

The trial wave function for N particles is given by

$$\Psi_T(\mathbf{r}) = \Psi_T(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N, \alpha, \beta) = \left[\prod_i g(\alpha, \beta, \mathbf{r}_i) \right] \left[\prod_{j < k} f(a, |\mathbf{r}_j - \mathbf{r}_k|) \right], \quad (1)$$

where

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

and

$$f(a, |\mathbf{r}_i - \mathbf{r}_j|) = \begin{cases} 0 & |\mathbf{r}_i - \mathbf{r}_j| \leq a \\ (1 - \frac{a}{|\mathbf{r}_i - \mathbf{r}_j|}) & |\mathbf{r}_i - \mathbf{r}_j| > a. \end{cases} \quad (3)$$

Defining $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$ and $u(r_{ij}) = \ln f(r_{ij})$, this can be rewritten as

$$\Psi_T(\mathbf{r}) = \left[\prod_i \phi(\mathbf{r}_i) \right] \exp \left(\sum_{j < m} u(r_{jm}) \right)$$

The gradient with respect to particle k is then:

$$\begin{aligned} \nabla_k \Psi_T(\mathbf{r}) &= \nabla_k \left(\left[\prod_i \phi(\mathbf{r}_i) \right] \exp \left(\sum_{j < m} u(r_{jm}) \right) \right) \\ &= \left(\nabla_k \left[\prod_i \phi(\mathbf{r}_i) \right] \right) \exp \left(\sum_{j < m} u(r_{jm}) \right) + \left[\prod_i \phi(\mathbf{r}_i) \right] \left(\nabla_k \exp \left(\sum_{j < m} u(r_{jm}) \right) \right) \\ &= \nabla_k \phi(\mathbf{r}_k) \left[\prod_{i \neq k} \phi(\mathbf{r}_i) \right] \exp \left(\sum_{j < m} u(r_{jm}) \right) \\ &\quad + \left[\prod_i \phi(\mathbf{r}_i) \right] \exp \left(\sum_{j < m} u(r_{jm}) \right) \sum_{l \neq k} \nabla_k u(r_{kl}) \end{aligned}$$

where we used the product rule for gradients and the fact that only $\phi(\mathbf{r}_k)$ and $\exp(\sum_{l \neq k} u(r_{kl}))$ are functions of \mathbf{r}_k .

The second derivative divided by the trial wave function is then given by

$$\begin{aligned}
\frac{1}{\Psi_T(\mathbf{r})} \nabla_k^2 \Psi_T(\mathbf{r}) &= \frac{1}{\Psi_T(\mathbf{r})} \nabla_k \cdot (\nabla_k \Psi_T(\mathbf{r})) \\
&= \frac{1}{\Psi_T(\mathbf{r})} \nabla_k \cdot \left(\nabla_k \phi(\mathbf{r}_k) \left[\prod_{i \neq k} \phi(\mathbf{r}_i) \right] \exp \left(\sum_{j < m} u(r_{jm}) \right) \right) \\
&\quad + \frac{1}{\Psi_T(\mathbf{r})} \nabla_k \cdot \left(\left[\prod_i \phi(\mathbf{r}_i) \right] \exp \left(\sum_{j < m} u(r_{jm}) \right) \sum_{l \neq k} \nabla_k u(r_{kl}) \right) \\
&= \frac{1}{\Psi_T(\mathbf{r})} (\nabla_k^2 \phi(\mathbf{r}_k)) \left[\prod_{i \neq k} \phi(\mathbf{r}_i) \right] \exp \left(\sum_{j < m} u(r_{jm}) \right) \\
&\quad + \frac{1}{\Psi_T(\mathbf{r})} \left(\left[\prod_{i \neq k} \phi(\mathbf{r}_i) \right] \exp \left(\sum_{j < m} u(r_{jm}) \right) \nabla_k \phi(\mathbf{r}_k) \cdot \sum_{l \neq k} \nabla_k u(r_{kl}) \right) \\
&\quad + \frac{1}{\Psi_T(\mathbf{r})} \left(\left[\prod_{i \neq k} \phi(\mathbf{r}_i) \right] \exp \left(\sum_{j < m} u(r_{jm}) \right) \nabla_k \phi(\mathbf{r}_k) \cdot \sum_{l \neq k} \nabla_k u(r_{kl}) \right) \\
&\quad + \frac{1}{\Psi_T(\mathbf{r})} \left[\prod_i \phi(\mathbf{r}_i) \right] \exp \left(\sum_{j < m} u(r_{jm}) \right) \left(\sum_{l \neq k} \nabla_k u(r_{kl}) \right)^2 \\
&\quad + \frac{1}{\Psi_T(\mathbf{r})} \left[\prod_i \phi(\mathbf{r}_i) \right] \exp \left(\sum_{j < m} u(r_{jm}) \right) \sum_{l \neq k} \nabla_k^2 u(r_{kl}) \\
&= \frac{\nabla_k^2 \phi(\mathbf{r}_k)}{\phi(\mathbf{r}_k)} + 2 \frac{\nabla_k \phi(\mathbf{r}_k)}{\phi(\mathbf{r}_k)} \cdot \sum_{l \neq k} \nabla_k u(r_{kl}) \\
&\quad + \sum_{l \neq k} \nabla_k u(r_{kl}) \cdot \sum_{i \neq k} \nabla_k u(r_{ki}) \\
&\quad + \sum_{l \neq k} \nabla_k^2 u(r_{kl})
\end{aligned}$$

