Appendix J

Anderson impurity model: chain representation

This appendix explains the mapping of the Anderson impurity model (8.8)–(8.11) onto a semi-infinite chain. For simplicity, we may assume that the hybridization parameters V_p are real. The goal is to transform the impurity and bath annihilation operators $\{d, c_{p_1}, c_{p_2}, \ldots\}$ to new operators $\{d, c_1, c_2, \ldots\}$ such that $H_0 + H_{\rm bath} + H_{\rm mix}$ becomes tridiagonal:

$$\begin{pmatrix} d^\dagger & c_{p_1}^\dagger & c_{p_2}^\dagger & c_{p_3}^\dagger & \ldots \end{pmatrix} UU^T \begin{pmatrix} -\mu & V_{p_1} & V_{p_2} & V_{p_3} & \ldots \\ V_{p_1} & \varepsilon_{p_1} & & & \\ V_{p_2} & & \varepsilon_{p_2} & & \\ V_{p_3} & & & \varepsilon_{p_3} & \\ \vdots & & & & \ddots \end{pmatrix} UU^T \begin{pmatrix} d \\ c_{p_1} \\ c_{p_2} \\ c_{p_3} \\ \vdots \end{pmatrix}$$

$$= \begin{pmatrix} d^\dagger & c_1^\dagger & c_2^\dagger & c_3^\dagger & \ldots \end{pmatrix} \begin{pmatrix} -\mu & -V & & & \\ -V & \tilde{\varepsilon}_1 & -t_1 & & \\ & -t_1 & \tilde{\varepsilon}_2 & -t_2 & \\ & & -t_2 & \tilde{\varepsilon}_3 & \ddots \\ & & & \ddots & \ddots \end{pmatrix} \begin{pmatrix} d \\ c_1 \\ c_2 \\ c_3 \\ \vdots \end{pmatrix}.$$

The symmetric and orthogonal matrix U associated with this tranformation can be constructed as a product of *Householder transformations*

$$h_v = 1 - \frac{2\vec{v}\vec{v}^T}{|\vec{v}|^2}, \tag{J.1}$$

which describe mirror operations. Let us assume that the bath has N sites. In the first step, we choose v such that the vector $\vec{V} = (V_{p_1}\ V_{p_2}\ V_{p_3}\ \cdots V_{p_N})^T$ is mapped onto the first element $\vec{e}_1$: $\vec{v}_1 = \vec{V} \mp |V|\vec{e}_1 \Rightarrow h_{v_1}\vec{V} = \pm|V|\vec{e}_1$, with $|V|^2 = \sum_{p=1}^N |V_p|^2$. Defining the block matrix

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$$U_1 = \left(\begin{array}{c|c} 1 & \\ \hline & h_{v_1} \end{array}\right) \tag{J.2}$$

with diagonal blocks of dimension 1 and N, respectively, we obtain the transformed Hamiltonian

$$U_1 \left(\begin{array}{c|ccc} -\mu & V_{p_1} & V_{p_2} & \cdots \\ \hline V_{p_1} & \varepsilon_{p_1} & & \\ V_{p_2} & & \ddots & \\ \vdots & & & \end{array}\right) U_1 = \left(\begin{array}{c|ccc} -\mu & \pm|V| & 0 & \cdots \\ \hline \pm|V| & & & \\ 0 & & A_2 & \\ \vdots & & & \end{array}\right). \tag{J.3}$$

We can now repeat the procedure, and define a transformation h_{v_2} that maps the vector defined by the off-diagonal elements in the first column of the $N \times N$ matrix A_2 onto $\vec{e}_2$. The Householder matrix

$$U_2 = \left(\begin{array}{cc|c} 1 & 0 & \\ 0 & 1 & \\ \hline & & h_{v_2} \end{array}\right) \tag{J.4}$$

with diagonal blocks of dimension 2 and $N-1$ may then be used to bring the Hamiltonian into tridiagonal form up to the second row and column. The transformation U for an impurity model with N bath sites eventually becomes

$$U = U_1 U_2 \cdots U_{N-1}. \tag{J.5}$$

In the case of multi-orbital systems with diagonal baths, similar transformations map the system onto a star-shaped geometry, with the impurity site at the center.

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