We start with the block tri-diagonal Hamiltonian

$$H = \begin{pmatrix} H_s & T_s & & & & \\ T_s^\dagger & H & T & & & \\ & T^\dagger & \ddots & \ddots & & \\ & & \ddots & H & T & \\ & & & T^\dagger & \ddots & \ddots \\ & & & & \ddots & \end{pmatrix} \tag{1}$$

where, H is the Hamiltonian for a principal layer, T is the inter-layer interaction, and the subscript s denotes surface layer. The Green's function matrix is defined by $G = (z - H)^{-1}$, where z can be $i\omega_n$, $\omega + i\delta$, or $\omega - i\delta$ for Matsubara, retarded, or advanced Green's functions, respectively.

$$\begin{pmatrix} z-H_s & -T_s & & \\ -T_s^\dagger & z-H & -T & \\ & -T^\dagger & z-H & \ddots \\ & & \ddots & \ddots \end{pmatrix} \begin{pmatrix} G_{00} & G_{01} & G_{02} & \\ G_{10} & G_{11} & G_{12} & \cdots \\ G_{20} & G_{21} & G_{22} & \\ & \vdots & & \ddots \end{pmatrix} = \begin{pmatrix} I & & & \\ & I & & \\ & & I & \\ & & & \ddots \end{pmatrix} \tag{2}$$

Block multiplying out, we get the relations

$$(z - H_s)G_{0,j} = \delta_{0,j} + T_s G_{1,j} \tag{3}$$

$$(z - H)G_{1,j} = \delta_{1,j} + T_s^\dagger G_{0,j} + T G_{2,j} \tag{4}$$

$$(z - H)G_{i,j} = \delta_{i,j} + T^\dagger G_{i-1,j} + T G_{i+1,j} \qquad i > 1 \tag{5}$$

We define

$$\varepsilon_s^{(n+1)} = \varepsilon_s^{(n)} + \alpha_s^{(n)} \left(z - \varepsilon^{(n)}\right)^{-1} \beta_s^{(n)} \qquad \varepsilon^{(n+1)} = \varepsilon^{(n)} + \alpha^{(n)} \left(z - \varepsilon^{(n)}\right)^{-1} \beta^{(n)} + \beta^{(n)} \left(z - \varepsilon^{(n)}\right)^{-1} \alpha^{(n)} \tag{6}$$

$$\alpha_s^{(n+1)} = \alpha_s^{(n)} \left(z - \varepsilon^{(n)}\right)^{-1} \alpha^{(n)} \qquad \alpha^{(n+1)} = \alpha^{(n)} \left(z - \varepsilon^{(n)}\right)^{-1} \alpha^{(n)} \tag{7}$$

$$\beta_s^{(n+1)} = \beta^{(n)} \left(z - \varepsilon^{(n)}\right)^{-1} \beta_s^{(n)} \qquad \beta^{(n+1)} = \beta^{(n)} \left(z - \varepsilon^{(n)}\right)^{-1} \beta^{(n)} \tag{8}$$

with the initial conditions

$$\varepsilon_s^{(0)} = H_s \qquad \alpha_s^{(0)} = T_s \qquad \beta_s^{(0)} = T_s^\dagger \tag{9}$$

$$\varepsilon^{(0)} = H \qquad \alpha^{(0)} = T \qquad \beta^{(0)} = T^\dagger \tag{10}$$

Eqs. (3-5) become

$$\left(z - \varepsilon_s^{(0)}\right) G_{0,j} = \delta_{0,j} + \alpha_s^{(0)} G_{1,j} \tag{11}$$

$$\left(z - \varepsilon^{(0)}\right) G_{1,j} = \delta_{1,j} + \beta_s^{(0)} G_{0,j} + \alpha^{(0)} G_{2,j} \tag{12}$$

$$\left(z - \varepsilon^{(0)}\right) G_{i,j} = \delta_{i,j} + \beta^{(0)} G_{i-1,j} + \alpha^{(0)} G_{i+1,j} \qquad i > 1 \tag{13}$$

Consider the subset of even indices. Plugging in eq. (12) into eq. (11), we get

$$\left(z - \varepsilon_s^{(0)}\right) G_{0,2j} = \delta_{0,j} + \alpha_s^{(0)} G_{1,2j} \tag{14}$$

$$\left(z - \varepsilon_s^{(0)}\right) G_{0,2j} = \delta_{0,j} + \alpha_s^{(0)} (z - \varepsilon^{(0)})^{-1} \left(\beta_s^{(0)} G_{0,2j} + \alpha^{(0)} G_{2,2j}\right) \tag{15}$$

$$\left(z - \varepsilon_s^{(0)} - \alpha_s^{(0)} (z - \varepsilon^{(0)})^{-1} \beta_s^{(0)}\right) G_{0,2j} = \delta_{0,j} + \alpha_s^{(0)} (z - \varepsilon^{(0)})^{-1} \alpha^{(0)} G_{2,2j} \tag{16}$$

Using eq. (6), we get

$$\left(z - \varepsilon_s^{(1)}\right) G_{0,2j} = \delta_{0,j} + \alpha_s^{(1)} G_{2,2j} \tag{17}$$

