Lecture 3 MF theory of BEC : static properties

$$i\hbar \frac{\partial}{\partial t}\phi = -\frac{\hbar^2}{2m}\nabla^2\phi + V_{ext}\phi + g|\phi|^2\phi$$

$$\int \phi^*\phi \, d^3r = N \quad , \quad n(r) = |\phi(r)|^2$$

* all bosons share same wavefunction $\bar{\phi}(r) = \frac{\phi(r)}{\sqrt{N}}$

$$|N:\phi\rangle = \frac{1}{\sqrt{N!}}\left(\int d^3r \, \phi(r)\hat{\psi}^+(r)\right)^N |vac\rangle$$

evolution of many body state approximately restricted to $|N\,\phi\rangle$ space, with ϕ evolving according to GPE.

* quantum matter field $\hat{\psi}$ replaced by classical field $\phi = \langle\hat{\psi}\rangle$

Usual in nonlinear optics : $E = \langle\hat{E}\rangle$,

Maxwell's equations + $\chi^{(3)}$ nonlinearity $\longleftrightarrow$ GPE.

The many-body Hamiltonian

equivalent forms.

$$H = \sum_i \frac{\vec{P}_i^2}{2m} + V_{ext}(R_i) + \sum_{i<j} V_{int}(|R_i - R_j|)$$

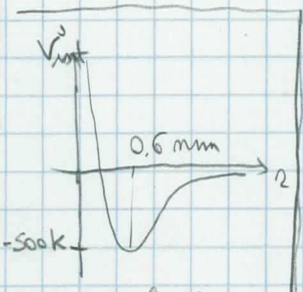
1st quantization

$$H = \int d^3r \left[\frac{\hbar^2}{2m}(\vec{\nabla}\hat{\psi}^+)(\vec{\nabla}\hat{\psi}) + V_{ext}(r)\,\hat{\psi}^+(r)\hat{\psi}(r)\right] +$$

$$+ \frac{1}{2}\int d^3r \, d^3r' \; V_{int}(|r-r'|)\,\hat{\psi}^+(r)\hat{\psi}^+(r')\hat{\psi}(r')\hat{\psi}(r).$$

2nd quantization

Interaction term



potential for Cs

- one could keep full atom-atom potential in V^0_{int}, but theory very complicated as energy scale of V^0_{int} is orders of magnitude higher than energy scale of BEC dynamics.

Moreover: BEC is metastable against solidification in minimum of V^0_{int}

- BEC physics only involves low-energy collisions.

  $\left[\varepsilon_{kin} \simeq k_B T, \frac{\hbar^2}{2m}\left(1/d\right)^2, \mu\right]$

- low-energy collisions characterized by a single parameter, the s-wave scattering length a

- one can replace true V^0_{int} by a "model potential" V_{int} that gives the same a

  * hard sphere potential → ok for numerics QMC
  * for theory → good to have potential which can be treated within 1st Born approximation.

$$V_{int}(r) = \frac{4\pi\hbar^2 a}{m}\,\delta(r)\left[\frac{\partial}{\partial r}(r\,\cdot)\right]$$

→ is a Dirac-δ on regular $\psi_{reg}(r)$

→ eliminates $\frac{A}{r}$ divergences in $\psi(r) = \frac{A}{r} + \psi_{reg}(r)$.

Simplest "proof" of GPE:

$$i\hbar \frac{d}{dt} \langle \hat{\psi} \rangle = \langle [\hat{\psi}, \hat{H}] \rangle =$$

$$= \langle \underbrace{-\frac{\hbar^2}{2m} \nabla^2 \hat{\psi} + V_{ext} \hat{\psi}}_{\text{no difficulty}} + \int d r' \, V_{int}(r - r') \, \hat{\psi}^+(r') \hat{\psi}(r') \hat{\psi}(r) \rangle$$

Approximation $\quad \langle \hat{\psi}^+(r') \hat{\psi}(r') \hat{\psi}(r) \rangle \simeq \langle \hat{\psi}^+(r') \rangle \langle \hat{\psi}(r') \rangle \langle \hat{\psi}(r) \rangle$

Setting $\quad \phi(r) = \langle \hat{\psi}(r) \rangle$

$$\Longrightarrow \quad i\hbar \frac{d}{dt} \phi = -\frac{\hbar^2}{2m} \nabla^2 \phi + V_{ext} \phi + \int d^3 r' \, V_{int}(r - r') \, |\phi(r')|^2 \phi(r)$$

For $\quad V_{int}(r) = $ pseudo-potential

$$i\hbar \frac{d}{dt} \phi = -\frac{\hbar^2}{2m} \nabla^2 \phi + V_{ext} \phi + g |\phi|^2 \phi \qquad \underline{\text{GPE}}$$

ii) Stationary state of the GPE

$$\phi(r) = \phi_0(r)\, e^{-i\mu t/\hbar}$$

$$\mu \phi_0 = -\frac{\hbar^2}{2m}\nabla^2\phi_0 + V_{ext}\,\phi_0 + g|\phi_0|^2\phi_0 .$$

General properties of lowest-μ solution:

- ϕ_0 is non-degenerate
- ϕ_0 is real (i.e. same phase everywhere)
- ϕ_0 is nodeless.

