6.4 Comparison of Schrieffer-Wolff transformation and URG

The Schrieffer-Wolff transformation The general method of Schrieffer-Wolff transformation involves defining a unitarily transformed Hamiltonian

$$\mathcal{H}_{eff} = e^{-\lambda\hat{S}}\mathcal{H}e^{\lambda\hat{S}} \tag{269}$$

where $\mathcal{H} = H_0 + V$, $H_0 = \epsilon_s n_2 + \epsilon_d n_1 + U n_{1\uparrow}n_{1\downarrow}$ and $V = -t\sum_\sigma \left(c^\dagger_{1\sigma}c_{2\sigma} + c^\dagger_{2\sigma}c_{1\sigma}\right)$. Unitarity of the transformation requires $\hat{S}^\dagger = -S$. Expanding $\mathcal{H}_{eff}$ upto second order in λ gives

$$\mathcal{H}_{eff} \simeq H_0 + \lambda\left(V + \left[H_0, \hat{S}\right]\right) + \frac{\lambda^2}{2}\left(\left[V, \hat{S}\right] + \left[\left[H_0, \hat{S}\right], \hat{S}\right]\right) \tag{270}$$

To extract the low energy physics, we set the first order term to zero, giving us the condition $\left[\hat{S}, H_0\right] = V$. The effective Hamiltonian then simplifies to

$$\mathcal{H}_{eff} \simeq H_0 + \frac{1}{2}\left[V, \hat{S}\right] \tag{271}$$

To find $\hat{S}$, we take the ansatz[1]

$$\hat{S} = \sum_\sigma (A + Bn_{1\overline{\sigma}})(c^\dagger_{1\sigma}c_{2\sigma} - c^\dagger_{2\sigma}c_{1\sigma}) \tag{272}$$

Using this ansatz, we get

$$= \sum_\sigma (A + Bn_{1\overline{\sigma}})(\epsilon_s - \epsilon_d - Un_{1\overline{\sigma}})(c^\dagger_{1\sigma}c_{2\sigma} - c^\dagger_{2\sigma}c_{1\sigma}) \tag{273}$$

Comparing with V, we get the following expressions for the coefficients A and B:

$$A = \frac{t}{\epsilon_d - \epsilon_s} \quad B = \frac{Ut}{(\epsilon_d - \epsilon_s)(\epsilon_s - \epsilon_d - U)} \tag{274}$$

The effective Hamiltonian becomes

$$\mathcal{H}_{eff} = \epsilon_d n_1 + \epsilon_s n_2 + Un_{1\uparrow}n_{1\downarrow} + \frac{2t^2(n_2 - n_1)}{\epsilon_s - \epsilon_d} + \frac{2t^2U}{(\epsilon_s - \epsilon_d)(\epsilon_s - \epsilon_d - U)}\sum_\sigma n_{1\overline{\sigma}}\left(n_{2\sigma} - n_{1\sigma}\right) \tag{275}$$

[1]motivated by Advanced Solid State Physics, Philiip Philips

Finally, I set $\epsilon_s = \epsilon_d + \frac{U}{2}$. The journey via SWT is shown:

$$\mathcal{H}(\text{exact}) = \begin{array}{c} \begin{matrix} |\uparrow,\uparrow\rangle & |\downarrow,\downarrow\rangle & |\uparrow,\downarrow\rangle & |\downarrow,\uparrow\rangle & |\uparrow\downarrow,0\rangle & |0,\uparrow\downarrow\rangle \end{matrix} \\ \begin{pmatrix} 2\epsilon_d + \frac{U}{2} & & & & & \\ & 2\epsilon_d + \frac{U}{2} & & & & \\ & & 2\epsilon_d + \frac{U}{2} & & t & -t \\ & & & 2\epsilon_d + \frac{U}{2} & -t & t \\ & & t & -t & 2\epsilon_d + U & \\ & & -t & t & & 2\epsilon_d + U \end{pmatrix} \end{array} \tag{276}$$

