Computational physics: Project 1

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(Dated: March 1, 2024)

SECTION 1

The local energy is given by

$$E_L = \frac{1}{\Psi_T} H \Psi_T \tag{1}$$

with

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

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

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

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

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

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

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