We wish to compute the wavefunction which minimizes the expectation value of the Hartree-Fock Hamiltonian:

$$\hat{H} = \sum_i -\frac{\hbar^2}{2m}\nabla^2_{\vec{x}_i} + \sum_{i<j} V(\vec{x}_i, \vec{x}_j) .$$

Elsewhere, we have computed that the expectation value of this Hamiltonian in the Slater determinant state is given by

$$\langle \hat{H} \rangle = \sum_i \int d^3x \, \nabla\phi_i^*(\vec{x}) \cdot \nabla\phi_i(\vec{x}) +$$

$$\frac{1}{2}\sum_{i,j} \int d^3x_1 d^3x_2 V(\vec{x}_1, \vec{x}_2)\Big(|\phi_i(\vec{x}_1)|^2 |\phi_j(\vec{x}_2)|^2 -$$

$$\phi_j^*(\vec{x}_1)\phi_i^*(\vec{x}_2)\phi_i(\vec{x}_1)\phi_j(\vec{x}_2)\Big).$$

We will now compute the functional derivative of this Hamiltonian with respect to the single particle wavefunctions. (In fact, we will differentiate with respect to the complex conjugate of the single-particle wavefunctions to get nicer equations.

First, we differentiate the kinetic term.

$$\frac{\delta\langle T\rangle}{\delta\phi_k^*(\vec{z})} = -\nabla\cdot\left(-\frac{\hbar^2}{2m}\nabla\phi_k(\vec{z})\right) = \boxed{\frac{\hbar^2}{2m}\nabla^2\phi_k(\vec{z})} .$$

Next, we differentiate the potential term. We shall first do this the long and tedious way, using the definition of the functional derivative. We will subsequently compute the result again using the known results of functional differentiation.

$$\frac{\delta\langle V\rangle}{\delta\phi_k^*(\vec{z})} = \lim_{\varepsilon\to 0}\frac{1}{\varepsilon}\left(\langle V\rangle[\phi_k^*+\varepsilon\delta] - \langle V\rangle[\phi_k^*]\right)$$

$$=\lim_{\varepsilon\to 0}\frac{1}{\varepsilon}\left\{\frac{1}{2}\int d^3x_1 d^3x_2 V(\vec{x}_1,\vec{x}_2)\sum_{i,j}\Big[(\phi_i^*(\vec{x}_1)+\varepsilon\delta_{ik}\delta(\vec{x}_1-\vec{z}))\right.$$

$$\cdot\left(\phi_j^*(\vec{x}_2)+\varepsilon\delta_{jk}\delta(\vec{x}_2-\vec{z})\right)\phi_i(\vec{x}_1)\phi_j(\vec{x}_2) -$$

$$\left(\left(\phi_j^*(\vec{x}_1)+\varepsilon\delta_{jk}\delta(\vec{x}_1-\vec{z})\right)\left(\phi_i^*(\vec{x}_2)+\varepsilon\delta_{ik}\delta(\vec{x}_2-\vec{z})\right)\phi_i(\vec{x}_1)\phi_j(\vec{x}_2)\right)$$

$$\left.-\left(\phi_i^*(\vec{x}_1)\phi_j^*(\vec{x}_2)\phi_i(\vec{x}_1)\phi_j(\vec{x}_2) - \phi_j^*(\vec{x}_1)\phi_i^*(\vec{x}_2)\phi_i(\vec{x}_1)\phi_i(\vec{x}_2)\right)\Big]\right\}$$

$$=\frac{1}{2}\int d^3x_1 d^3x_2 V(\vec{x}_1,\vec{x}_2)\sum_{i,j}\Big[\Big(\phi_i^*(\vec{x}_1)\delta_{jk}\delta(\vec{x}_2-\vec{z})+$$

$$\phi_j^*(\vec{x}_2)\delta_{ik}\delta(\vec{x}_1-\vec{z})\Big)\phi_i(\vec{x}_1)\phi_j(\vec{x}_2) -$$

$$\left(\phi_j^*(\vec{x}_1)\delta_{ik}\delta(\vec{x}_2-\vec{x})+\phi_i^*(\vec{x}_2)\delta_{jk}\delta(\vec{x}_1-\vec{z})\right)\phi_i(\vec{x}_1)\phi_j(\vec{x}_2)\Big]$$

$$=\frac{1}{2}\int d^3x_1 V(\vec{x}_1,\vec{z})\sum_i|\phi_i(\vec{x}_1)|^2\phi_k(\vec{z}) +$$

$$\frac{1}{2}\int d^3x_2 V(\vec{z},\vec{x}_2)\sum_j|\phi_j(\vec{x}_2)|^2\phi_k(\vec{z}) -$$

$$\frac{1}{2}\int d^3x_1\, V(\vec{x}_1,\vec{z})\sum_j \phi_j^*(\vec{x}_1)\phi_j(\vec{z})\phi_k(\vec{x}_1) -$$

$$\frac{1}{2}\int d^3x_2\, V(\vec{z},\vec{x}_2)\sum_i \phi_i^*(\vec{x}_2)\phi_i(\vec{z})\phi_k(\vec{x}_2) =$$

$$\boxed{\int d^3x_1\, \frac{1}{2}\left(V(\vec{x}_1,\vec{z})+V(\vec{z},\vec{x}_1)\right)\cdot \left[\sum_i |\phi_i(\vec{x}_1)|^2\phi_k(\vec{z}) - \phi_i^*(\vec{x}_1)\phi_i(\vec{z})\,\phi_k(\vec{x}_1)\right]}$$

