Cold atoms

Lecture 4. 1st November, 2006

Interacting bosons in the trap

Are the interactions important?

In the dilute gaseous atomic clouds in the traps, the interactions are incomparably weaker than in liquid helium.

That permits to develop a perturbative treatment and to study in a controlled manner many particle phenomena difficult to attack in HeII.

Several roles of the interactions

- the atomic collisions take care of thermalization
- the mean field component of the interactions determines most of the deviations from the non-interacting case

• beyond the mean field, the interactions change the quasi-particles and result into superfluidity even in these dilute systems

Fortunate properties of the interactions

1. Strange thing: the cloud lives for seconds, or even minutes at temperatures, at which the atoms should form a crystalline cluster. Why?

For binding of two atoms, a third one is necessary to carry away the released binding energy and momentum. Such ternary collisions are very unlikely in the rare cloud, however.

- 2. The interactions are elastic and spin independent: they do not spoil the separation of the hyperfine atomic species and preserve thus the identity of the atoms.
- 3. At the very low energies in question, the effective interaction is typically weak and repulsive ... which enhances the formation and stabilization of the condensate.

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Interatomic interactions



For neutral atoms, the pairwise interaction has two parts

- van der Waals force $\propto \frac{1}{r^6}$
- strong repulsion at shorter distances due to the Pauli principle for electrons
- Popular model is the 6-12 potential:

$$U_{\text{TRUE}}(r) = 4\varepsilon \left(\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right)$$

Example:

Ar $\varepsilon = 1.6 \times 10^{-22} \text{ J} \sigma = 0.34 \text{ nm}$

 ${\cal E}$ corresponds to ~12 K!!

Many bound states, too.



Interatomic interactions

The repulsive part of the potential – not well known The attractive part of the potential can be measured with precision

$$U_{\text{TRUE}}(r) = \text{repulsive part} - \frac{C_6}{r^6}$$

Even this permits to define a characteristic length

"local kinetic energy" \approx "local potential energy" $\frac{\hbar^2}{2m} \frac{1}{\beta_6^2} \approx \frac{C_6}{\beta_6^6}$ $\beta_6 = \left(2mC_6\hbar^{-2}\right)^{1/4}$

Scattering length, pseudopotential

Beyond the potential radius, say 3σ , the scattered wave propagates in free space

For small energies, the scattering is purely isotropic, the *s*-wave scattering. The outside wave is

$$\psi \propto \frac{\sin(kr + \delta_0)}{r}$$

For very small energies the radial part becomes just

$$r - a_s$$
, a_s ... the scattering length

This may be extrapolated also into the interaction sphere (we are not interested in the short range details)

Equivalent potential ("pseudopotential")

$$U(r) = g \cdot \delta(r)$$
$$g = \frac{4\pi a_s \hbar^2}{m}$$

Experimental data

	C_6 (a.u.)	$\beta_{\rm 6}$ (a.u.)	<i>a</i> ₀ (a.u.)
⁷ Li ₂	1388 ^a	65	-27.3 ^b
23 Na ₂	1472 ^c	89	77.3 ^d
³⁹ K ₂	3897 ^e	129	$-33^{\rm f}$
⁸⁵ Rb ₂	4700 ^g	164	- 369 ^g
⁸⁷ Rb ₂	4700 ^g	165	106 ^g
¹³³ Cs ₂	6890 ^h	197	2400 ^h

Many-body Hamiltonian

$$\hat{H} = \sum_{a} \frac{1}{2m} p_{a}^{2} + V(\mathbf{r}_{a}) + \frac{1}{2} \sum_{a \neq b} U(\mathbf{r}_{a} - \mathbf{r}_{b})$$

We start from the mean field approximation.

This is an educated way, similar to (almost identical with) the Hartree approximation for many electron systems.

