Instructions on self consistency

January 11, 2024

In the following I am explaining how to do the DMFT self-consistency for heterostructures as the one illustrated in Fig. 1. Fig. 1 depicts a heterostructure in 2D with two semi-finite leads on the left and right and a slab in the middle with three layers. In general, the dimensionality of the system and the thickness of the slab material as well as the Coulomb interactions can vary. The number of slab-layers is indicated by the parameter l (in Fig. 1 we have $l = 3$) and the initial state has an antiferromagnetic order between vertical layers. A constant electric field with strength E is applied along the diagonal, which introduces a phase to the hopping v_0.

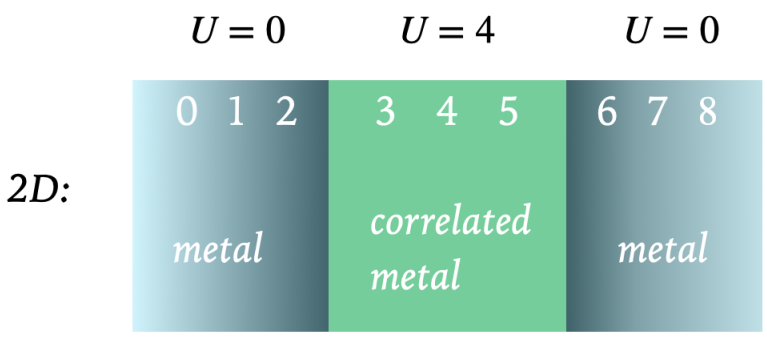

Figure 1: heterostructure model with $l = 3$.

We start by defining the hopping terms between different neighbors, which can be divided into three sorts: left and right hopping terms, which differ only by a minus sign in the exponent due to the direction of the electric field and the hopping term between sites of the same layer, which is a combination of an incoming and outgoing field. The number of nearest neighbors in the same layer grows as the spatial dimension of the material is increased. For a constant electric field with field strength E the hopping amplitudes are

$$v_{\text{left}}(t_1, t_2) = \frac{v(t_1)\overline{v}(t_2)}{\dim * 2}$$

and

$$v_{\text{right}}(t_1, t_2) = \frac{v(t_2)\overline{v}(t_1)}{\text{dim} * 2}$$

with $v(t) = v_0 * \exp(-iEt)$ and $\overline{v}(t) = v_0 * \exp(iEt)$. The coupling between sites of the same layer is

$$v_{\text{layer}} = (v + \bar{v}) * (1 - 1/\text{dim})$$

for one and two dimensions and

$$v_{\text{layer}} = (v + \bar{v}) * (1 - 2/\text{dim}) + v_0/\text{dim}$$

for three dimensions. The parameter *dim* is the spatial dimension of the system and $v_0 = 1$.

After computing the Green's functions for the impurity sites 1 to 8, we can update the hybridization functions for each site using the self-consistency:

$$\Delta^{\sigma}_{\text{site}} = v_{\text{left}} * \text{Green}^{\sigma}_{site-1} + v_{\text{layer}} * \text{Green}^{\sigma}_{\text{site}} + v_{\text{right}} * \text{Green}^{\sigma}_{\text{site}+1}.$$

for sites $1...N-1$. The hybridization function or the first and the last site are given by:

$$\Delta^{\sigma}_{0} = v_{\text{left}} * \text{Green}^{\bar{\sigma}}_{0} + v_{\text{layer}} * \text{Green}^{\sigma}_{0} + v_{\text{right}} * \text{Green}^{\sigma}_{1},$$

$$\Delta^{\sigma}_{\text{N}} = v_{\text{left}} * \text{Green}^{\sigma}_{\text{N}-1} + v_{\text{layer}} * \text{Green}^{\sigma}_{\text{N}} + v_{\text{right}} * \text{Green}^{\bar{\sigma}}_{\text{N}}.$$