$\longrightarrow$ mathematical proof ?

physical examples:

a) 1D box with hard walls

$$V_{ext}(x) = 0 \quad \text{for } x > 0, \quad = \infty \quad \text{for } x < 0 .$$

$$\text{i.e. } \psi(x) = 0 \quad \text{at } x = 0 .$$

$$\mu\phi_0 = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\phi_0 + g|\phi_0|^2\phi_0$$

$$\begin{cases} \dfrac{d^2}{dx^2}\phi_0 = \dfrac{2m}{\hbar^2}\left(g\,\phi_0^{\,3} - \mu\phi_0\right) \\ \phi_0(0) = 0 \\ \phi_0(\infty) = \phi_0^{asympt} \end{cases} \implies \mu = g\,|\phi_0^{asympt}|^2$$

Adimensional form :

$$y = \frac{\phi_0(x)}{\phi_0^{asympt}} \quad , \quad X = x/\xi \quad \text{with} \quad \xi = \left(\frac{\hbar^2}{2mg|\phi_0^{asympt}|^2}\right)^{1/2}$$

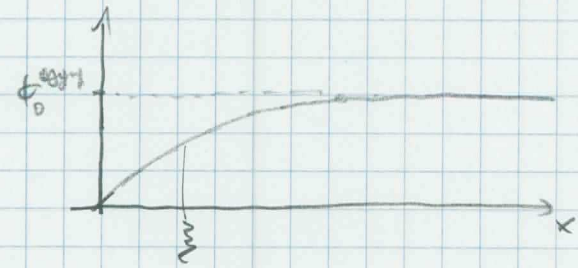
(healing length)

$$\cancel{\frac{\phi_0^{asympt}}{\xi^2}}\frac{d^2}{dX^2}y = \cancel{\frac{2mg}{\hbar^2}(\phi_0^{asympt})^3}\, y^3 - \cancel{\frac{2mg}{\hbar^2}(\phi_0^{asympt})^3}\, y$$

$$y'' = y^3 - y$$

solution $\quad y(X) = \text{th}\, X$

<u>So</u>: $\quad \phi_0(x) = \phi_0^{asympt}\ \text{th}(x/\xi)$



* effect of wall "heals" over a length scale ξ

* far from wall $\longrightarrow$ density constant

* solves paradox of BEC dependence on boundary condition

b) <u>Harmonic trap</u> $\quad V_{ext} = \frac{1}{2} m \omega^2 r^2$

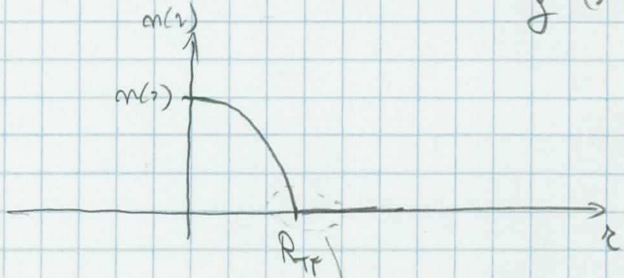
$$\mu \phi_0 = -\frac{\hbar^2}{2m}\nabla^2\phi_0 + \frac{1}{2} m\omega^2 r^2 \phi_0 + g\phi_0^2\phi_0$$

Thomas-Fermi approx: neglects $\frac{\hbar^2}{2m}\nabla^2\phi_0$ term

$$\left(\frac{1}{2} m \omega^2 r^2 + g\phi_0^2\right)\phi_0 = \mu\, \phi_0$$

density profile $(\phi_0(r))^2 = n(r)$ follows inverted parabola.

$$n(r) = \frac{1}{g}\left(\mu - V_{ext}(r)\right)$$



→ quantum pressure term active only in this region.

→ smoothens density profile

→ tail extends beyond R_{TF}

c) Soliton with attractive interactions $g<0$

- $g<0$ means negative compressibility $\partial n/\partial\mu < 0$
  so uniform system unstable
- look for localized solutions.

