Cold atoms

Lecture 3.

17. October 2007

BEC for interacting particles

Description of the interaction

Mean field approximation: GP equation

Variational properties of the GP equation

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.

# Fortunate properties of the interactions

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    Quasi-Equilibrium

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Interatomic interactions
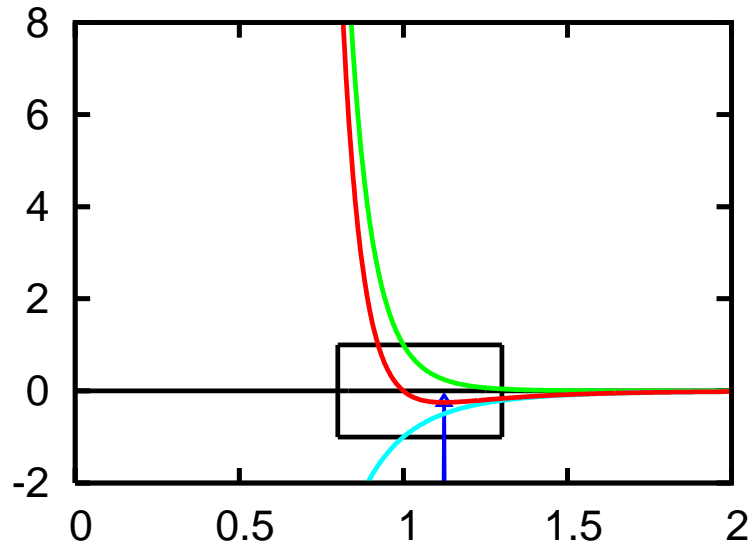
For neutral atoms, the pairwise interaction has two parts

• van der Waals force $\quad \propto \dfrac{1}{r^6}$

• strong repulsion at shorter distances due to the Pauli principle for electrons
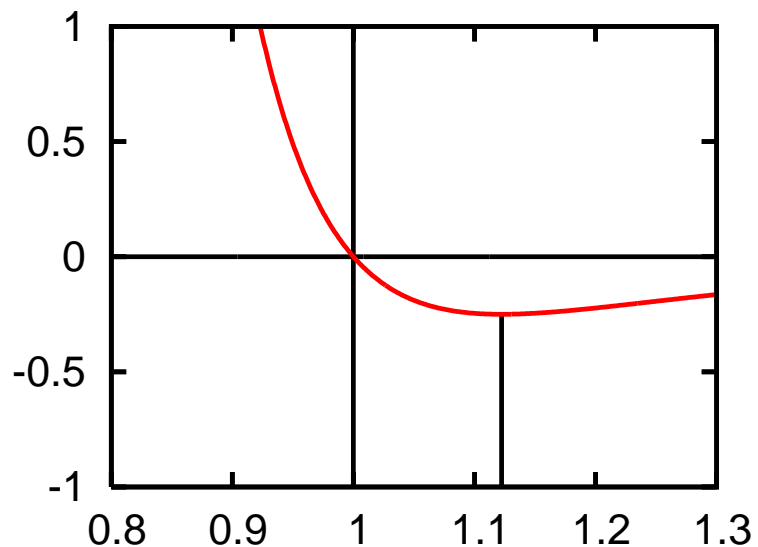
Popular model is the 6-12 potential:

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

Example:

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

ε corresponds to ~12 K!!

Many bound states, too.

