

## Exercise 2:

a) Deduce the expression for the expectation value of the Hamiltonian:

$$H = \sum_{i=1}^N \left[ \frac{p_i^2}{2m} + V(r_i) \right] + U_0 \sum_{i<j} \delta(r_i - r_j)$$

and,

$$E = \langle \Psi | H | \Psi \rangle = \sum_{i=1}^N \int d^3r \frac{\hbar^2}{2m} |\nabla_{r_i} \Psi(r_1, \dots, r_N)|^2 + \sum_{i=1}^N \int d^3r V(r_i) |\Psi(r_1, \dots, r_N)|^2 +$$

$$U_0 \sum_{i<j} \int d^3r |\Psi(r_1, \dots, r_N)|^2 \delta(r_i - r_j)$$

where,

$$\Psi(r_1, \dots, r_N) = \prod_{i=1}^N \phi(r_i)$$

$$\int d^3r_i |\phi(r_i)|^2 = 1$$

so,

$$E = \frac{\hbar^2}{2m} \sum_{i=1}^N \int \prod_{j=1}^N d^3r_j |\nabla_{r_i} \phi(r_j)|^2 + \sum_{i=1}^N \int \prod_{j=1}^N d^3r_j V(r_i) |\phi(r_j)|^2 +$$

$$U_0 \sum_{i<j} \int \prod_{j=1}^N d^3r_j |\phi(r_j)|^2 \delta(r_i - r_j)$$

we make,

$$E = \frac{\hbar^2}{2m} \sum_{i=1}^N \int \prod_{j=1}^N d^3r_j |\nabla_{r_i} \phi(r_j)|^2 + \sum_{i=1}^N \int \prod_{j=1}^N d^3r_j V(r_i) |\phi(r_j)|^2 +$$

$$U_0 \int \prod_{i=1}^N d^3r_i |\phi(r_i)|^2 \left\{ \sum_{i<j} \int \prod_{j=1}^N d^3r_j |\phi(r_j)|^2 \delta(r_i - r_j) \right\}$$

where,

$$\sum_{i=1}^N \int \prod_{j=1}^N d^3r_j |\nabla_{r_i} \phi(r_j)|^2 = \sum_{i=1}^N \int d^3r_i |\nabla_{r_i} \phi(r_i)|^2 = N \int d^3r |\nabla_r \phi(r)|^2$$

$$\sum_{i=1}^N \int \prod_{j=1}^N d^3r_j V(r_i) |\phi(r_j)|^2 = \sum_{i=1}^N \int d^3r_j V(r_j) |\phi(r_j)|^2 = N \int d^3r V(r) |\phi(r)|^2$$

and,

$$\int \prod_{i=1}^N d^3 r_i |\phi(r_i)|^2 \left\{ \sum_{i < j} \int \prod_{j=1}^N d^3 r_j |\phi(r_j)|^2 \delta(r_i - r_j) \right\} =$$

$$\frac{1}{2} \sum_i \int \prod_{i=1}^N d^3 r_i |\phi(r_i)|^2 \left\{ \sum_j \int \prod_{j=1}^N d^3 r_j |\phi(r_j)|^2 \delta(r_i - r_j) \right\}$$

so,

$$\sum_j \int \prod_{j=1}^N d^3 r_j |\phi(r_j)|^2 \delta(r_i - r_j) = N |\phi(r_i)|^2$$

replacing in the expectation value of the hamiltonian,

$$E = N \int d^3 r \frac{\hbar^2}{2m} |\nabla_r \phi(r)|^2 + N \int d^3 r V(r) |\phi(r)|^2 +$$

$$U_0 \frac{N}{2} \sum_{i=1}^N \int d^3 r_i |\phi(r_i)|^2 |\phi(r_i)|^2$$

finally,

$$E = N \int d^3 r \frac{\hbar^2}{2m} |\nabla_r \phi(r)|^2 + N \int d^3 r V(r) |\phi(r)|^2 +$$

$$U_0 \frac{N^2}{2} \int d^3 r |\phi(r)|^4$$

$$E = N \int d^3 r \left[ \frac{\hbar^2}{2m} |\nabla \phi(r)|^2 + V(r) |\phi(r)|^2 + U_0 \frac{N}{2} |\phi(r)|^4 \right]$$

b) obtain time-independent GPE. from:

$$E(\psi) = \int d^3 r \left[ \frac{\hbar^2}{2m} |\nabla \psi(r)|^2 + V(r) |\psi(r)|^2 + \frac{1}{2} U_0 |\psi(r)|^4 \right]$$

and,

$$N = \int d^3 r |\psi(r)|^2$$

by using Lagrange multipliers,

$$\delta E - \mu \delta N = 0$$

and,

$$\frac{\partial E}{\partial \psi^*} \delta \psi^* + \frac{\partial E}{\partial (\nabla \psi^*)} \delta (\nabla \psi^*) - \mu \frac{\partial N}{\partial \psi^*} \delta \psi^* = 0$$

$$\frac{\partial E}{\partial \psi^*} \delta \psi^* + \frac{\partial E}{\partial (\nabla \psi^*)} \nabla (\delta \psi^*) - \mu \frac{\partial N}{\partial \psi^*} \delta \psi^* = 0$$

and,

$$\left\{ \frac{\partial E}{\partial \psi^*} - \nabla \left( \frac{\partial E}{\partial (\nabla \psi^*)} \right) - \mu \frac{\partial N}{\partial \psi^*} \right\} \delta \psi^* + \nabla \left( \frac{\partial E}{\partial (\nabla \psi^*)} \delta \psi^* \right) = 0$$

$$\frac{\partial E}{\partial \psi^*} = \int d^3 r [V(r) \psi(r) + U_0 |\psi(r)|^2 \psi(r)]$$

$$\frac{\partial E}{\partial (\nabla \psi^*)} = \int d^3 r \frac{\hbar^2}{2m} \nabla \psi(r)$$

$$\frac{\partial N}{\partial \psi^*} = \int d^3 r \psi(r)$$

replacing,

$$\int d^3 r \left\{ V(r) \psi(r) + U_0 |\psi(r)|^2 \psi(r) - \nabla \left( \frac{\hbar^2}{2m} \nabla \psi(r) \right) - \mu \psi(r) \right\} \delta \psi^* +$$

$$\int d^3 r \nabla \left( \frac{\partial E}{\partial (\nabla \psi^*)} \delta \psi^* \right) = 0$$

and,

$$\int d^3 r \left\{ -\frac{\hbar^2}{2m} \nabla^2 \psi(r) + V(r) \psi(r) + U_0 |\psi(r)|^2 \psi(r) - \mu \psi(r) \right\} \delta \psi^* = 0$$

a GPE is,

$$-\frac{\hbar^2}{2m} \nabla^2 \psi(r) + V(r) \psi(r) + U_0 |\psi(r)|^2 \psi(r) = \mu \psi(r)$$

c) with for uniform gas  $V(r) = 0$ ,  $\psi(r) \approx cte$ , defining  $g = U_0$ ,  $g |\psi|^2 = \mu$ . We can consider the time-dependende GPE.

$$i\hbar \frac{\partial \psi(r, t)}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi(r) + g |\psi(r)|^2 \psi(r)$$