where we used the product rule for divergences and gradients. The expressions for the gradient of $u(r_{ik})$ can be reexpressed using the chain rule. We have that, by the chain rule

$$\frac{\partial u(r_{ki})}{\partial x_k} \hat{\mathbf{x}}_{\mathbf{k}} = \frac{\partial r_{ki}}{\partial x_k} \frac{\partial u(r_{ki})}{\partial r_{ki}} \hat{\mathbf{x}}_{\mathbf{k}} = u'(r_{ki}) \frac{x_k - x_i}{r_{ki}} \hat{\mathbf{x}}_{\mathbf{k}}$$

and we get the equivalent expressions for the partial derivatives with respect to y_k and z_k due to symmetry. Combining these, we get

$$\nabla_k u(r_{ki}) = \frac{(\mathbf{r}_k - \mathbf{r}_i)}{r_{ki}} u'(r_{ki})$$

Similarly, we get for the second partial derivative that

$$\begin{aligned}\frac{\partial^2 u(r_{ki})}{\partial x_k^2} &= \frac{\partial}{\partial x_k} \left(u'(r_{ki}) \frac{x_k - x_i}{r_{ki}} \right) = \frac{\partial u'(r_{ki})}{\partial x_k} \frac{x_k - x_i}{r_{ki}} + u'(r_{ki}) \frac{\partial}{\partial x_k} \left(\frac{x_k - x_i}{r_{ki}} \right) \\ &= u''(r_{ki}) \frac{(x_k - x_i)^2}{r_{ki}^2} + u'(r_{ki}) \left(\frac{1}{r_{ki}} - \frac{(x_k - x_i)^2}{r_{ki}^3} \right)\end{aligned}$$

and again, we get equivalent expressions for the second partial derivatives with respect to y_k and z_k . Because $(x_k - x_i)^2 + (y_k - y_i)^2 + (z_k - z_i)^2 = r_{ki}^2$, the Laplacian becomes

$$\nabla_k^2 u(r_{kl}) = u''(r_{ki}) \frac{r_{ki}^2}{r_{ki}^2} + u'(r_{ki}) \left(\frac{3}{r_{ki}} - \frac{r_{ki}^2}{r_{ki}^3} \right) = u''(r_{kj}) + \frac{2}{r_{kj}} u'(r_{kj})$$

Inserting this in the expression for the second derivative, we get Morten's result.