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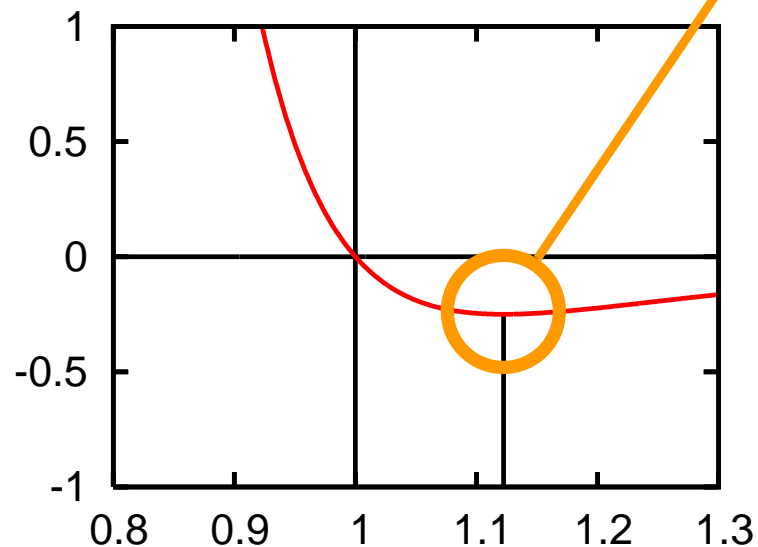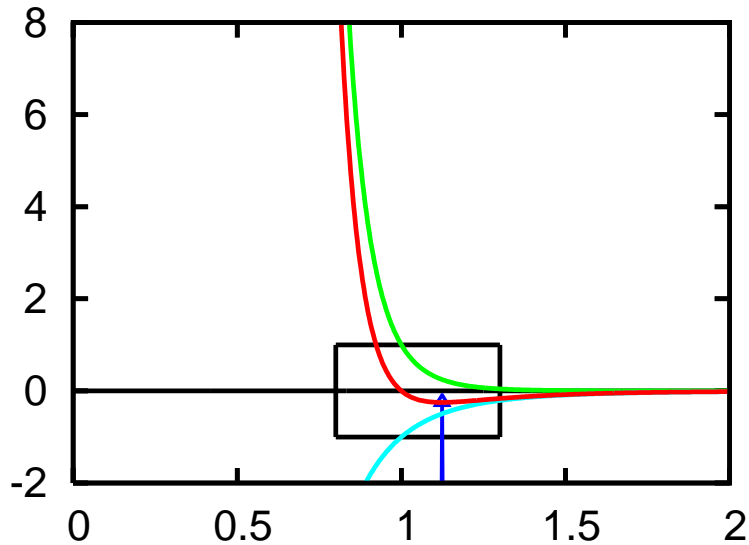
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Interatomic interactions

The repulsive part of the potential – not well known

The attractive part of the potential can be measured with precision

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

Even this permits to define a characteristic length

"local kinetic energy" $\approx$ "local potential energy"

$$\frac{h^2}{2m} \frac{1}{\beta_6^2} \approx \frac{C_6}{\beta_6^6}$$

$$\beta_6 = \left(2mC_6 h^{-2}\right)^{1/4}$$

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For the 6 - 12 potential

$$C_6 = 4\varepsilon \cdot \sigma^6 \qquad \beta_6 = \sigma\left(4\varepsilon \cdot 2m\sigma^2\text{h}^{-2}\right)^{1/4}$$

Interatomic interactions

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rough estimate of the last bound state energy

$$: \; k_{\text{B}}T_C \approx \; \text{collision energy of the}$$

condensate atoms

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

$$r - a_s, \quad a_s \ \dots \text{ the scattering length}$$

This may be extrapolated also into the interaction sphere

(we are not interested in the short range details)

Equivalent potential ("pseudopotential")

$$\boxed{\begin{array}{c} U(r) = g \cdot \delta(\boldsymbol{r}) \\[2mm] g = \dfrac{4\pi a_s \mathrm{h}^2}{m} \end{array}}$$

Experimental data

	C_6 (a.u.)	β_6 (a.u.)	a_s (a.u.)
$^7\text{Li}_2$	1388 [a]	65	-27.3 [b]
$^{23}\text{Na}_2$	1472 [c]	89	77.3 [d]
$^{39}\text{K}_2$	3897 [e]	129	-33 [f]
$^{85}\text{Rb}_2$	4700 [g]	164	-369 [g]
$^{87}\text{Rb}_2$	4700 [g]	165	106 [g]
$^{133}\text{Cs}_2$	6890 [h]	197	2400 [h]

Experimental data

1 a.u. = 1 bohr ≈ 0.053 nm

	C_6 (a.u.)	β_6 (a.u.)	nm	a_s (a.u.)	nm
$^7\text{Li}_2$	1388 [a]	65	3.4	−27.3 [b]	-1.4
$^{23}\text{Na}_2$	1472 [c]	89	4.7	77.3 [d]	4.1
$^{39}\text{K}_2$	3897 [e]	129	6.8	−33 [f]	-1.7
$^{85}\text{Rb}_2$	4700 [g]	164	8.7	−369 [g]	-1.9
$^{87}\text{Rb}_2$	4700 [g]	165	8.7	106 [g]	5.6
$^{133}\text{Cs}_2$	6890 [h]	197	10.4	2400 [h]	127.2

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$^{39}\text{K}_2$	3897 [e]	129	6.8	-33 [f]	-1.7	weak attraction
$^{85}\text{Rb}_2$	4700 [g]	164	8.7	-369 [g]	-19.5	intermediate attraction
$^{87}\text{Rb}_2$	4700 [g]	165	8.7	106 [g]	5.6	weak repulsion **ok**
$^{133}\text{Cs}_2$	6890 [h]	197	10.4	2400 [h]	127.2	strong resonant repulsion

"well behaved; monotonous increase

seemingly erratic, very interesting physics of scattering resonances behind

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Mean-field treatment of interacting atoms

Many-body Hamiltonian and the Hartree approximation

$$\hat{H} = \sum_a \frac{1}{2m} p_a^2 + V(\mathbf{r}_a) + \frac{1}{2} \sum_{a \ne b} \sum U(\mathbf{r}_a - \mathbf{r}_b)$$

We start from the mean field approximation.

