

# Computational physics: Project 1

Jon Aleksander Prøitz  
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## SECTION 1

The local energy is given by

$$E_L = \frac{1}{\Psi_T} H \Psi_T \quad (1)$$

with

$$H = \sum_i^N \left( \frac{-\hbar^2}{2m} \nabla_i^2 + V_{\text{ext}} \right) + \sum_{i < j}^N V_{\text{int}} \quad (2)$$

$$V_{\text{ext}}(\mathbf{r}) = \begin{cases} \frac{1}{2} m \omega_{ho}^2 r^2 & (S) \\ \frac{1}{2} m [\omega_{ho}^2 (x^2 + y^2) + \omega_z^2 z^2] & (E) \end{cases} \quad (3)$$

$$V_{\text{int}}(|\mathbf{r}_i - \mathbf{r}_j|) = \begin{cases} \infty & |\mathbf{r}_i - \mathbf{r}_j| \leq a \\ 0 & |\mathbf{r}_i - \mathbf{r}_j| > a \end{cases} \quad (4)$$

$$\Psi_T(\mathbf{r}) = \Psi_T(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N, \alpha, \beta) = \left[ \prod_i g(\alpha, \beta, \mathbf{r}_i) \right] \left[ \prod_{j < k} f(a, |\mathbf{r}_j - \mathbf{r}_k|) \right], \quad (5)$$

for  $a = 0$ ,  $\beta = 1$ , note that in 1D

$$\frac{1}{\Psi_T} \frac{\partial^2 \Psi_T}{\partial x^2} = -2\alpha \frac{1}{\Psi_T} \frac{\partial \Psi_T}{\partial x} (x \Psi_T) = 2\alpha (2\alpha x^2 - 1) \quad (6)$$

$$\frac{1}{\Psi_T} \sum_{i=1}^d \frac{\partial^2 \Psi_T}{\partial x_i^2} = 2\alpha \left( 2\alpha \sum_{i=1} x_i^2 - d \right) \quad (7)$$