Emin Haux Notes

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Important equations

$$E\left[f_n, \psi_n\right] = \sum_n f_n \left\langle \psi_n \left| -\frac{1}{2}\nabla^2 + V_{\text{ext}} \right| \psi_n \right\rangle + \frac{1}{2}\int \frac{\rho(\mathbf{r})\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}\,\mathrm{d}\mathbf{r}\,\mathrm{d}\mathbf{r}' + E_{\text{XC}}\left[\rho(\mathbf{r})\right] \tag{1}$$

$$F\left[f_n, \psi_n\right] = E\left[f_n, \psi_n\right] - T\,S\left[f_n\right] \tag{2}$$

$$S\left[f_n\right] = -k\sum_n f_n \ln f_n + (1-f_n)\ln\left(1-f_n\right) \tag{3}$$

$$L\left[f_n, \psi_n\right] = F\left[f_n, \psi_n\right] - \sum_{nn'} \lambda_{nn'}\left(\langle\psi_n|\psi_n\rangle - \delta_{nn'}\right) - \mu\left(\sum_n f_n - N\right) \tag{4}$$

Important equations

$$\frac{\partial L}{\partial \langle \psi_n |} = f_n H |\psi_n\rangle - \sum_{n'} \lambda_{nn'} |\psi_{n'}\rangle \tag{5}$$

$$\frac{\partial L}{\partial f_n} = \langle \psi_n \mid H \mid \psi_n \rangle - \epsilon_n \tag{6}$$

Modified Lagrangian

$$\tilde{L}\left[\eta_{mm'}, \psi_m\right] := L\left[\sum_m U_{mn}\left[\eta\right]\psi_m, f_n\left[\eta\right]\right] \tag{7}$$