This is an educated way, similar to (almost identical with) the HARTREE APPROXIMATION we know for many electron systems.

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

$$\hat{H}_{GP} = \sum_a \frac{1}{2m} p_a^2 + V(\mathbf{r}_a) + V_H(\mathbf{r}_a)$$

$$V_H(\mathbf{r}_a) = \int d\mathbf{r}_b U(\mathbf{r}_a - \mathbf{r}_b) n(\mathbf{r}_b) = g \cdot n(\mathbf{r}_a)$$

$$n(\mathbf{r}) = \sum_\alpha n_\alpha \left| \varphi_\alpha(\mathbf{r}) \right|^2$$

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

$\rightarrow$ ADDITIONAL NOTES

self-consistent system

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Many-body Hamiltonian and the Hartree approximation

$$\hat{H} = \sum_a \frac{1}{2m} p_a^2 + V(\boldsymbol{r}_a) + \frac{1}{2} \sum_{a \neq b} \sum U(\boldsymbol{r}_a - \boldsymbol{r}_b)$$

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$$V_H(\boldsymbol{r}_a) = \int d\boldsymbol{r}_b U(\boldsymbol{r}_a - \boldsymbol{r}_b) n(\boldsymbol{r}_b), \ \ U(r) = \frac{e'^2}{r}$$

$$n(\boldsymbol{r}) = \sum_{E_\alpha < \mu} \left| \varphi_\alpha(\boldsymbol{r}) \right|^2$$

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

Hartree approximation at zero temperature

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

$$\left(\frac{1}{2m} p^2 + V(r) + gN \left| \varphi_0 (r) \right|^2 \right) \varphi_0 (r) = E_0 \varphi_0 (r)$$

This is a single self-consistent equation for a single orbital, the simplest HF like theory ever.

Gross-Pitaevskii equation at zero temperature

Consider a condensate. Then all occupied orbit... single self-consistent equation for a single orbital

$$\left(\frac{1}{2m} p^2 + V(r) + gN|\varphi_0(r)|^2 \right)\varphi_0(r) = E_0\varphi_0(r)$$

Putting

$$\Psi(r) = \sqrt{N} \cdot \varphi_0(r)$$

we obtain a closed equation for the order parameter:

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

This is the celebrated Gross-Pitaevskii equation.

Gross-Pitaevskii equation at zero temperature

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The lowest level coincides with the chemical potential

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This is the celebrated Gross-Pitaevskii equation.

- has the form of a simple non-linear Schrödinger equation

- concerns a macroscopic quantity Ψ

- suitable for numerical solution.

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Gross-Pitaevskii equation – "Bohmian" form

For a static condensate, the order parameter has ZERO PHASE.
Then

$$\Psi(r) = \sqrt{N} \cdot \varphi_0(r) = \sqrt{n(r)}$$

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

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The Gross-Pitaevskii equation

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

becomes

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$$\underbrace{-\frac{h^2}{2m} \frac{\Delta\sqrt{n(r)}}{\sqrt{n(r)}}}_{\text{Bohm's quantum potential}} + \underbrace{V(r) + g\, n(r)}_{\text{the effective mean-field potential}} = \mu$$

Gross-Pitaevskii equation – variational interpretation

This equation results from a variational treatment of the
Energy Functional

$$E[n] = \int d^3 r \left\{ \frac{h^2}{2m} \left(\nabla \sqrt{n(r)} \right)^2 + V(r) n(r) + \frac{1}{2} g\, n^2(r) \right\}$$

It is required that

$$E[n] = \min$$

with the auxiliary condition

$$N[n] = N$$

$\rightarrow$ ADDITIONAL NOTES

that is

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

which is the GP equation written for the particle density (previous slide).