* Stationary ϕ_0 is minimizer of $E_{GP}(\phi)$

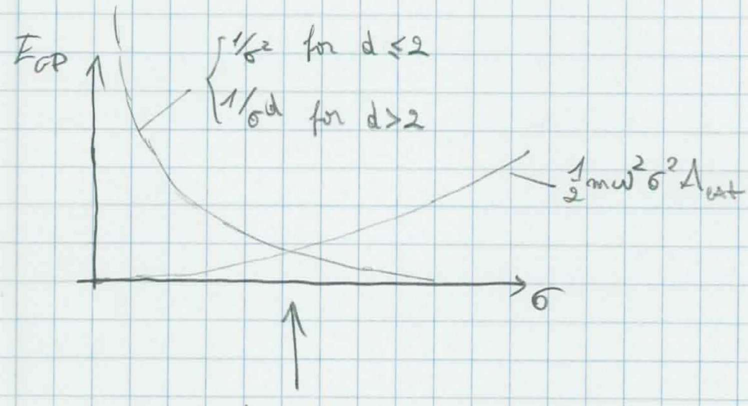
$$E_{GP}(\phi) = \int d^3r \; \frac{\hbar^2}{2m}|\nabla\phi|^2 + V_{ext}|\phi|^2 + \frac{g}{2}|\phi|^4$$

Gaussian ansatz: $\phi = \phi_{max}\, e^{-r^2/2\sigma^2} = C\sqrt{\frac{N}{\sigma^d}}\, e^{-r^2/2\sigma^2}$

variational calculation in σ

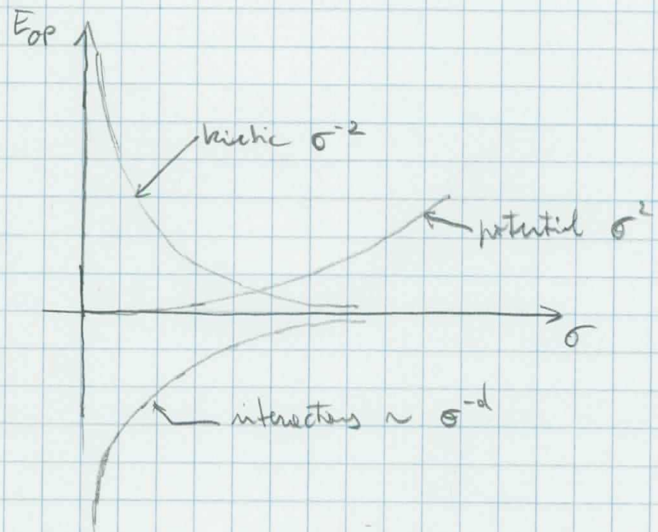
$$E_{op}^{gauss}(\sigma) \sim \frac{\hbar^2}{2m\sigma^2} A_{kin} + \frac{1}{2} m\omega^2 \sigma^2 A_{ext} + \frac{g}{2\sigma^d} A_{int}$$

i) $g > 0$



exists an energy minimum at finite σ.

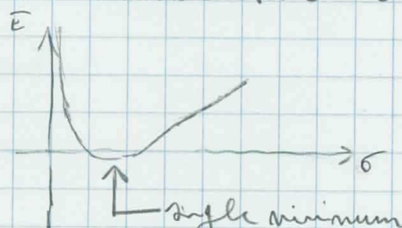
ii) $g < 0$



* for $d < 2$ kinetic energy dominates over interactions for $\sigma \to 0$

single minimum at finite σ

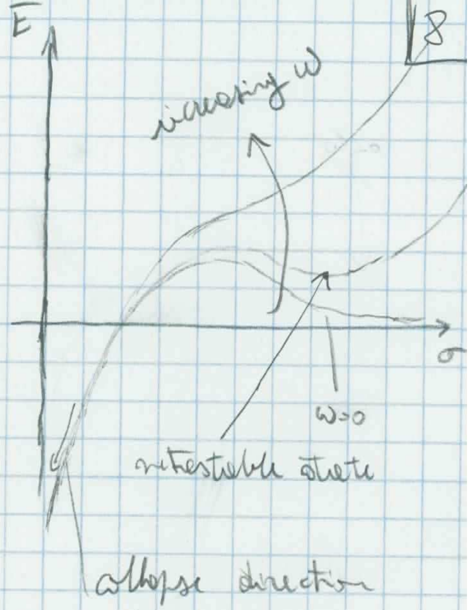
↳ SOLITON wavepacket



* for $d > 2$ interaction energy dominates over kinetic for $\sigma \to 0$

system may collapse $\sigma \to 0$

but <u>metastable states also possible</u>.



$\Rightarrow$ if trapping not too strong a metastable state is possible at a finite σ.

equivalently: metastable state exists for not too large N

$\Rightarrow$ solves a debate whether BEC is possible with $g<0$. (unlucky Hulet)

Full calculation of SOLITON state:

$$\phi_0(x) = \sqrt{\frac{\hbar^2}{m|g|\xi^2}} \cdot \frac{1}{2\cosh(x/2\xi)}$$

* total N and size ξ related by $N = \frac{\hbar^2}{m|g|\xi}$

  → more atoms, more compressed soliton

  → stronger interaction, more compressed.

Physically: particles bound by potential created by themselves.

Bibliography

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  [soliton physics]