Most of the interactions is indeed absorbed into the mean field and what remains are explicit quantum correlation corrections

$$\hat{H}_{GP} = \sum_{a} \frac{1}{2m} p_{a}^{2} + V(r_{a}) + V_{H}(r_{a}) \qquad \rightarrow \text{ADDITIONAL NOTES}$$

$$V_{H}(r_{a}) = \int dr_{b} U(r_{a} - r_{b}) n(r_{b}) = g \cdot n(r_{a}) \qquad \text{self-consistent}$$

$$n(r) = \sum_{\alpha} n_{\alpha} \left| \varphi_{\alpha} \left(r \right) \right|^{2} \qquad \text{self-consistent}$$

$$\left(\frac{1}{2m} p^{2} + V(r) + V_{H}(r) \right) \varphi_{\alpha} \left(r \right) = E_{\alpha} \varphi_{\alpha} \left(r \right)$$

$$11$$

Gross-Pitaevskii equation at zero temperature

Consider a condensate. Then all occupied orbitals are the same and

$$\left(\frac{1}{2m}p^{2}+V(\boldsymbol{r})+gN\left|\boldsymbol{\varphi}_{0}\left(\boldsymbol{r}\right)\right|^{2}\right)\boldsymbol{\varphi}_{0}\left(\boldsymbol{r}\right)=E_{0}\boldsymbol{\varphi}_{0}\left(\boldsymbol{r}\right)$$

Putting

$$\Psi(\boldsymbol{r}) = \sqrt{N} \cdot \boldsymbol{\varphi}_0(\boldsymbol{r})$$

we obtain a closed equation for the order parameter:

$$\left(\frac{1}{2m}p^2 + V(\boldsymbol{r}) + g\left|\boldsymbol{\Psi}(\boldsymbol{r})\right|^2\right)\boldsymbol{\Psi}(\boldsymbol{r}) = \boldsymbol{\mu}\boldsymbol{\Psi}(\boldsymbol{r})$$

This is the celebrated Gross-Pitaevskii equation.

It is a simple non-linear Schrödinger equation, suitable for numerical solution.

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How much is it??

For a static condensate, the order parameter has ZERO PHASE. Then $\Psi(\mathbf{r}) = \sqrt{N} \cdot \varphi_0(\mathbf{r}) = \sqrt{n(\mathbf{r})}$

$$\int \mathrm{d}^3 \mathbf{r} \left| \boldsymbol{\Psi}(\mathbf{r}) \right|^2 = \int \mathrm{d}^3 \mathbf{r} \cdot n(\mathbf{r}) = N$$

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The Gross-Pitaevskii equation

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becomes

$$-\frac{\hbar^2}{2m}\frac{\Delta\sqrt{n(\mathbf{r})}}{\sqrt{n(\mathbf{r})}} + V(\mathbf{r}) + g\,\mathbf{n}(\mathbf{r}) = \mu$$

For a static condensate, the order parameter has ZERO PHASE. Then $\Psi(\mathbf{r}) = \sqrt{N} \cdot \varphi_0(\mathbf{r}) = \sqrt{n(\mathbf{r})}$

$$N[n] = \int d^3 \mathbf{r} |\Psi(\mathbf{r})|^2 = \int d^3 \mathbf{r} \cdot n(\mathbf{r}) = N$$

The Gross-Pitaevskii equation

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becomes



This equation results from a variational treatment of the Energy Functional

$$E[n] = \int d^3 \mathbf{r} \left\{ \frac{\hbar^2}{2m} \left(\nabla \sqrt{n(\mathbf{r})} \right)^2 + V(\mathbf{r}) n(\mathbf{r}) + g n^2(\mathbf{r}) \right\}$$

It is required that

$$E[n] = \min$$

with the auxilliary condition

$$N[n] = N$$

that is

$$\delta(E[n] - \mu N[n]) = 0$$

which is the GP equation written for the particle density. From there,

$$\frac{\delta E[n]}{\delta N[n]} = \mu$$

Interacting atoms in a parabolic trap



Without interaction, the condensate would occupy the ground state of the oscillator

(dashed - - - - -)

In fact, there is a significant broadening of the condensate in the experiment, perfectly reproduced by the solution of the GP equation

Qualitative

for g>0, repulsion, both inner "quantum pressure" and the interaction broaden the condensate.

for g<0, attraction, "quantum pressure" and the interaction compete, the condensate shrinks and becomes metastable. Onset of instability with respect to three particle recombination processes

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<u>Quantitative</u>

The decisive parameter for the "importance" of interactions is

$$\frac{E_{\text{INT}}}{E_{\text{KIN}}} \quad \frac{gNn}{N\hbar\omega} \quad \frac{N^2 a_s a_0^{-3}}{N a_0^{-2}} = \frac{N a_s}{a_0}$$



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The minimum of the $\tilde{E}(\tilde{\sigma})$ curve gives the condensate size for a given η . With increasing η , the condensate stretches with an asymptotic power law $\tilde{\sigma}_{\min} \propto \eta^{1/5}$

For $-0.27 < \eta < 0$, the condensate is metastable, below $\eta_c = -0.27$, it becomes unstable and shrinks to a 'zero' volume.