$$\Bigg\downarrow \text{SWT} \tag{277}$$

$$\mathcal{H}_{eff} = \begin{pmatrix} 2\epsilon_d + \frac{U}{2} & & & & & \\ & 2\epsilon_d + \frac{U}{2} & & & & \\ & & 2\epsilon_d + \frac{U}{2} - \frac{8t^2}{U} & & & \\ & & & 2\epsilon_d + \frac{U}{2} - \frac{8t^2}{U} & & \\ & & & & 2\epsilon_d + U + \frac{8t^2}{U} & \\ & & & & & 2\epsilon_d + U + \frac{8t^2}{U} \end{pmatrix} \tag{278}$$

$$\Bigg\downarrow \epsilon_d = -\frac{U}{2} \text{ (particle-hole symmetry)} \tag{279}$$

$$= \begin{pmatrix} -\frac{U}{2} & & & & & \\ & -\frac{U}{2} & & & & \\ & & -\frac{U}{2} - \frac{8t^2}{U} & & & \\ & & & -\frac{U}{2} - \frac{8t^2}{U} & & \\ & & & & \frac{U}{2} + \frac{8t^2}{U} & \\ & & & & & \frac{U}{2} + \frac{8t^2}{U} \end{pmatrix} \tag{280}$$

In the final matrix, the first four states form the lower band, with energies around $-\frac{U}{2}$, and the last two form the upper band, with energies around $\frac{U}{2}$. They are separated by a gap of U. The appearance of $\frac{t^2}{U}$ means that this is equivalent to performing a second-order perturbation-theoretic calculation in the parameter $\frac{t}{U}$.

The Unitary RG On the other hand, the path via the URG goes as

$$\mathcal{H}(\text{exact}) = \begin{array}{c} \begin{matrix} |\uparrow,\uparrow\rangle & |\downarrow,\downarrow\rangle & |\uparrow,\downarrow\rangle & |\downarrow,\uparrow\rangle & |\uparrow\downarrow,0\rangle & |0,\uparrow\downarrow\rangle \end{matrix} \\ \begin{pmatrix} 2\epsilon_d + \frac{U}{2} & & & & & \\ & 2\epsilon_d + \frac{U}{2} & & & & \\ & & 2\epsilon_d + \frac{U}{2} & & t & -t \\ & & & 2\epsilon_d + \frac{U}{2} & -t & t \\ & & t & -t & 2\epsilon_d + U & \\ & & -t & t & & 2\epsilon_d + U \end{pmatrix} \end{array}$$

$$\Big\downarrow \text{URG}$$

$$\begin{pmatrix} 2\epsilon_d + \frac{U}{2} & & & & & \\ & 2\epsilon_d + \frac{U}{2} & & & & \\ & & 2\epsilon_d + \frac{U}{2} & 2t & & \\ & & 2t & 2\epsilon_d + U & & \\ & & & & 2\epsilon_d + \frac{U}{2} & \\ & & & & & 2\epsilon_d + U \end{pmatrix}$$

$$\Big\downarrow \epsilon_d = -\frac{U}{2} \text{ (particle-hole symmetry)}$$

$$
= \begin{pmatrix} -\frac{U}{2} & & & & & \\ & -\frac{U}{2} & & & & \\ & & -\frac{U}{2} & 2t & & \\ & & 2t & 0 & & \\ & & & & -\frac{U}{2} & \\ & & & & & \frac{U}{2} \end{pmatrix}
$$

- First thing to note is that the eigenvalues and vectors are preserved in this process, because the transformations are unitary (instead of perturbative).

- Another thing to note is that under the action of the RG, the matrix has become block-diagonalized; there are three 2×2 disconnected blocks; the top and bottom blocks are diagonal, the middle one is not.

- Thirdly, since the process is non-perturbative, the upper and lower bands are not yet completely manifest; they appear only in the limit of large U. Most of the states are already present though, as seen in the already-diagonal blocks. Applying that limit on the exact eigenstates obtained from the middle block do indeed give the remaining states of the lower and upper bands, that is, $-\frac{U}{2} - \frac{8t^2}{U}, \frac{U}{2} + \frac{8t^2}{U}$.