* Expansion on a harmonic osaillator basis *

Let's consider the HF equation:

$$-\frac{\hbar^2}{2m}\nabla^2\phi_k(\vec{r}) + U(r)\phi_k(\vec{r}) - \int d^3r_1\, W(\vec{r},\vec{r}_1)\,\phi_k(\vec{r}_1) = \varepsilon_k \phi_k(\vec{r}) \qquad 1)$$

Let $\varphi_k^\alpha(\vec{r})$ be the harmonic oscillator eigenfunctions

$$H^{HO}\varphi_k^\alpha = \left(-\frac{\hbar^2}{2m}\nabla^2 + \frac{1}{2}m\omega^2 r^2\right)\varphi_k^\alpha(\vec{r}) = \varepsilon^{HO}_{\alpha,k}\varphi_k^\alpha(\vec{r}) \qquad 2)$$

We consider $\phi_k(\vec{r}) = \sum_\alpha a_{\alpha,k}\,\varphi_k^\alpha(\vec{r}) \qquad 3)$

with $a_{\alpha,k}$ real coefficients. Obviously the orthonormalization of the ϕ_k implies $\sum_\alpha a_{\alpha,k}^2 = 1$

Subtracting the h.o. hamiltonian to 1):

$$U(r)\sum_\alpha a_{\alpha,k}\varphi_k^\alpha(\vec{r}) - \int d^3r_1\, W(\vec{r},\vec{r}_1)\sum_\alpha a_{\alpha,k}\varphi_k^\alpha(\vec{r}_1) - \frac{1}{2}m\omega^2r^2\sum_\alpha a_{\alpha,k}\varphi_k^\alpha(\vec{r})$$

$$= \left(\varepsilon_k - H^{HO}\right)\sum_\alpha a_{\alpha,k}\varphi_k^\alpha(\vec{r}) = \varepsilon_k\sum_\alpha a_{\alpha,k}\varphi_k^\alpha(\vec{r}) - \sum_\alpha \varepsilon^{HO}_{\alpha,k}\varphi_k^\alpha(\vec{r}) \qquad 5)$$

Multiplying by $\varphi_k^{*\beta}(\vec{r})$ and integrating on $\vec{r}$

$$\sum_\alpha a_{\alpha,k}\left\{\int d^3r\,\varphi_k^{*\beta}(\vec{r})\left[U(r) - \frac{1}{2}m\omega^2r^2\right]\varphi_k^\alpha(\vec{r}) - \int d^3r_1\, W(\vec{r},\vec{r}_1)\varphi_k^\alpha(\vec{r}_1) + \varepsilon^{HO}_{\alpha,k}\delta_{\alpha\beta}\right\}$$

$$= \varepsilon_k a_{\beta,k} \qquad 6)$$

This is a diagonalization problem.