Gross-Pitaevskii equation – chemical potential

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chemical potential by definition

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

chemical potential by definition

Interacting atoms in a constant potential

The simplest case of all: a homogeneous gas

In an extended homogeneous system (… Born-Kármán boundary condition),

the GP equation simplifies

$$n(\boldsymbol{r}) = n \equiv \frac{N}{V} = \text{const.} \qquad V(\boldsymbol{r}) = V = \text{const.}$$

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

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The repulsive interaction increases the chemical potential

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total energy	internal pressure
$\mathcal{E} = \frac{1}{2} g n^2 \cdot \mathcal{V}$	$\mathcal{P} = -\dfrac{\partial \mathcal{E}}{\partial \mathcal{V}} = \frac{1}{2} g n^2$

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$$E = \tfrac{1}{2}\frac{N^2}{V}$$

The simplest case of all: a homogeneous gas

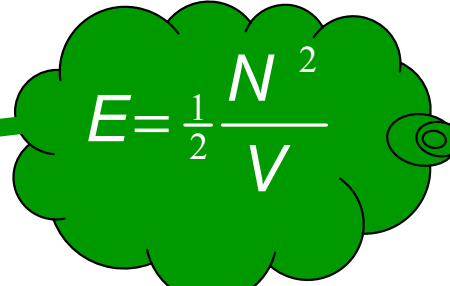- In an extended homogeneous system (… Born-Kármán boundary condition), the GP equation simplifies

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$$E = \tfrac{1}{2} \frac{N^2}{V}$$

If $g < 0$, it would be $\dfrac{\partial n}{\partial \mu} < 0$

and the gas would be thermodynamically unstable.

The simplest case of all: a homogeneous gas

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The repulsive interaction increases the chemical potential

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total energy	internal pressure
$\mathcal{E} = \frac{1}{2}gn^2 \cdot \mathcal{V}$	$\mathcal{P} = -\frac{\partial \mathcal{E}}{\partial \mathcal{V}} = \frac{1}{2}gn^2$

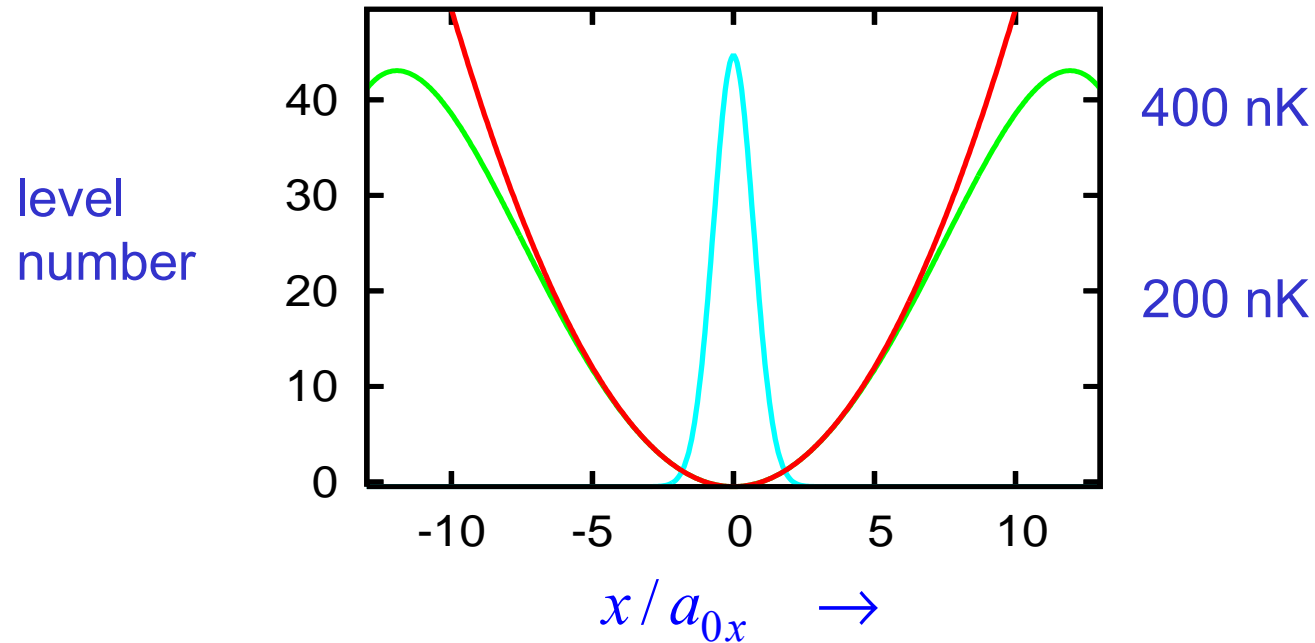$$E = \tfrac{1}{2}\frac{N^2}{V}$$

impossible!!!

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and the gas would be thermodynamically unstable.

