7.8 APPENDIX: THE SCHRIEFFER-WOLFF TRANSFORMATION

In this Appendix, we present the complete derivation of the exchange interaction in the Kondo Hamiltonian from the Anderson Hamiltonian. Because the Anderson Hamiltonian contains empty as well as doubly occupied impurity states, a transformation that generates the Kondo Hamiltonian is equivalent to a diagonalization of the Anderson Hamiltonian in the subspace of the singly occupied impurity states. This diagonalization is carried out by the Schrieffer-Wolff transformation [SW1966].

We first separate the Anderson Hamiltonian into a *zero*th-order part,

$$H_0 = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} n_{\mathbf{k}\sigma} + \epsilon_d \sum_{\sigma} n_{d\sigma} + U n_{d\uparrow} n_{d\downarrow}, \tag{7.108}$$

and a perturbed part,

$$H_1 = \sum_{\mathbf{k}} V_{\mathbf{k}d} \left(a^\dagger_{\mathbf{k}\sigma} a_{d\sigma} + a^\dagger_{d\sigma} a_{\mathbf{k}\sigma}\right). \tag{7.109}$$

To proceed, we perform a canonical or similarity transformation, S, on the original Hamiltonian:

$$\begin{aligned}\tilde{H} &= e^S H e^{-S} \\ &= H + [S, H] + \frac{1}{2}[S, [S, H]] + \cdots.\end{aligned}$$

Note that since e^S is unitary, S must be antihermitian. If we choose S so as to cancel the linear dependence

$$H_1 + [S, H_0] = 0 \tag{7.110}$$

on the perturbation H_1, the new Hamiltonian to lowest order becomes

$$\tilde{H} = H_0 + \frac{1}{2}[S, H_1], \tag{7.111}$$

and, hence, incorporates charge fluctuations to second order in $V_{\mathbf{k}d}$. The similarity transformation method is a general way of performing perturbative analyses, once a small quantity has been identified.

The explicit form of S can be constructed by noting that because $[S, H_0] = -H_1$, the operator S must contain terms $\propto a^\dagger_{\mathbf{k}\sigma} a_{d\sigma}$; furthermore, its commutator with $U n_{d\uparrow} n_{d\downarrow}$ yields $\propto n_{d-\sigma} a^\dagger_{\mathbf{k}\sigma} a_{d\sigma}$. This suggests that we try a transformation of the form

$$S = \sum_{\mathbf{k},\sigma} \left(A_{\mathbf{k}} + B_{\mathbf{k}} n_{d-\sigma}\right) a^\dagger_{\mathbf{k}\sigma} a_{d\sigma} - h.c., \tag{7.112}$$

where $A_{\mathbf{k}}$ and $B_{\mathbf{k}}$ are c-numbers to be determined by Eq. (7.110).

Using the commutators

$$\begin{aligned}\left[n_{d\sigma}, a_{d\sigma'}\right] &= -\delta_{\sigma\sigma'} a_{d\sigma}, \\ \left[n_{d\sigma}, n_{d\sigma'}\right] &= 0 \\ \left[n_{d\sigma} n_{d-\sigma}, a_{d\sigma'}\right] &= -\delta_{\sigma\sigma'} n_{d-\sigma} a_{d\sigma} - \delta_{-\sigma\sigma'} n_{d\sigma} a_{d\sigma'},\end{aligned} \tag{7.113}$$

together with the relation $[A, B^{\dagger}] = -[A, B]^{\dagger}$ provided $A = A^{\dagger}$, we straightforwardly evaluate the commutator of H_0 with S and find

$$
\begin{aligned}
[H_0, S] &= \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} \left(A_{\mathbf{k}} + B_{\mathbf{k}} n_{d-\sigma}\right) a^{\dagger}_{\mathbf{k}\sigma} a_{d\sigma} + h.c. \\
&\quad + \sum_{\mathbf{k},\sigma} \epsilon_d \left(-A_{\mathbf{k}} - B_{\mathbf{k}} n_{d-\sigma}\right) a^{\dagger}_{\mathbf{k}\sigma} a_{d\sigma} + h.c. \\
&\quad + U \sum_{\mathbf{k},\sigma} \left(-A_{\mathbf{k}} n_{d-\sigma} - B_{\mathbf{k}} n_{d-\sigma}\right) a^{\dagger}_{\mathbf{k}\sigma} a_{d\sigma} + h.c. \\
&= \sum_{\mathbf{k},\sigma} [(\epsilon_{\mathbf{k}} - \epsilon_d) A_{\mathbf{k}} \\
&\quad + (\epsilon_{\mathbf{k}} - \epsilon_d - U) n_{d-\sigma} B_{\mathbf{k}} - A_{\mathbf{k}} U n_{d-\sigma}] a^{\dagger}_{\mathbf{k}\sigma} a_{d\sigma} + h.c., \qquad (7.114)
\end{aligned}
$$

where $h.c.$ denotes the hermitian conjugate. In order to satisfy Eq. (7.110), we require that $(\epsilon_{\mathbf{k}} - \epsilon_d) A_{\mathbf{k}} = V_{\mathbf{k}d}$ and $(\epsilon_{\mathbf{k}} - \epsilon_d - U) B_{\mathbf{k}} - A_{\mathbf{k}} U = 0$, so that

$$A_{\mathbf{k}} = \frac{V_{\mathbf{k}d}}{\epsilon_{\mathbf{k}} - \epsilon_d}$$

and

$$B_{\mathbf{k}} = V_{\mathbf{k}d} \left[\frac{1}{\epsilon_{\mathbf{k}} - (\epsilon_d + U)} - \frac{1}{\epsilon_{\mathbf{k}} - \epsilon_d} \right].$$

Equation (7.112), coupled with the definitions of the constants $A_{\mathbf{k}}$ and $B_{\mathbf{k}}$, specifies the Schrieffer-Wolff transformation.