We can also derive this result more directly using what we know of functional derivatives. In particular, functional derivatives obey the product rule:

$$\frac{\delta}{\delta f(z)}\int dx\,dy\, f(x)f(y)H(x,y) = \int dx\, f(x)\, \frac{\delta}{\delta f(z)}\int f(y)H(x,y)dy$$

$$+\int dy\, f(y)\,\frac{\delta}{\delta f(z)}\int f(x)\,H(x,y)\,dy\,.$$

Thus, it follows that

$$\frac{\delta\langle V\rangle}{\delta\phi_k^*(\vec{z})} = \frac{\delta}{\delta\phi_k^*(\vec{z})}\Big\{\frac{1}{2}\sum_{i,j}\int d^3x_1 d^3x_2 V(\vec{x}_1,\vec{x}_2)\left(|\phi_i(\vec{x}_1)|^2|\phi_j(\vec{x}_2)|^2 -\right.$$

$$\phi_j^*(\vec{x}_1)\phi_i^*(\vec{x}_2)\phi_i(\vec{x}_1)\phi_j(\vec{x}_2)\Big]\Big)\Big\} =$$

$$\frac{1}{2}\sum_j \int d^3x_2\, V(\vec{z},\vec{x}_2)|\phi_j(\vec{x}_2)|^2 \phi_k(\vec{z})$$

$$+\frac{1}{2}\sum_i \int d^3x_1\, V(\vec{x}_1,\vec{z})\,|\phi_i(\vec{x}_1)|^2 \phi_k(\vec{z})$$

$$-\frac{1}{2}\sum_i \int d^3x_2\, V(\vec{z},\vec{x}_2)\,\phi_i^*(\vec{x}_2)\phi_i(\vec{z})\phi_k(\vec{x}_2)$$

$$-\frac{1}{2}\sum_j \int d^3x_1\, V(\vec{x}_1,\vec{z})\,\phi_j^*(\vec{x}_1)\phi_j(\vec{z})\phi_k(\vec{x}_1) \quad =$$

$$\boxed{\int d^3x_1\, \frac{1}{2}\left(V(\vec{x}_1,\vec{z})+V(\vec{z},\vec{x}_1)\right) \cdot \left[\sum_i |\phi_i(\vec{x}_1)|^2 \phi_k(\vec{z}) - \phi_i^*(\vec{x}_1)\phi_i(\vec{z})\,\phi_k(\vec{x}_1)\right]}$$

So indeed, we get the same result in fewer steps, at the expense of more mental accounting!

In any case, we now combine these results and conclude that the single-particle wavefunction which makes the expectation value of the Hartree-Fock Hamiltonian stationary obeys

$$\frac{\hbar^2}{2m}\nabla^2\phi_k(\vec{z}) + \int d^3x_1 \; \frac{1}{2}\left(V(\vec{x}_1,\vec{z}) + V(\vec{z},\vec{x}_1)\right) \cdot$$

$$\left[\sum_i |\phi_i(\vec{x}_1)|^2 \phi_k(\vec{z}) - \phi_i^*(\vec{x}_1)\phi_i(\vec{z})\,\phi_k(\vec{x}_1)\right] = 0$$

$$\Longleftrightarrow$$

$$-\frac{\hbar^2}{2m}\nabla^2\phi_k(\vec{z}) = \int d^3x_1 \; \frac{1}{2}\left(V(\vec{x}_1,\vec{z}) + V(\vec{z},\vec{x}_1)\right) \cdot$$

$$\left[\sum_i |\phi_i(\vec{x}_1)|^2 \phi_k(\vec{z}) - \phi_i^*(\vec{x}_1)\phi_i(\vec{z})\,\phi_k(\vec{x}_1)\right]$$

And indeed, assuming the potential is symmetric, we have

$$\boxed{-\frac{\hbar^2}{2m}\nabla^2\phi_k(\vec{z}) = \int d^3x_1\, V(\vec{x}_1,\vec{z})\left[\sum_i |\phi_i(\vec{x}_1)|^2 \phi_k(\vec{z}) - \phi_i^*(\vec{x}_1)\phi_i(\vec{z})\,\phi_k(\vec{x}_1)\right]}$$