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Interacting atoms in a parabolic trap

Reminescence: The trap potential and the ground state

level number

400 nK

200 nK

x/a_{0x} →

^{87}Rb

$a_0 = 1\mu m$

hω=10 nK

$N \sim 10^6$ at.

$$\psi_0(x,y,z) = \phi_{0x}(x)\phi_{0y}(y)\phi_{0z}(z)$$

$$\phi_0(u) = \frac{1}{\sqrt{a_0\pi}}e^{-\frac{u^2}{2a_0^2}}, \quad \boxed{a_0 = \sqrt{\frac{h}{m\omega}}}, \quad E_0 = \frac{1}{2}h\omega = \frac{1}{2}\cdot\frac{h^2}{ma_0^2} = \frac{1}{2}\cdot\frac{h^2}{Mu_m a_0^2}$$

$$V(u) = \frac{1}{2}m\omega^2 u^2 = \frac{1}{2}h\omega\left(\frac{u}{a_0}\right)^2$$

• characteristic energy

• characteristic length

Parabolic trap with interactions

GP equation for a spherical trap (… the simplest possible case)

$$\left(-\frac{h^2}{2m}\Delta + \frac{1}{2}m\omega^2 r^2 + g\left|\Psi(r)\right|^2 \right)\Psi(r) = \mu\Psi(r)$$

Where is the particle number N? (… a little reminder)

$$\int d^3 r \left|\Psi(r)\right|^2 = \int d^3 r \cdot n(r) = N$$

Parabolic trap with interactions

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$$\left(-\frac{h^2}{2m}\Delta + \frac{1}{2}m\omega^2 r^2 + g\left|\Psi(r)\right|^2 \right)\Psi(r) = \mu\Psi(r)$$

Where is the particle number N? (… a little reminder)

$$\int d^3 r \left|\Psi(r)\right|^2 = \int d^3 r \cdot n(r) = N$$

Dimensionless GP equation for the trap $\quad r = \tilde{r} \cdot a_0 \quad energy = \widetilde{energy} \cdot h\omega$

$$\left(-\frac{h^2}{2ma_0^2}\tilde{\Delta} + \frac{1}{2}m\omega^2 a_0^2\tilde{r}^2 + \frac{4\pi h^2 a_s}{m}\left|\Psi(\tilde{r}\cdot a_0)\right|^2 \right)\Psi(\tilde{r}\cdot a_0) = \tilde{\mu}h\omega\Psi(\tilde{r}\cdot a_0)$$

$$\Psi(\tilde{r}\cdot a_0) = \tilde{\Psi}(\tilde{r})\sqrt{\frac{N}{a_0^3}} \quad \Leftrightarrow \quad \int d^3\tilde{r}\left|\tilde{\Psi}(\tilde{r})\right|^2 = 1$$

$$\left(-\tilde{\Delta} + \tilde{r}^2 + \frac{8\pi a_s N}{a_0}\left|\tilde{\Psi}(\tilde{r})\right|^2 \right)\tilde{\Psi}(\tilde{r}) = \tilde{\mu}\tilde{\Psi}(\tilde{r})$$

Parabolic trap with interactions

GP equation for a spherical trap (… the simplest possible case)

$$\left(-\frac{\hbar^2}{2m}\Delta + \frac{1}{2}m\omega^2 r^2 + g\left|\Psi(r)\right|^2 \right)\Psi(r) = \mu\Psi(r)$$

Where is the particle number N? (… a little reminder)

