

### About the local spin density functional

Since

$$T_s[n_\uparrow, n_\downarrow] = \sum_{a\sigma} \left\langle \phi_{a\sigma} \left| \frac{1}{2} \nabla^2 \right| \phi_{a\sigma} \right\rangle$$

we can see that

$$T_s[n_\uparrow, n_\downarrow] = T_s[n_\uparrow, 0] + T_s[0, n_\downarrow]$$

and, for a spin-unpolarized case,

$$T_s[n] = T_s\left[\frac{1}{2}n, 0\right] + T_s\left[0, \frac{1}{2}n\right] = 2T_s\left[0, \frac{1}{2}n\right].$$

Then,

$$T_s[n_\uparrow, n_\downarrow] = \frac{1}{2}T_s[2n_\uparrow] + \frac{1}{2}T_s[2n_\downarrow].$$

The non-interacting kinetic energy functional can be expressed through a single component functional.

For the Thomas Fermi model, we can expand the kinetic energy functional as

$$T[n] = T_0[n] + T_2[n] + T_4[n] + \dots$$

where

$$T_0[n] = \frac{3}{10} (3\pi^2)^{2/3} \int d\mathbf{r} n(\mathbf{r})^{5/3}$$

$$T_2[n] = \frac{1}{72} \int d\mathbf{r} \frac{|\nabla n(\mathbf{r})|^2}{n(\mathbf{r})}$$

$$T_4[n] = \frac{1}{540(3\pi^2)^{2/3}} \int d\mathbf{r} n(\mathbf{r})^{1/3} \left[ \left( \frac{\nabla^2 n(\mathbf{r})}{n(\mathbf{r})} \right)^2 - \frac{9}{8} \frac{\nabla^2 n(\mathbf{r})}{n(\mathbf{r})} \left| \frac{\nabla n(\mathbf{r})}{n(\mathbf{r})} \right|^2 + \frac{1}{3} \left| \frac{\nabla n(\mathbf{r})}{n(\mathbf{r})} \right|^4 \right].$$

This can be proved by following steps (sketch):

Within the Hartree-Fock, the one-body Green's function can be written as

$$G(\mathbf{r}, \mathbf{r}'; E) = \sum_i \phi_i(\mathbf{r}) \phi_i(\mathbf{r}') \exp[-i\epsilon_i E] = \sum_i \phi_i(\mathbf{r}) \phi_i(\mathbf{r}') \exp[-i\hat{H}E],$$

from which the density matrix is given by

$$n(\mathbf{r}, \mathbf{r}') = \int_{-\infty-i\eta}^{\infty-i\eta} \frac{dE}{2\pi i E} e^{i\mu E} G(\mathbf{r}, \mathbf{r}'; E).$$

One can show, without derivation here, that the Thomas Fermi Green's function is

$$G_{\text{TF}}(\mathbf{r}, \mathbf{r}'; E) = \left( \frac{1}{2\pi i E} \right)^{3/2} \exp \left[ \frac{i(\mathbf{r} - \mathbf{r}')^2}{2E} - iEV \left( \frac{\mathbf{r} + \mathbf{r}'}{2} \right) \right].$$

When retaining the mass and the Planck constant, it is

$$G_{\text{TF}}(r, r'; E) = \left( \frac{m}{2\pi i \hbar E} \right)^{3/2} \exp \left[ \frac{im(\mathbf{r} - \mathbf{r}')^2}{2\hbar E} - \frac{iE}{\hbar} V \left( \frac{\mathbf{r} + \mathbf{r}'}{2} \right) \right].$$

When expanding it with respect to  $\hbar$ , we obtain the kinetic energy functional as

$$t(\mathbf{r}) = \frac{\hbar^2}{10\pi^2 m} \left( \frac{2m}{\hbar^2} \right)^{\frac{5}{2}} (\mu - V(\mathbf{r}))^{\frac{5}{2}} \theta(\mu - V(\mathbf{r})) \left( 1 - \frac{5}{8} \frac{\hbar^2}{2m} \left\{ \frac{5}{3} \nabla^2 V(\mathbf{r}) (\mu - V(\mathbf{r}))^{-2} - \frac{3}{4} (\nabla V(\mathbf{r}))^2 (\mu - V(\mathbf{r}))^{-3} \right\} \right)$$

and the electron density as

$$n(\mathbf{r}) = \frac{1}{3\pi^2} \left( \frac{2m}{\hbar^2} \right)^{\frac{3}{2}} (\mu - V(\mathbf{r}))^{\frac{3}{2}} \theta(\mu - V(\mathbf{r})) \left( 1 - \frac{1}{8} \frac{\hbar^2}{2m} \left\{ \nabla^2 V(\mathbf{r}) (\mu - V(\mathbf{r}))^{-2} + \frac{1}{4} (\nabla V(\mathbf{r}))^2 (\mu - V(\mathbf{r}))^{-3} \right\} \right)$$

Then one can relate the kinetic energy with the electron density as

$$t_2(\mathbf{r}) = \frac{3}{10} \left( \frac{\hbar^2}{m} \right) (2\pi^2)^{2/3} c_k n(\mathbf{r})^{5/3} + \frac{11}{98} \left( \frac{\hbar^2}{m} \right) \frac{(\nabla n(\mathbf{r}))^2}{n(\mathbf{r})} + \frac{1}{6} \left( \frac{\hbar^2}{m} \right) \nabla^2 n(\mathbf{r})$$

Likewise, we can derive the form for  $t_4$  and relate it with the density.

The form for  $T[n]$  can be used derive the form for  $T[n_\uparrow, n_\downarrow]$ . When, for example, the relative spin-polarization is constant of space as

$$n_\uparrow(\mathbf{r}) = 1/2 (1 + x)n(\mathbf{r}) \text{ and } n_\downarrow(\mathbf{r}) = 1/2 (1 - x)n(\mathbf{r}).$$

and

we obtain

$$T_0[n_\uparrow, n_\downarrow] = 1/2 \left[ (1 + x)^{\frac{5}{3}} + (1 - x)^{\frac{5}{3}} \right] T_0[n]$$

$$T_2[n_\uparrow, n_\downarrow] = T_2[n]$$

$$T_4[n_\uparrow, n_\downarrow] = 1/2 \left[ (1 + x)^{\frac{1}{3}} + (1 - x)^{\frac{1}{3}} \right] T_4[n].$$

For the exchange, when describing the exchange energy  $E_x$  using the Kohn-Sham orbitals, not describing  $E_x$  of the Hartree-Fock,

$$E_x[n_\uparrow, n_\downarrow] = 1/2 E_x[2n_\uparrow] + 1/2 E_x[n_\downarrow]$$

and

$$E_x[n_\uparrow, n_\downarrow] = 1/2 \left[ (1 + x)^{\frac{4}{3}} + (1 - x)^{\frac{4}{3}} \right] E_x[n].$$