Construction of GPE

$$H_N = \sum_{i=1}^{N} \left(-\frac{\hbar^2}{2m} \Delta_i + V(x_i) \right) + \sum_{1 \le j < k \le N} V_{int}(x_j - x_k)$$

$\Psi_N := \Psi_N(x_1, \dots, x_N, t) \in L^2(\mathbb{R}^{3N} \times \mathbb{R})$ is symmetric w.r.t. any permutation of pos. x_j. (Indistinguishability of particles ?)

In ultracold regime, 1st approximation $\Rightarrow$ $V_{int}(x_j - x_k) = g\,\delta(x_j - x_k)$ where $g = \dfrac{4\pi\hbar^2 a_s}{m}$

This approx. is valid for $a_s \ll$ average dist. btw. particles. (Dilute Gases)

For BEC, Hartree ansatz can be used $\Psi_N(x_1, \dots, x_N, t) = \prod_{j=1}^{N} \phi_n(x_j, t)$ where all particles are in same q-state.

$$\int_{\mathbb{R}^3} |\phi_H(x_j, t)|^2 d^3x_j = 1$$

$$H_N = \sum_{j=1}^{N} H_{j,non} + \sum_{1 \le j < k \le N} g\,\delta(x_j - x_k)$$

$\langle E \rangle = ?$

* Without Hartree Approx., $|\Psi_N\rangle = \sum_{i_1, \dots, i_N} C_{i_1, \dots, i_N} |\phi_{i_1}\rangle \otimes \cdots |\phi_{i_N}\rangle$

With Hartree Approx., $|\Psi_N\rangle = |\phi_1\rangle \otimes \cdots \otimes |\phi_N\rangle$

$$\langle E \rangle = \sum_{j=1}^{N} \langle \Psi_N | H_{j,non} | \Psi_N \rangle + \sum_{1 \le j < k \le N} g \langle \Psi_N | \delta(x_j - x_k) | \Psi_N \rangle$$

$$\langle \Psi_N | H_{j,non} | \Psi_N \rangle = \int d^3x_1' \dots d^3x_N'\, d^3x_1'' \dots d^3x_N''\, \langle \phi_1 | x_1' \rangle \langle x_1' | \otimes \cdots \otimes \langle \phi_N | x_N' \rangle \langle x_N' | \left(\mathbb{1} \otimes \cdots \otimes H_{j,non} \otimes \cdots \otimes \mathbb{1} \right) |x_1''\rangle \langle x_1'' | \phi_1 \rangle \otimes \cdots \otimes |x_N''\rangle \langle x_N'' | \phi_N \rangle$$

$$= \int d^3x_j'\, d^3x_j''\, \langle \phi_j | x_j' \rangle \langle x_j' | H_{j,non} | x_j'' \rangle \langle x_j'' | \phi_j \rangle$$

Since $H_{j,non}$ is diagonal operator, $\left(-\frac{\hbar^2}{2m}\Delta_{x_j'} + V(x_j')\right)\delta(x_j' - x_j'') = \langle x_j' | H_{j,non} | x_j'' \rangle$

$$\Rightarrow \langle \Psi_N | H_{j,non} | \Psi_N \rangle = \int d^3x_j' \, d^3x_j'' \, \phi^*(x_j') \left(-\frac{\hbar^2}{2m}\Delta_{x_j'} + V(x_j')\right)\delta(x_j' - x_j'')\,\phi(x_j'')$$

$$= \int d^3x_j' \, \phi^*(x_j') \left(-\frac{\hbar^2}{2m}\nabla^2_{x_j'} + V(x_j')\right)\phi(x_j')$$

By integration by parts; $du = d^3x_j' \, \nabla^2_{x_j'}\phi(x_j')$, $u = \nabla_{x_j'}\phi(x_j')$ & $v = \phi^*(x_j')$, $dv = dx_j' \, \nabla_{x_j'}\phi^*(x_j')$

$$= \int d^3x_j' \left(+\frac{\hbar^2}{2m}\left|\nabla_{x_j'}\phi(x_j')\right|^2 + V(x_j')\left|\phi(x_j')\right|^2\right)$$

$$\langle \Psi_N | \delta(x_i - x_j) | \Psi_N \rangle \overset{?}{=}$$

$$\sum_{1\le j<k\le N} \delta(x_j - x_k) = \underbrace{\delta(x_1 - x_2) + \delta(x_1 - x_3) + \delta(x_2 - x_3) + \cdots}$$

$\frac{N(N-1)}{2}$ is the number of Dirac-Delta func.

$$\Rightarrow \sum_{1\le j<k\le N} \langle \Psi_N | \delta(x_i - x_j) | \Psi_N \rangle = \frac{N(N-1)}{2} \int d^3x \, |\phi(x)|^4$$

$$\langle E\rangle = N\int_{\mathbb{R}^3}\left[\frac{\hbar^2}{2m}|\nabla\phi_H(\vec{x},t)|^2 + V(x)|\phi_H(\vec{x},t)|^2 + \frac{N-1}{2}g|\phi_H(\vec{x},t)|^4\right]d^3x$$

with redefination, $\phi(\vec{x},t) - \sqrt{N}\,\phi_H(\vec{x},t)$ & assumption of $N >> 1$

$$\langle E\rangle = \int_{\mathbb{R}^3}\left[\frac{\hbar^2}{2m}|\nabla\phi(\vec{x},t)|^2 + V(\vec{x})|\phi(\vec{x},t)|^2 + \frac{1}{2}g|\phi(\vec{x},t)|^4\right]d^3x \quad ?$$

Now, we will use similar relation from Classical Hamiltonian Mechanics.

$q(t)$ & $p(t)$ are canonical variables, $H \equiv H(q,p)$; $\dot{q} = \frac{\partial H}{\partial p}$ & $\dot{p} = -\frac{\partial H}{\partial q}$ where $\{q,\vec{p}\} = 1$

Likewise, in our case, ϕ & ϕ^* taken as conjugate variables. $\{\phi(\vec{x}),\phi^*(\vec{y})\} = \frac{1}{i\hbar}\delta(\vec{x}-\vec{y})$

$$\Rightarrow i\hbar\,\partial_t\phi = \frac{\delta E}{\delta\phi^*}, \quad -i\hbar\,\partial_t\phi^* = \frac{\delta E}{\delta\phi}$$

$$i\hbar\frac{\partial\phi}{\partial t} = \left(-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{x}) + \frac{g}{2}|\phi(\vec{x},t)|^2\right)\phi(\vec{x},t)$$

How can we get ground state from an Ordinary function?

Any function, $\Psi(z,0)=\sum c_i\phi_i(z)$; for time-indep. Hamiltonian, $\Psi(z,t)=e^{-iHt/\hbar}\Psi(z,0)=\sum_n c_n e^{-iE_n t/\hbar}\phi_n(z)$

with Wick Rotation $t=-i\tau$, $\Psi(z,\tau)=\sum_n c_n e^{-E_n\tau/\hbar}\phi_n(z)$

Since $E_0<E_1<\dots$, for large τ, major contr. from ground state,

$$\Psi(z,\tau)\propto e^{-E_0\tau/\hbar}\phi_0(z)$$

$\mathcal{H}=\sum_{i=1}^{n} p_i\dot{q}_i-\mathcal{L}(q,\dot{q},t)$, In our case, while constructing to have ~~constant~~ stationary action, we treat like looking expectation values. Such that we multiply Sch. eqn. by ϕ^*

$$S=\int dt\int d^3x\,\psi^*(i\hbar\partial_t-\hat{H})\psi$$