Next, consider $G_{2,2j}$.

$$\left(z - \varepsilon^{(0)}\right) G_{2,2j} = \delta_{2,2j} + \beta^{(0)} G_{1,2j} + \alpha^{(0)} G_{3,2j} \tag{18}$$

$$\left(z - \varepsilon^{(0)}\right) G_{2,2j} = \delta_{2,2j} + \beta^{(0)} \left(z - \varepsilon^{(0)}\right)^{-1} \left(\beta_s^{(0)} G_{0,2j} + \alpha^{(0)} G_{2,2j}\right) + \alpha^{(0)} \left(z - \varepsilon^{(0)}\right)^{-1} \left(\beta^{(0)} G_{2,2j} + \alpha^{(0)} G_{4,2j}\right) \tag{19}$$

$$\left(z - \varepsilon^{(1)}\right) G_{2,2j} = \delta_{1,j} + \beta_s^{(1)} G_{0,2j} + \alpha^{(1)} G_{4,2j} \tag{20}$$

Next, consider even indices with $i > 1$.

$$\left(z - \varepsilon^{(0)}\right) G_{2i,2j} = \delta_{2i,2j} + \beta^{(0)} G_{2i-1,2j} + \alpha^{(0)} G_{2i+1,2j} \tag{21}$$

$$\left(z - \varepsilon^{(0)}\right) G_{2i,2j} = \delta_{2i,2j} + \beta^{(0)} \left(z - \varepsilon^{(0)}\right)^{-1} \left(\beta^{(0)} G_{2i-2,2j} + \alpha^{(0)} G_{2i,2j}\right) + \alpha^{(0)} \left(z - \varepsilon^{(0)}\right)^{-1} \left(\beta^{(0)} G_{2i,2j} + \alpha^{(0)} G_{2i+2,2j}\right) \tag{22}$$

$$\left(z - \varepsilon^{(1)}\right) G_{2i,2j} = \delta_{i,j} + \beta^{(1)} G_{2(i-1),2j} + \alpha^{(1)} G_{2(i+1),2j} \tag{23}$$

The relations for even indices are

$$\left(z - \varepsilon_s^{(1)}\right) G_{0,2j} = \delta_{0,j} + \alpha_s^{(1)} G_{2,2j} \tag{24}$$

$$\left(z - \varepsilon^{(1)}\right) G_{2,2j} = \delta_{1,j} + \beta_s^{(1)} G_{0,2j} + \alpha^{(1)} G_{4,2j} \tag{25}$$

$$\left(z - \varepsilon^{(1)}\right) G_{2i,2j} = \delta_{i,j} + \beta^{(1)} G_{2(i-1),2j} + \alpha^{(1)} G_{2(i+1),2j} \qquad i > 1 \tag{26}$$

which is isomorphic to eqs. (11-13). I.e., if we consider indices in multiples of 4, we get

$$\left(z - \varepsilon_s^{(2)}\right) G_{0,4j} = \delta_{0,j} + \alpha_s^{(2)} G_{4,4j} \tag{27}$$

$$\left(z - \varepsilon^{(2)}\right) G_{4,4j} = \delta_{1,j} + \beta_s^{(2)} G_{0,4j} + \alpha^{(2)} G_{8,4j} \tag{28}$$

$$\left(z - \varepsilon^{(2)}\right) G_{4i,4j} = \delta_{i,j} + \beta^{(2)} G_{4(i-1),4j} + \alpha^{(2)} G_{4(i+1),4j} \qquad i > 1 \tag{29}$$

After n iterations, we get

$$\left(z - \varepsilon_s^{(n)}\right) G_{0,2^n j} = \delta_{0,j} + \alpha_s^{(n)} G_{2^n,2^n j} \tag{30}$$

$$\left(z - \varepsilon^{(n)}\right) G_{2^n,2^n j} = \delta_{1,j} + \beta_s^{(n)} G_{0,2^n j} + \alpha^{(n)} G_{2^{n+1},2^n j} \tag{31}$$

$$\left(z - \varepsilon^{(n)}\right) G_{2^n i,2^n j} = \delta_{i,j} + \beta^{(n)} G_{2^n(i-1),2^n j} + \alpha^{(n)} G_{2^n(i+1),2^n j} \qquad i > 1 \tag{32}$$

The $\varepsilon^{(n)}$ describe an effective layer that contains the interactions of $2^n - 1$ layers. The $\alpha^{(n)}$ and $\beta^{(n)}$ are effective hoppings between effective layers with lattice constant $2^n a$. After many iterations, the interactions between effective layers become weak compared to the interactions within the effective layer. Therefore,

$$\left(z - \varepsilon_s^{(n)}\right) G_{0,2^n j} \approx \delta_{0,j} \qquad \left(z - \varepsilon^{(n)}\right) G_{2^n,2^n j} \approx \delta_{1,j} \tag{33}$$

or

$$\left(z - \varepsilon_s^{(n)}\right)^{-1} \xrightarrow{n\to\infty} G_{00} \qquad \left(z - \varepsilon^{(n)}\right)^{-1} \xrightarrow{n\to\infty} G_{2^n,2^n} \tag{34}$$