Sample calculation

For the 1s orbital of hydrogen

$$\phi(\vec{r}) = \exp(-r) \qquad (1.1)$$

..\WaveFunction\Del2.doc

$$\nabla^2 f(|\vec{r}-\vec{a}|) = \left\{ 2\frac{f'(|\vec{r}-\vec{a}|)}{|\vec{r}-\vec{a}|} + f''(|\vec{r}-\vec{a}|) \right\} \qquad (1.2)$$

In Hartrees the Schrödinger equation is [..\WaveFunction\SeqnVariance.docx]

$$-\frac{\nabla^2\phi}{2} - \frac{1}{r}\phi = E_H\phi \qquad (1.3)$$

At the origin

$$\begin{aligned} \phi'(\vec{r}) &= -\exp(-r) \\ \phi''(\vec{r}) &= \exp(-r) \end{aligned} \qquad (1.4)$$

So that the value of E_H is ½

The expectation value of V is

$$\langle V \rangle = \frac{\int_0^\infty r\exp(-2r)\,dr}{\int_0^\infty r^2\exp(-2r)\,dr}$$

Use importance sampling with g(r) = exp(-αr) [ImportanceSampling.doc]

$$I = \frac{1}{\alpha}\int_0^1 \exp(\alpha r(t))\,r(t)\exp(-2r(t))\,dt$$