Here are the analytic expressions for the quantum force and the second derivative: The quantum force $\frac{2\nabla\psi}{\psi}$ for particle k is given by:

$$\begin{aligned}\frac{2\nabla_k\psi}{\psi} &= \frac{2\nabla_k\phi(\mathbf{r}_k) \left[\prod_{i \neq k} \phi(\mathbf{r}_i) \right] \exp \left(\sum_{j < m} u(r_{jm}) \right) + 2 \left[\prod_i \phi(\mathbf{r}_i) \right] \exp \left(\sum_{j < m} u(r_{jm}) \right) \sum_{l \neq k} \nabla_k u(r_{kl})}{\psi} \\ &= \frac{-4\alpha(x_k \hat{x}_k + y_k \hat{y}_k + \beta z_k \hat{z}_k) \psi + 2\psi \sum_{l \neq k} \nabla_k u(r_{kl})}{\psi} \\ &= -4\alpha(x_k \hat{x}_k + y_k \hat{y}_k + \beta z_k \hat{z}_k) + 2 \sum_{l \neq k} \frac{(\mathbf{r}_k - \mathbf{r}_l)}{r_{kl}} u'(r_{kl}) \\ &= -4\alpha(x_k \hat{x}_k + y_k \hat{y}_k + \beta z_k \hat{z}_k) + 2 \sum_{l \neq k} \frac{(\mathbf{r}_k - \mathbf{r}_l)}{r_{kl}} \frac{-a}{ar_{kl} - r_{kl}^2} \\ &= -4\alpha(x_k \hat{x}_k + y_k \hat{y}_k + \beta z_k \hat{z}_k) - \sum_{l \neq k} \frac{2a}{ar_{kl}^2 - r_{kl}^3} (\mathbf{r}_k - \mathbf{r}_l)\end{aligned}$$

Now let's have a good look at the best that we call second derivative / kinetic energy. We have the formula given by

$$\begin{aligned}
\frac{1}{\Psi_T(\mathbf{r})} \nabla_k^2 \Psi_T(\mathbf{r}) &= \frac{\nabla_k^2 \phi(\mathbf{r}_k)}{\phi(\mathbf{r}_k)} + 2 \frac{\nabla_k \phi(\mathbf{r}_k)}{\phi(\mathbf{r}_k)} \cdot \sum_{l \neq k} \nabla_k u(r_{kl}) \\
&\quad + \sum_{l \neq k} \nabla_k u(r_{kl}) \cdot \sum_{i \neq k} \nabla_k u(r_{ki}) \\
&\quad + \sum_{l \neq k} \nabla_k^2 u(r_{kl}) \\
&= [4\alpha^2 [x_k^2 + y_k^2 + \beta^2 z_k^2] - 4\alpha - 2\alpha\beta] - 4\alpha(x_k \hat{x}_k + y_k \hat{y}_k + \beta z_k \hat{z}_k) \cdot \sum_{j \neq k} \frac{-a}{ar_{kj}^2 - r_{kj}^3} (\mathbf{r}_k - \mathbf{r}_j) \\
&\quad + \sum_{k \neq i} \sum_{k \neq j} \frac{(\mathbf{r}_k - \mathbf{r}_i) \cdot (\mathbf{r}_k - \mathbf{r}_j)}{r_{ki} r_{kj}} \frac{a^2}{(ar_{kj}^2 - r_{kj}^3)(ar_{ki}^2 - r_{ki}^3)} \\
&\quad + \sum_{k \neq j} \frac{a(a - 2r_{kj})}{r_{kj}^2 (a - r_{kj})^2} - \frac{2a}{(ar_{kj}^2 - r_{kj}^3)} \\
&= [4\alpha^2 [x_k^2 + y_k^2 + \beta^2 z_k^2] - 4\alpha - 2\alpha\beta] - 4\alpha(x_k \hat{x}_k + y_k \hat{y}_k + \beta z_k \hat{z}_k) \cdot \sum_{j \neq k} \frac{-a}{ar_{kj}^2 - r_{kj}^3} (\mathbf{r}_k - \mathbf{r}_j) \\
&\quad + 2 \sum_{k \neq i, k \neq j, i \leq j} \frac{(\mathbf{r}_k - \mathbf{r}_i) \cdot (\mathbf{r}_k - \mathbf{r}_j)}{r_{ki} r_{kj}} \frac{a^2}{(ar_{kj}^2 - r_{kj}^3)(ar_{ki}^2 - r_{ki}^3)} \\
&\quad + \sum_{k \neq j} \frac{-a^2}{r_{kj}^2 (a - r_{kj})^2}
\end{aligned}$$