The end

On the way to the mean-field Hamiltonian

ADDITIONAL NOTES On the way to the mean-field Hamiltonian

① First, the following <u>exact</u> transformations are performed

$$\hat{H} = \sum_{a} \frac{1}{2m} p_{a}^{2} + \sum_{a} \hat{V}(r_{a}) + \frac{1}{2} \sum_{a \neq b} \hat{U}(r_{a} - r_{b})$$

$$\hat{V} = \sum_{a} V(r_{a}) = \int d^{3}r V(r) \sum_{a} \delta(r - r_{a}) \equiv \int d^{3}r V(r) \cdot \hat{n}(r)$$

$$particle density operator$$

$$\hat{U} = \frac{1}{2} \sum_{a \neq b} \sum_{b} U(r_{a} - r_{b}) = \frac{1}{2} \int d^{3}r d^{3}r' U(r - r') \sum_{a \neq b} \delta(r - r_{a}) \delta(r' - r_{b})$$

$$= \frac{1}{2} \int d^{3}r d^{3}r' U(r - r') \sum_{a} \delta(r - r_{a}) \left\{ \sum_{b} \delta(r' - r_{b}) - \frac{TRICK!!}{\delta(r' - r')} \right\}$$

$$\hat{H} = \hat{W} + \int d^{3}r V(r) \cdot \hat{n}(r) + \frac{1}{2} \int d^{3}r d^{3}r' U(r - r') \hat{n}(r) \left\{ \hat{n}(r') - \delta(r - r') \right\}$$

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On the way to the mean-field Hamiltonian

② Second, a specific many-body state is chosen, which defines the mean field:

$$\Psi \to n(\mathbf{r}) = \left\langle \hat{n}(\mathbf{r}) \right\rangle \equiv \left\langle \Psi \right| \hat{n}(\mathbf{r}) \left| \Psi \right\rangle$$

Then, the operator of the (quantum) density fluctuation is defined:

$$\hat{n}(\mathbf{r}) = n(\mathbf{r}) + \Delta \hat{n}(\mathbf{r})$$

$$\hat{n}(\boldsymbol{r})\hat{n}(\boldsymbol{r'}) = \hat{n}(\boldsymbol{r})n(\boldsymbol{r'}) + n(\boldsymbol{r})\hat{n}(\boldsymbol{r'}) + \Delta\hat{n}(\boldsymbol{r})\Delta\hat{n}(\boldsymbol{r'}) - n(\boldsymbol{r})n(\boldsymbol{r'})$$

The Hamiltonian, still exactly, becomes

$$\hat{H} = \hat{W} + \int d^3r \left\{ V(r) + \int d^3r' U(r-r')n(r') \right\} \cdot \hat{n}(r)$$

$$-\frac{1}{2} \int d^3r d^3r' U(r-r')n(r)n(r')$$

$$+\frac{1}{2} \int d^3r d^3r' U(r-r') \left\{ \Delta \hat{n}(r) \Delta \hat{n}(r') - \hat{n}(r) \delta(r-r') \right\}$$

ADDITIONAL NOTES On the way to the mean-field Hamiltonian

③ In the last step, the third line containing exchange, correlation and the self-interaction correction is neglected. The mean-field Hamiltonian of the main lecture results:



REMARKS

• Second line ... an additive constant compensation for doublecounting of the Hartree interaction energy

• In the original (variational) Hartree approximation, the self-interaction is not left out, leading to non-orthogonal Hartree orbitals

