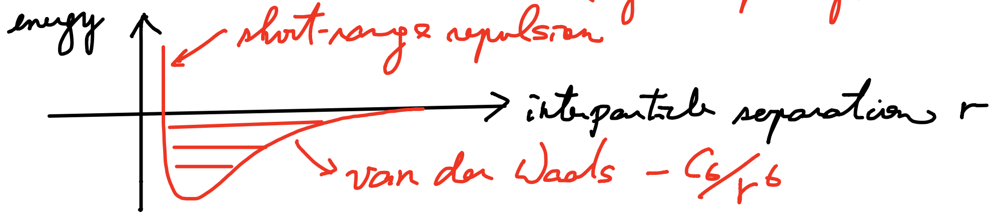


We get $\psi(r) = \frac{e^{-ikr}}{r} - S\,\frac{e^{ikr}}{r}$ Scattering matrix $S = e^{i2\delta}$

incident wave   outgoing wave   scattering phase shift

$= \frac{1}{r} e^{i\delta} \sin(kr+\delta)$

interaction between 2 atoms in the ground state :
(ignore spin for now)



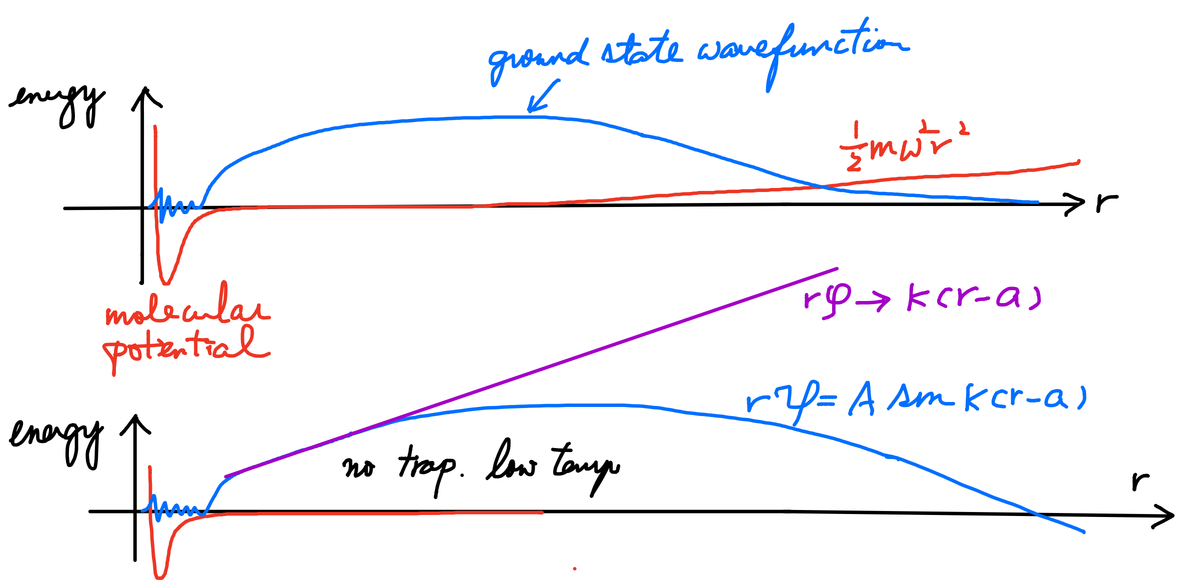
Consider 2 atoms in a trap.

$$H = P_1^2/2m + P_2^2/2m + V(x_1) + V(x_2) + U(|x_1 - x_2|)$$

$$= P^2/2M + p^2/2\mu + V(x_{cm}) + V(r) + U(r)$$

Since trap size is typically $\gg$ molecular potential length

$$H_r = -\frac{\hbar^2}{2\mu}\nabla^2 + U(r) + \cancelto{0}{V(r)}$$



Note that we have assumed s-wave scattering implicitly!

S-wave scattering length: offset of the $l=0$ radial wavefunction.

scattering length

$$\lim_{r\to 0}\lim_{k\to 0}\frac{r\psi}{(r\psi)'} = \lim_{k\cdot r\to 0}\frac{\sin kr+\delta}{k\cos kr+\delta} = \boxed{\lim_{k\to 0}\frac{\tan\delta}{k} = -a}$$

$$\lim_{k\to 0}\psi \to \frac{A}{r}(r-a) = A(1-\frac{a}{r})$$

$$-\frac{\hbar^2}{2\mu}\nabla^2\psi = -\frac{\hbar^2}{2\mu}(-Aa)\nabla^2\frac{1}{r} = -\frac{\hbar^2}{m}a\,4\pi\delta(r)A$$

$$-\frac{\hbar^2}{2\mu}\nabla^2\psi + \underline{\underline{\frac{4\pi a\hbar^2}{m}}}\,\delta(r)\left[\partial_r r\psi\right] = 0$$

$\hookrightarrow \approx \psi$ why?

$\Rightarrow$ This is the Schroedinger's eqn with an effective interaction potential $\underline{\underline{g\delta(r)}}$!

Final result: Coupling constant $g = 4\pi a\hbar^2/m$

$$\boxed{i\hbar\partial_t\psi(x) = \left[P^2/2m + V(x) + \frac{4\pi a\hbar^2}{m}|\psi|^2\right]\psi}$$

Additional assumptions we have made:

1. Short-range interactions
2. low-temp scattering (s-wave scattering)

References: Modern Quantum mechanics, JJ Sakurai. Chap. 7
RMP 82. 1225 (2010)