Density Functional Theory (DFT)

Schroedinger equation

$$\left(-\frac{\hbar^2}{2m}\sum_j \nabla_j^2 + \sum_j v(r_j) + \frac{1}{2}\sum_{j\neq j'} \frac{1}{|r_j - r_{j'}|} - E\right)\Psi = 0$$

$v(r)$

$$\Psi = \Psi(r_1, r_2, \ldots r_N) \quad \text{(spin ignored)}$$

DFT

$n(r)$

$$E_{v(r)}[n(r)] = \int v(r)\, n(r)\, dr + T[n(r)] + \left\{\frac{1}{2}\frac{1}{|r-r'|} n(r)\, n'(r)\, dr dr'.\right.$$

$\rho_1(r) \equiv$ density of particles "1"

$$\rho_1(r) = N_1 \int dr_2' dr_3' \ldots dr_{N_1}' \, dr_1'' \ldots dr_{N_2}'' \left| \Phi(r_1' \ldots r_{N_1}' r_1'' \ldots r_{N_2}'') \right|^2$$

no dr_1

Self-bound Systems

To save writing, deal only with neutrons and ignore protons. If mass-center is "free"

$$\Phi_K(r_1, r_2, \ldots r_K) = \exp(iKR)\, \Phi(r_1, r_2 \ldots r_N)$$

K = total momentum

R = center of mass,

$$R \equiv N^{-1}(r_1 + \ldots + r_N)$$

$$r_j' \equiv r_j - R$$

Wave-packets

$$\Psi_K \equiv \sum_{K'} A(K')\, \Phi_{K'} \; ; \; A(K') = A\, e^{-\sigma(K'-K)^2}$$