Variational approach to the condensate ground state

Variational estimate of the condensate properties

VARIATIONAL PRINCIPLE OF QUANTUM MECHANICS
 The ground state and energy are uniquely defined by

$$E = \left\langle \Psi \middle| \hat{H} \middle| \Psi \right\rangle \leq \left\langle \Psi' \middle| \hat{H} \middle| \Psi' \right\rangle \quad \text{for all } \left| \Psi' \right\rangle \in \mathcal{H}_N^S, \left\langle \Psi' \middle| \Psi' \right\rangle = 1$$

In words, $|\Psi'\rangle$ is a normalized symmetrical wave function of *N* particles. The minimum condition in the variational form is

 $\delta \langle \Psi | \hat{H} | \Psi \rangle = 0$ equivalent with the SR $\hat{H} | \Psi \rangle = E | \Psi \rangle$

ARTREE VARIATIONAL ANSATZ FOR THE CONDENSATE WAVE F.
 For our many-particle Hamiltonian,

$$\hat{H} = \sum_{a} \frac{1}{2m} p_{a}^{2} + V(\mathbf{r}_{a}) + \frac{1}{2} \sum_{a \neq b} \sum_{b} U(\mathbf{r}_{a} - \mathbf{r}_{b}), \quad U(\mathbf{r}) = g \cdot \delta(\mathbf{r})$$

the true ground state is approximated by the condensate for non-interacting particles (Hartree Ansatz, here identical with the symmetrized Hartree-Fock)

$$\Psi(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_p,\ldots,\mathbf{r}_N) = \varphi_0(\mathbf{r}_1)\varphi_0(\mathbf{r}_2)\cdots\varphi_0(\mathbf{r}_p)\cdots\varphi_0(\mathbf{r}_N)$$

Variational estimate of the condensate properties

Here, φ_0 is a normalized real spinless orbital. It is a functional variable to be found from the variational condition

$$\delta \mathcal{E}[\varphi_0] = \delta \langle \Psi[\varphi_0] | \hat{H} | \Psi[\varphi_0] \rangle = 0 \quad \text{with} \quad \langle \Psi[\varphi_0] | \Psi[\varphi_0] \rangle = 1 \Leftrightarrow \langle \varphi_0 | \varphi_0 \rangle = 1$$

Explicit calculation yields

$$\mathcal{E}[\varphi_0] = \frac{\hbar^2}{2m} N \int \mathrm{d}^3 \mathbf{r} \left(\nabla \varphi_0(\mathbf{r}) \right)^2 + N \int \mathrm{d}^3 \mathbf{r} V(\mathbf{r}) \left(\varphi_0(\mathbf{r}) \right)^2 + \frac{1}{2} N \left(N - 1 \right) g \int \mathrm{d}^3 \mathbf{r} \left(\varphi_0(\mathbf{r}) \right)^4$$

Variation of energy with the use of a Lagrange multiplier:

$$\delta \Big\{ N^{-1} \mathcal{E}[\varphi_0] - \mu \big\langle \varphi_0 \big| \varphi_0 \big\rangle \Big\} \qquad \qquad \varphi_0 = \varphi_0(\mathbf{r}), \ \delta \varphi_0 = \delta \varphi_0(\mathbf{r})$$

$$=\frac{2\hbar^2}{2m}\int \mathrm{d}^3 r \,\,\delta\varphi_0 \cdot (-\Delta\varphi_0) + 2\int \mathrm{d}^3 r \,\,\delta\varphi_0 \cdot (V(r) - \mu)\varphi_0 + \frac{4}{2}(N-1)g\int \mathrm{d}^3 r \,\,\delta\varphi_0 \cdot \varphi_0^3$$

This results into the GP equation derived here in the variational way:

$$\frac{1}{2m}p^{2}+V(\mathbf{r})+(N-\mathbf{1})g\left|\varphi_{0}(\mathbf{r})\right|^{2}\right)\varphi_{0}(\mathbf{r})=\mu\varphi_{0}(\mathbf{r})$$

eliminates self-interaction

Variational estimate of the condensate properties

2 ANNEX Interpretation of the Lagrange multiplier μ

The idea is to identify it with the chemical potential. First, we modify the notation to express the particle number dependence

