Computational physics: Project 1

Jon Aleksander Prøitz
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SECTION 1

The local energy is given by

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

with

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

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

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

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

with

$$g(\alpha, \beta, \mathbf{r}_i) = exp\left[-\alpha \left(x_i^2 + y_i^2 + \beta z_i^2 \right) \right] \tag{6}$$

$$f(a, |\mathbf{r}_i - \mathbf{r}_j|) = \begin{cases} 0 & |\mathbf{r}_i - \mathbf{r}_j| \leq a \\ (1 - \frac{a}{|\mathbf{r}_i - \mathbf{r}_j|}) & |\mathbf{r}_i - \mathbf{r}_j| > a. \end{cases} \tag{7}$$

for $a = 0$, $\beta = 1$, note that in one dimension for one particle

$$\frac{1}{\Psi_T} \frac{\partial^2 \Psi_T}{\partial x^2} = -2\alpha \frac{1}{\Psi_T} \frac{\partial \Psi_T}{\partial x} \left(x \Psi_T \right) = 2\alpha \big(2\alpha x^2 - 1 \big) \tag{8}$$

Due to the symmetric properties of the trial wavefunction we note that with $\nabla^2 = \sum_{i=1} \frac{\partial^2}{\partial x_i^2}$

$$\frac{1}{\Psi_T} \sum_{i=1}^{d} \frac{\partial^2 \Psi_T}{\partial x_i^2} = 2\alpha \left(2\alpha \sum_{i=1}^{d} x_i^2 - d \right) = 2\alpha \left(2\alpha r^2 - d \right) \tag{9}$$

where d is the number of dimensions. Hence

$$E_L = \sum_{i}^{N} \left(\frac{-\hbar^2}{2m} 2\alpha \left(2\alpha r_i^2 - d \right) + \frac{1}{2} m \omega_{ho}^2 r_i^2 \right) = \sum_{i}^{N} \frac{d}{2} \hbar \omega_{ho} = \frac{Nd}{2} \hbar \omega_{ho} \tag{10}$$

with $\alpha = 1/2a_{ho}^2$ and $a_{ho} = \sqrt{\hbar/m\omega_{ho}}$

$$\mathbf{F} = \frac{2\nabla\Psi_T}{\Psi_T} = -4\alpha\sum_{i=1}^{d} x_i\hat{\mathbf{x}}_i \tag{11}$$

Define $g(\alpha,\beta,\mathbf{r}_i) = \phi(\mathbf{r}_i)$ and $r_{jm} = |\mathbf{r}_j - \mathbf{r}_m|$, such that

$$\Psi_T = \left[\prod_i \phi(\mathbf{r}_i)\right] e^{\sum_{j<m}\ln f(r_{jm})} = \left[\prod_i \phi(\mathbf{r}_i)\right] e^{\sum_{j<m} u(r_{jm})} \tag{12}$$

with $u(r_{jm}) = \ln f(r_{jm})$. The derivative of particle k is then

$$\nabla_k\Psi_T = \nabla_k\left[\prod_i \phi(\mathbf{r}_i)\right] e^{\sum_{j<m} u(_{jm})} + \left[\prod_i \phi(\mathbf{r}_i)\right] \nabla_k\left(e^{\sum_{j<m} u(r_{jm})}\right) \tag{13}$$

we note that in the frist term only particle k is affected by the derivation, such that

$$\nabla_k\prod_i \phi(\mathbf{r}_i) = \nabla_k\phi(\mathbf{r}_i)\left[\prod_{i\neq k}\phi(\mathbf{r}_i)\right] \tag{14}$$

while the second term

$$\nabla_k\left(e^{\sum_{j<m} u(r_{jm})}\right) = e^{\sum_{j<m} u(r_{jm})}\nabla_k\sum_{j<m} u(r_{jm}) = e^{\sum_{j<m} u(r_{jm})}\sum_{k\neq l}\nabla_k u(r_{kl}) \tag{15}$$

such that

$$\nabla_k\Psi_T = \nabla_k\phi(\mathbf{r}_i)\left[\prod_{i\neq k}\phi(\mathbf{r}_i)\right] e^{\sum_{j<m} u(_{jm})} + \left[\prod_i \phi(\mathbf{r}_i)\right] e^{\sum_{j<m} u(r_{jm})}\sum_{k\neq l}\nabla_k u(r_{kl}) \tag{16}$$