$$\int d^3 r \left|\Psi(r)\right|^2 = \int d^3 r \cdot n(r) = N$$

Dimensionless GP equation for the trap $r = \rho \cdot a_0$ energy $= $ energy $\cdot \hbar\omega$
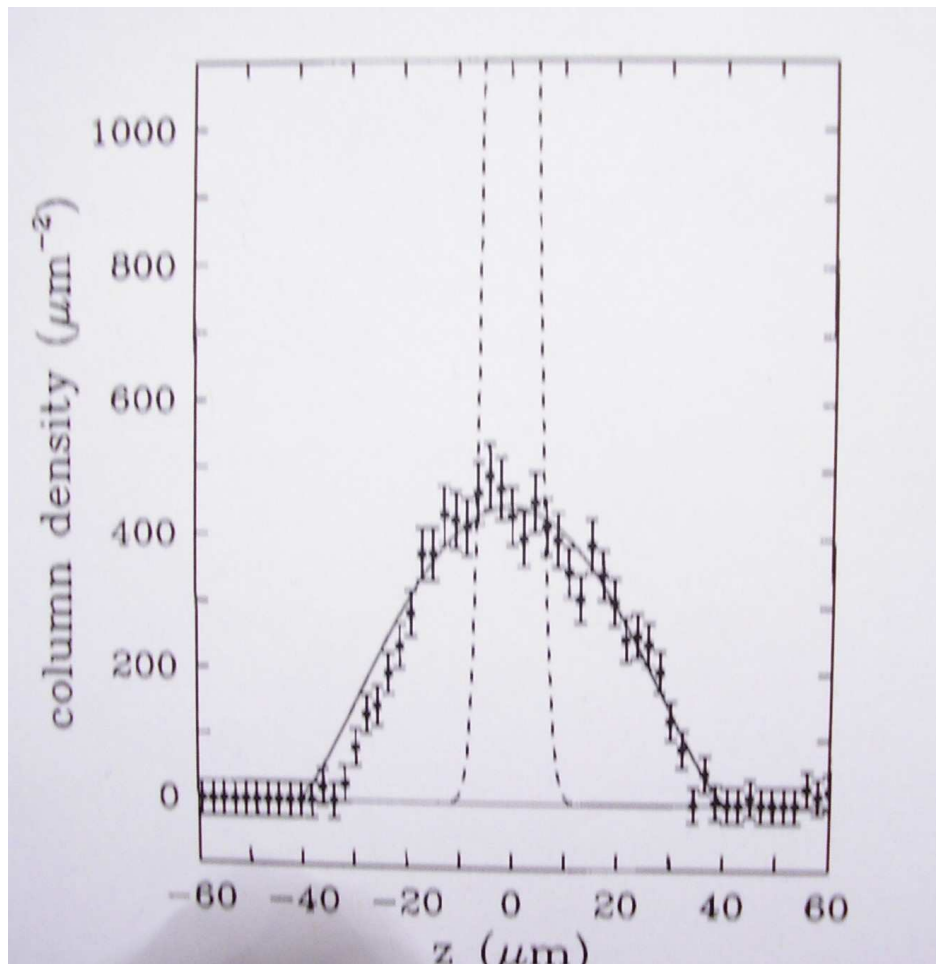
$$\left(-\frac{\hbar^2}{2ma_0^2}\Delta_\rho + \frac{1}{2}m\omega^2 a_0^2 \rho^2 + \frac{4\pi\hbar^2 a_s}{m}\left|\Psi(\rho a_0)\right|^2 \right)\Psi(\rho a_0) = \mu\,\hbar\omega\,\Psi(\rho a_0)$$

$$\Psi(\rho a_0) = \Psi(\rho)\sqrt{\frac{N}{a_0^3}} \quad\Leftrightarrow\quad \int d^3\rho\left|\Psi(\rho)\right|^2 = 1$$

$$\left(-\Delta_\rho + \rho^2 + \frac{8\pi a_s N}{a_0}\left|\Psi(\rho)\right|^2 \right)\Psi(\rho) = \mu\,\Psi(\rho)$$

$\equiv 2\gamma$

a single dimensonless parameter

Importance of the interaction – synopsis

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

(dashed - - - - -)

In fact, there is a significant broadening of the condensate of 80 000 sodium atoms in the experiment by *Hau et al.* (1998),

perfectly reproduced by the solution of the GP equation

Importance of the interaction

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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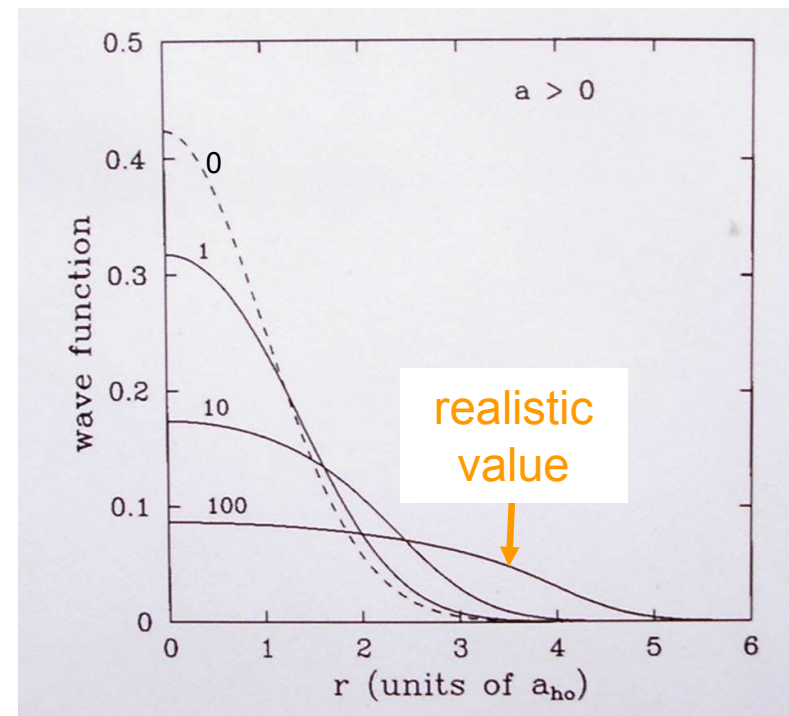
Quantitative