$$\mathcal{E}_{N}[\boldsymbol{\varphi}] = N\left\{ \left\langle \boldsymbol{\varphi} \middle| \frac{1}{2m} p^{2} \middle| \boldsymbol{\varphi} \right\rangle + \left\langle \boldsymbol{\varphi} \middle| \boldsymbol{V} \middle| \boldsymbol{\varphi} \right\rangle + \frac{1}{2} (N-1) g \int d^{3} \boldsymbol{r} \, \boldsymbol{\varphi}^{4} \right\}$$
$$E_{N} = \mathcal{E}_{N}[\boldsymbol{\varphi}_{0N}], \quad \left(\frac{1}{2m} p^{2} + V(\boldsymbol{r}) + (N-1) g \left| \boldsymbol{\varphi}_{0N}(\boldsymbol{r}) \right|^{2} \right) \boldsymbol{\varphi}_{0}(\boldsymbol{r}) = \mu_{N} \boldsymbol{\varphi}_{0N}(\boldsymbol{r})$$

The first result is that μ is not the average energy per particle:

$$E_{N} / N = \mathcal{E}_{N} [\varphi_{0N}] / N = \langle \varphi_{0N} | \frac{1}{2m} p^{2} | \varphi_{0N} \rangle + \langle \varphi_{0N} | V | \varphi_{0N} \rangle + \frac{1}{2} (N-1) g \int d^{3}r \, \varphi_{0N}^{4}$$

from the GPE $\mu_{N} = \langle \varphi_{0N} | \frac{1}{2m} p^{2} | \varphi_{0N} \rangle + \langle \varphi_{0N} | V | \varphi_{0N} \rangle + (N-1) g \int d^{3}r \, \varphi_{0N}^{4}$

Variational estimate of the condensate properties

Compare now systems with *N* and *N* -1 particles:

 $E_{N} = \underbrace{\mathcal{E}_{N}\left[\varphi_{0N}\right]}_{N} = \underbrace{\mathcal{E}_{N-1}\left[\varphi_{0N}\right]}_{N-1} + \mu_{N} \ge \underbrace{\mathcal{E}_{N-1}\left[\varphi_{0,N-1}\right]}_{N-1} + \mu_{N} = E_{N-1} + \mu_{N}$ $\mu_{N} \dots \text{ energy to remove a particle without relaxation of the condensate principle for GPE}$

In the "thermodynamic" asymptotics of large N, the inequality tends to equality. This only makes sense, and can be proved, for g > 0.

Reminescent of the Derivation:

theorem in the HF theory of atoms.

 $\mathcal{E}_{N}[\varphi] = N\langle \varphi | \frac{1}{2m} p^{2} | \varphi \rangle + N\langle \varphi | V | \varphi \rangle + \frac{1}{2} N(N-1)g \int d^{3}r \varphi^{4}$ $\mathcal{E}_{N-1}[\varphi] = (N-1)\langle \varphi | \frac{1}{2m} p^{2} | \varphi \rangle + (N-1)\langle \varphi | V | \varphi \rangle + \frac{1}{2} (N-1)(N-2)g \int d^{3}r \varphi^{4}$ $\mathcal{E}_{N} - \mathcal{E}_{N-1} = \underbrace{\langle \varphi | \frac{1}{2m} p^{2} | \varphi \rangle + \langle \varphi | V | \varphi \rangle + \frac{1}{2} (N(N-1) - (N-1)(N-2))g \int d^{3}r \varphi^{4}}_{\mu_{N} \text{ for } \varphi \mapsto \varphi_{0N}} \int d^{3}r \varphi^{4}$

Variational estimate of the condensate properties

③ SCALING ANSATZ FOR A SPHERICAL PARABOLIC TRAP

The potential energy has the form

$$V(\mathbf{r}) = \frac{1}{2}m\omega_0^2 \cdot r^2 = \frac{1}{2}m\omega_0^2(x^2 + y^2 + z^2)$$

Without interactions, the GPE reduces to the SE for isotropic oscillator

$$\left(\frac{1}{2m}p^2 + \frac{1}{2}m\omega_0^2 \cdot r^2\right)\varphi_0(\mathbf{r}) = \frac{3}{2}\hbar\omega_0\varphi_0(\mathbf{r})$$

The solution (for the ground state orbital) is

$$\varphi_{00}(\mathbf{r}) = A_0^3 e^{-\frac{1}{2} \cdot \frac{\mathbf{r}^2}{a_0^2}}, \quad a_0 = \sqrt{\frac{\hbar}{m\omega_0}}, \quad \hbar\omega_0 = \frac{\hbar^2}{ma_0^2} \quad A_0 = \left(a_0^2 \pi\right)^{-1/4}$$

