Extended Hubbard model:
Hamiltonian_extended_Hubbard_smod.F90

The Hamiltonian that we will consider here is given by:

$$\hat{H} = \sum_{b=\langle i,j\rangle} \sum_{\sigma=1}^{N} \left(\hat{c}^{\dagger}_{i,\sigma} T^{\sigma}_{i,j} \hat{c}^{\dagger}_{j,\sigma} + \text{H.c.} \right) + \sum_{b=\langle i,j\rangle} \frac{V_{i,j}}{2N} \left([n_i - N/2] + s_V [n_j - N/2] \right)^2 + \sum_i \frac{U_i}{N} \left(n_i - \frac{N}{2} \right)^2 \quad (1)$$

The implementation supports all standard ALF lattices and the hopping as well as the interaction V are restricted to nearest neighbors. The parameter file for this specific model reads:

```
&VAR_extended_Hubbard      !! Variables for the Extended Hubbard
ham_T      = 1.d0          ! Hopping parameter
Ham_chem   = 0.d0          ! Chemical potential
Ham_U      = 1.d0          ! Hubbard interaction
Ham_V1     = 0.d0          ! nearest neighbor interaction
ham_T2     = 1.d0          ! For bilayer systems
Ham_U2     = 0.d0          ! For bilayer systems
Ham_V2     = 0.d0          ! For bilayer systems
ham_Tperp  = 0.d0          ! For bilayer systems
Ham_Vperp  = 0.d0          ! For bilayer systems
Ham_SV     = 1.0           ! = +/- 1: Sign convention for interaction
/
```

In the above `Ham_T, Ham_V, Ham_U` are the nearest neighbor hopping, nearest neighbor interaction and Hubbard repulsion on the the first layer. `Ham_T2, Ham_V2, Ham_U2` are the corresponding quantities on the second layer. `Ham_Tperp, Ham_Vperp` define the inter-layer couplings. Finally *Ham_chem* is the chemical potential. To use this Hamiltonian you have to specify:

```
&VAR_ham_name
ham_name = "extended_Hubbard"
/
```

in the `parameters` file.

In this formulation, there is some *double counting* of the Hubbard term. In particular expanding the square V-term gives the Hamiltonian:

$$\hat{H} = \sum_{b=\langle i,j\rangle} \sum_{\sigma=1}^{N} \hat{c}^{\dagger}_{i,\sigma} T^{\sigma}_{i,j} \hat{c}^{\dagger}_{j,\sigma} + \sum_{b=\langle i,j\rangle} \frac{s_V V_{i,j}}{N} \left([n_i - N/2] \right) \left([n_j - N/2] \right) + \sum_i \frac{U_i^{eff}}{N} \left(n_i - \frac{N}{2} \right)^2 \quad (2)$$

In the above

$$U_i^{eff} = U_i + \frac{1}{2} \sum_{b=(n,m)} V_b \left(\delta_{i,m} + s_V^2 \delta_{i,n} \right). \quad (3)$$

For the single layer lattices with uniform U and V, and $s_V = 1$, $U^{eff} = U + ZV$ where $Z = 4$ ($Z = 3$) for the square (honeycomb) lattice.

Note that the potential and total energies are defined as in the Hamiltonian. That is the file `Ener_scalJ` corresponds to $\langle \hat{H} \rangle$.