The decisive parameter for the "importance" of interactions is

$$\frac{E_{\text{INT}}}{E_{\text{KIN}}} : \frac{gNn}{Nh\omega} : \frac{N^2 a_s a_0^{-3}}{Na_0^{-2}} = \frac{Na_s}{a_0} \equiv \frac{\gamma}{4\pi}$$

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can vary
in a wide range

collective effect
weak or strong
depending on N

$= 1$
weak individual
collisions

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realistic
value

The end

On the way to the mean-field Hamiltonian

On the way to the mean-field Hamiltonian

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

$$\hat{H} = \sum_a \overset{\hat{W}}{\frac{1}{2m}} p_a^2 + \sum_a \overset{\hat{V}}{V(\pmb{r}_a)} + \frac{1}{2} \sum_{a \neq b} \overset{\hat{U}}{U(\pmb{r}_a - \pmb{r}_b)}$$

$$\hat{V} = \sum_a V(\pmb{r}_a) = \int d^3r\, V(\pmb{r}) \sum_a \delta(\pmb{r} - \pmb{r}_a) \equiv \int d^3r\, V(\pmb{r}) \cdot \hat{n}(\pmb{r})$$

particle density operator

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

$$= \frac{1}{2} \int d^3\pmb{r}\, d^3\pmb{r}'\, U(\pmb{r} - \pmb{r}') \underset{\hat{n}(\pmb{r})}{\sum_a \delta(\pmb{r} - \pmb{r}_a)} \left\{ \underset{\hat{n}(\pmb{r}')}{\sum_b \delta(\pmb{r}' - \pmb{r}_b)} - \overset{\boxed{\text{TRICK!!}}}{\delta(\pmb{r} - \pmb{r}')} \right\}$$

eliminates **SI**
(self-interaction)

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

On the way to the mean-field Hamiltonian

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

$$\Psi \rightarrow n(r) = \langle \hat{n}(r) \rangle \equiv \langle \Psi | \hat{n}(r) | \Psi \rangle$$

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

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

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

The Hamiltonian, still exactly, becomes

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

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

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

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:

$$V_H(r)$$

substitute back
$$\hat{n}(r) = \sum_a \delta(r - r_a)$$
and integrate

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

REMARKS

BACK

• Second line … an additive constant compensation for double-counting 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

① VARIATIONAL PRINCIPLE OF QUANTUM MECHANICS

The ground state and energy are uniquely defined by

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

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

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

② HARTREE VARIATIONAL ANSATZ FOR THE CONDENSATE WAVE F.

For our many-particle Hamiltonian,

$$\hat{H} = \sum_a \frac{1}{2m} p_a^2 + V(r_a) + \frac{1}{2} \sum_{a \neq b} \sum U(r_a - r_b), \quad U(r) = g \cdot \delta(r)$$

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

$$\Psi(r_1, r_2, \text{K}, r_p, \text{K}, r_N) = \varphi_0(r_1) \varphi_0(r_2) \text{L} \, \varphi_0(r_p) \text{L} \, \varphi_0(r_N)$$

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

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

Variation of energy with the use of a Lagrange multiplier:

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

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

BY PARTS

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

$$\left(\frac{1}{2m} p^2 + V(r) + (N\,\textbf{-1})\, g \left|\varphi_0(r)\right|^2 \right) \varphi_0(r) = \mu\varphi_0(r)$$

eliminates self-interaction

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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

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

$$E_N = \mathcal{E}_N[\varphi_{0N}], \quad \left(\frac{1}{2m}p^2 + V(r) + (N\,\textbf{-1})g|\varphi_{0N}(r)|^2\right)\varphi_0(r) = \mu_N\varphi_{0N}(r)$$

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

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

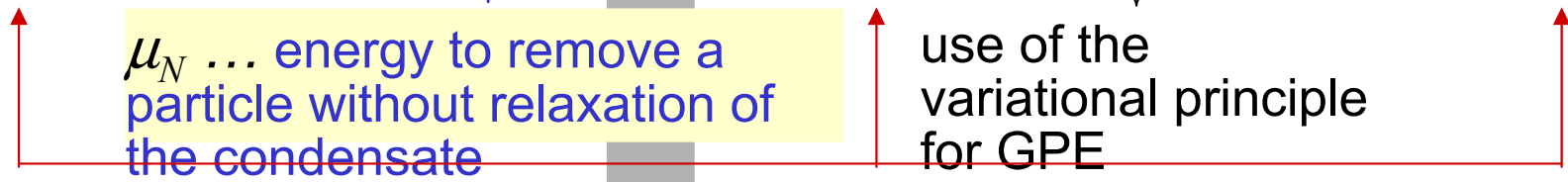from the GPE $\qquad \mu_N = \langle\varphi_{0N}|\frac{1}{2m}p^2|\varphi_{0N}\rangle + \langle\varphi_{0N}|V|\varphi_{0N}\rangle + (N-1)g\int d^3r\,\varphi_{0N}{}^4$