We (have used and) will need two integrals:

$$I_{1}(\sigma) = \int_{-\infty}^{+\infty} du e^{-\frac{u^{2}}{\sigma^{2}}} = \sigma \sqrt{\pi}, \quad I_{2}(\sigma) = \int_{-\infty}^{+\infty} du e^{-\frac{u^{2}}{\sigma^{2}}} u^{2} = \frac{1}{2}\sigma^{3}\sqrt{\pi}$$

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Variational estimate of the condensate properties

SCALING ANSATZ

The condensate orbital will be taken in the form

$$\varphi_0(\mathbf{r}) = A^3 e^{-\frac{1}{2} \cdot \frac{r^2}{b^2}}, \qquad A = (b^2 \pi)^{-1/4}$$

It is just like the ground state orbital for the isotropic oscillator, but with a rescaled size. This is reminescent of the well-known scaling for the ground state of the helium atom.

Next, the total energy is calculated for this orbital

$$\mathcal{E}[\varphi_{0}] = \frac{\hbar^{2}}{2m} N \int d^{3}r \left(\nabla \varphi_{0}(r) \right)^{2} + N \int d^{3}r V(r) \left(\varphi_{0}(r) \right)^{2} + \frac{1}{2} N \left(N - 1 \right) g \int d^{3}r \left(\varphi_{0}(r) \right)^{4}$$
$$= \frac{1}{2} \hbar \omega_{0} N A^{6} \left\{ \frac{a_{0}^{2}}{b^{4}} \int d^{3}r e^{-\frac{r^{2}}{b^{2}}} r^{2} + \frac{1}{a_{0}^{2}} \int d^{3}r e^{-\frac{r^{2}}{b^{2}}} r^{2} + (N - 1) A^{6} \frac{m a_{0}^{2}}{\hbar^{2}} g \int d^{3}r e^{-\frac{2r^{2}}{b^{2}}} \right\}$$

ADDITIONAL NOTES Variational estimate of the condensate properties For an explicit evaluation, we (have used and) will use the identities: $\frac{\hbar^2}{m} = \hbar \omega_0 a_0^2, \ m \omega_0^2 = \frac{\hbar \omega_0}{a_0^2}, \ A^2 = \frac{1}{I_1(b)} = \frac{1}{b\sqrt{\pi}}, \ g = \frac{4\pi \hbar^2 a_s}{m}$ $\mathcal{E}[\varphi_0] =$ The integrals, by the Fubini theorem, are a product of three: $=\hbar\omega_{0}N\left\{\frac{3I_{2}(b)\left(I_{1}(b)\right)^{2}}{2b\sqrt{\pi}\left(I_{1}(b)\right)^{2}}\left\{\frac{a_{0}^{2}}{b^{4}}+\frac{1}{a_{0}^{2}}\right\}+(N-1)\frac{1}{2b^{3}\pi^{3/2}}\frac{ma_{0}^{2}}{\hbar^{2}}\frac{4\pi\hbar^{2}a_{s}}{m}\frac{\left(I_{1}(b/\sqrt{2})\right)^{3}}{\left(I_{1}(b)\right)^{3}}\right\}\right\}$ Finally, $\mathcal{E}[\varphi_0] = \hbar \omega_0 N \left\{ \frac{3}{4} \right\} \left\{ \frac{a_0^2}{b^2} + \frac{b^2}{a_0^2} \right\} \left\{ + \frac{(N-1)}{\sqrt{2\pi}} \frac{a_s}{a_0} \cdot \frac{a_0^3}{b^3} \right\} \equiv \hbar \omega_0 N \cdot \tilde{E}(\tilde{\sigma})$ dimension-less energy per particle $\tilde{E}(\tilde{\sigma}) = \frac{3}{4} \left\{ \frac{1}{\tilde{\sigma}^2} + \tilde{\sigma}^2 \right\} + \eta \cdot \frac{1}{\tilde{\sigma}^3}$ $\tilde{\sigma} = \frac{b}{a}$ dimension-less orbital size

This expression is plotted in the figures in the main lecture.

