(1-6) <u>The Gross-Pitaevskii equation</u>

How describe BEC theoretically?

N bosons at zero temperature

Many-body wavefunction

$\psi(\vec{r}_1, \dots, \vec{r}_N, t)$

Schrödinger eqn.

$$i\hbar \frac{\partial \psi}{\partial t} = \sum_{j=1}^{N} \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial \vec{r}_j^{\,2}}\right) \psi + \sum_{j=1}^{N} V(\vec{r}_j) \psi$$

$$+ \frac{1}{2} \sum_{i \neq j} U_0 \, \delta(\vec{r}_i - \vec{r}_j) \psi(\vec{r}_1, \dots \vec{r}_i, \dots, \vec{r}_j, \dots, \vec{r}_N, t) = \hat{H} \psi$$

Model of <u>contact interaction</u>

<u>Assume:</u> All bosons are in the same single-particle state

$\Rightarrow$ <u>product state</u>

$$\boxed{\psi(\vec{r}_1, \dots, \vec{r}_N, t) = \prod_{j=1}^{N} \varphi(\vec{r}_j, t) \qquad \text{B.E.C. Ansatz}}$$

Insert in S.E. $[\text{let } \varphi_j = \varphi(\vec{r}_j, t)]$

$$i\hbar \sum_{j=1}^{N} \frac{\partial \varphi_j}{\partial t} \left(\prod_{j' \neq j} \varphi_{j'}\right) = -\frac{\hbar^2}{2m} \sum_{j=1}^{N} \nabla^2 \varphi_j \left(\prod_{j' \neq j} \varphi_{j'}\right)$$

$$+ \sum_{j=1}^{N} V(r_j) \varphi_j \left(\prod_{j' \neq j} \varphi_{j'}\right)$$

$$+ \frac{1}{2} \sum_{i \neq j} U_0 \varphi_i \varphi_j \delta(\vec{r}_i - \vec{r}_j) \left(\prod_{\substack{j' \neq i \\ j' \neq j}} \varphi_{j'}\right)$$

Multiply from left by $\varphi_1^* \varphi_2^* \varphi_3^* \varphi_4^* \dots \varphi_N^*$

and integrate $\int dr_1 \, dr_2 \dots dr_N$

$$i\hbar N \int dr \, \varphi^*(r) \frac{\partial}{\partial t} \varphi(r) = N \int dr \, \varphi^*(r) \left(-\frac{\hbar^2}{2m} \nabla^2 + V(r)\right) \varphi(r)$$

$$+N(N-1)\frac{U_0}{2}\underbrace{\int dr_i\, dr_j\, \varphi^*(r_i)\varphi^*(r_j)\,\delta(r_i-r_j)\,\varphi(r_j)\varphi(r_i)}$$

$$= N(N-1)\frac{U_0}{2}\int dr\, |\varphi(r)|^4$$

Finally, differentiate w.r.t. $\varphi^*(r)$ both sides

$$i\hbar\frac{\partial\varphi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\varphi + V(r)\varphi + (N-1)U_0|\varphi(r)|^2\varphi(r)$$

The Gross-Pitaevskii equation.

- Note 1: A many-body system described by a single PDE.

Note 2: A non-linear Schrodinger equation.
Similar equations in - optics.
- Ginzburg-Landau eqn.

Note 3: Compare Hartree-Fock theory.
A mean-field theory: Assumes particles are uncorrelated.

Assume time-independent state
$\Psi(\vec{r},t) = \Psi(r)e^{-i\lambda t/\hbar}$
where λ is some quantity with dimensions of energy

$\lambda\Psi = (R.H.S.)$

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Compute total energy

$$E = \int d^3r\, \psi^*(\vec{r}_1, \dots, \vec{r}_N)\, \hat{H}\, \psi(\vec{r}_1, \dots, \vec{r}_N)$$

$$= \int d^3r\, N \varphi^* \left[-\frac{\hbar^2}{2m}\nabla^2 + V(r) + \frac{N}{2} U_0 |\varphi|^2 \right] \varphi$$

Chemical potential

$$\mu = \frac{\partial E}{\partial N} = \int d^3r\, \varphi^* \underbrace{\left[-\frac{\hbar^2}{2m}\nabla^2 + V(r) + N U_0 |\varphi|^2 \right] \varphi}_{\text{GPE!}}$$

$$= \int d^3r\, \varphi^* \lambda \varphi = \lambda$$

$\therefore$ $\lambda = \mu$ the chemical potential of the system.

GPE is used to simulate
- ☆ Ground state in various traps
- ☆ Modes of oscillation
- ☆ Vortices, rotational states
- ☆ Even finite-T theory and T_c (with modifications!)
- ☆ etc. etc.

→ excellent agreement with experiment!!

Slides

Note: GPE is not the whole story.
Bogoliubov theory describes excitations above ground state