Variational estimate of the condensate properties

Compare now systems with N and N -1 particles:

$$E_N = \underbrace{\mathcal{E}_N[\varphi_{0N}] = \mathcal{E}_{N-1}[\varphi_{0N}] + \mu_N} \geq \underbrace{\mathcal{E}_{N-1}[\varphi_{0,N-1}] + \mu_N} = E_{N-1} + \mu_N$$

μ_N … energy to remove a particle without relaxation of the condensate

use of the variational principle for GPE

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

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Reminescent of the Koopmans' theorem in the HF theory of atoms.
Derivation:

$$\mathcal{E}_N[\varphi] = N\langle\varphi|\tfrac{1}{2m}p^2|\varphi\rangle + N\langle\varphi|V|\varphi\rangle + \tfrac{1}{2}N(N-1)g\int d^3r\,\varphi^4$$

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

$$\mathcal{E}_N - \mathcal{E}_{N-1} = \langle\varphi|\tfrac{1}{2m}p^2|\varphi\rangle + \langle\varphi|V|\varphi\rangle + \tfrac{1}{2}\big(N(N-1)-(N-1)(N-2)\big)g\int d^3r\,\varphi^4$$

$$\mu_N \text{ for } \varphi \text{ a } \varphi_{0N}$$

Variational estimate of the condensate properties

③ SCALING ANSATZ FOR A SPHERICAL PARABOLIC TRAP

The potential energy has the form

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

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

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

The solution (for the ground state orbital) is

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

We (have used and) will need two integrals:

$$I_1(\sigma) = \int\limits_{-\infty}^{+\infty} du \, e^{-\frac{u^2}{\sigma^2}} = \sigma\sqrt{\pi}, \quad I_2(\sigma) = \int\limits_{-\infty}^{+\infty} du \, e^{-\frac{u^2}{\sigma^2}} u^2 = \tfrac{1}{2}\sigma^3 \sqrt{\pi}$$

Variational estimate of the condensate properties

SCALING ANSATZ

The condensate orbital will be taken in the form

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

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

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

$$= \frac{1}{2}h\omega_0 N A^6 \left\{ \frac{a_0^2}{b^4}\int d^3r\, e^{-\frac{r^2}{b^2}}\, r^2 + \frac{1}{a_0^2}\int d^3r\, e^{-\frac{r^2}{b^2}}\, r^2 + (N-1)A^6\frac{ma_0^2}{h^2}g\int d^3r\, e^{-\frac{2r^2}{b^2}} \right\}$$

Variational estimate of the condensate properties

For an explicit evaluation, we (have used and) will use the identities:

$$\frac{h^2}{m} = h\omega_0 a_0^2, \quad m\omega_0^2 = \frac{h\omega_0}{a_0^2}, \quad A^2 = \frac{1}{I_1(b)} = \frac{1}{b\sqrt{\pi}}, \quad g = \frac{4\pi h^2 a_s}{m}$$

$\mathcal{E}[\varphi_0] =$

The integrals, by the Fubini theorem, are a product of three:

$$= h\omega_0 N \left\{ \frac{3 I_2(b)}{2b\sqrt{\pi}} \frac{\left(I_1(b)\right)^2}{\left(I_1(b)\right)^2} \left\{ \frac{a_0^2}{b^4} + \frac{1}{a_0^2} \right\} + (N-1) \frac{1}{2b^3 \pi^{3/2}} \frac{ma_0^2}{h^2} \frac{4\pi h^2 a_s}{m} \frac{\left(I_1(b/\sqrt{2})\right)^3}{\left(I_1(b)\right)^3} \right\}$$

Finally,

$$\mathcal{E}[\varphi_0] = h\omega_0 N \left\{ \frac{3}{4} \left\{ \frac{a_0^2}{b^2} + \frac{b^2}{a_0^2} \right\} + \frac{(N-1)}{\sqrt{2\pi}} \frac{a_s}{a_0} \cdot \frac{a_0^3}{b^3} \right\} \equiv h\omega_0 N \cdot E(\sigma)$$

$$E(\sigma) = \frac{3}{4} \left\{ \frac{1}{\sigma^2} + \sigma^2 \right\} + \eta \cdot \frac{1}{\sigma^3}$$

$$\sigma = \frac{b}{a_0}$$

dimension-less orbital size

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

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The end