

# Extended Hubbard model:

## Hamiltonian\_extended\_Hubbard\_smod.F90

The Hamiltonian that we will consider here is given by:

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

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:

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

In the above

$$U_i^{eff} = U_i + \sum_{b=(n,m)} V_b (\delta_{i,m} + \delta_{i,n}) \quad (3)$$

For the single layer lattices with uniform  $U$  and  $V$ ,  $U^{eff} = U + ZV$  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  $\langle \hat{H} \rangle$ .