To find the new Hamiltonian, we need to evaluate the commutator $[S, H_1]$:

$$
\begin{aligned}
[S, H_1] = \sum_{\mathbf{k},\sigma,\mathbf{k}',\sigma'} \{ & A_{\mathbf{k}} V_{\mathbf{k}'d} [\rho_{\mathbf{k}d\sigma}, (\rho_{\mathbf{k}'d\sigma'} + \rho^{\dagger}_{\mathbf{k}'d\sigma'})] \\
& - B^{*}_{\mathbf{k}} V_{\mathbf{k}'d} [n_{d-\sigma} \rho^{\dagger}_{\mathbf{k}d\sigma}, (\rho_{\mathbf{k}'d\sigma'} + \rho^{\dagger}_{\mathbf{k}'d\sigma'})] \\
& + B_{\mathbf{k}} V_{\mathbf{k}'d} [n_{d-\sigma} \rho_{\mathbf{k}d\sigma}, (\rho_{\mathbf{k}'d\sigma'} + \rho^{\dagger}_{\mathbf{k}'d\sigma'})] \\
& - A^{*}_{\mathbf{k}} V_{\mathbf{k}'d} [\rho^{\dagger}_{\mathbf{k}d\sigma}, (\rho_{\mathbf{k}'d\sigma'} + \rho^{\dagger}_{\mathbf{k}'\sigma'})] \}, \qquad (7.115)
\end{aligned}
$$

where we have simplified the notation by defining $\rho_{\mathbf{k}d\sigma} = a^{\dagger}_{\mathbf{k}\sigma} a_{d\sigma}$. At this stage, these commutators are useful:

$$[\rho_{\mathbf{k}d\sigma}, \rho_{\mathbf{k}'d\sigma'}] = 0$$

$$[\rho_{\mathbf{k}d\sigma}, \rho^{\dagger}_{\mathbf{k}'d\sigma'}] = \delta_{\sigma\sigma'}[-\delta_{\mathbf{k}\mathbf{k}'}n_{d\sigma} + a^{\dagger}_{\mathbf{k}\sigma}a_{\mathbf{k}'\sigma}]$$

$$[n_{d-\sigma}\rho_{\mathbf{k}d\sigma}, \rho_{\mathbf{k}'d\sigma'}] = -\delta_{\sigma'-\sigma}\rho_{\mathbf{k}d\sigma}\rho_{\mathbf{k}'d-\sigma}$$

$$[n_{d-\sigma}\rho_{\mathbf{k}d\sigma}, \rho^{\dagger}_{\mathbf{k}'d\sigma'}] = \delta_{-\sigma\sigma'}\rho_{\mathbf{k}d\sigma}\rho^{\dagger}_{\mathbf{k}'d-\sigma} + \delta_{\sigma\sigma'}(a^{\dagger}_{\mathbf{k}\sigma}a_{\mathbf{k}'\sigma}n_{d-\sigma} - \delta_{\mathbf{k}\mathbf{k}'}n_{d-\sigma}n_{d\sigma}).$$

Substituting these relationships into Eq. (7.115), we find

$$\begin{aligned}[S, H_1] = &- \sum_{\mathbf{k},\sigma}(A_{\mathbf{k}}V_{\mathbf{k}d} + B_k V_{\mathbf{k}d}n_{d-\sigma})n_{d\sigma} + h.c.\\ &+ \sum_{\mathbf{k},\mathbf{k}',\sigma} A_{\mathbf{k}}V_{\mathbf{k}'d}a^{\dagger}_{\mathbf{k}\sigma}a_{\mathbf{k}'\sigma} + h.c.\\ &- \sum_{\mathbf{k},\mathbf{k}',\sigma} B_{\mathbf{k}}V_{\mathbf{k}'d}\rho_{\mathbf{k}\sigma}\rho_{\mathbf{k}'-\sigma} + h.c.\\ &+ \sum_{\mathbf{k},\mathbf{k}',\sigma} B_{\mathbf{k}}V_{\mathbf{k}'d}[a^{\dagger}_{\mathbf{k}\sigma}a_{\mathbf{k}'\sigma}n_{d-\sigma} + \rho_{\mathbf{k}\sigma}\rho^{\dagger}_{\mathbf{k}'-\sigma}] + h.c.. \end{aligned} \quad (7.116)$$

Let us write the operators in the last term as

$$\begin{aligned}[a^{\dagger}_{\mathbf{k}\sigma}a_{\mathbf{k}'\sigma}n_{d-\sigma} + \rho_{\mathbf{k}d\sigma}\rho^{\dagger}_{\mathbf{k}'d-\sigma}] = &\frac{1}{2}(n_{d\sigma} + n_{d-\sigma})a^{\dagger}_{\mathbf{k}\sigma}a_{\mathbf{k}'\sigma}\\ &- \frac{1}{2}[(n_{d\sigma} - n_{d-\sigma})a^{\dagger}_{\mathbf{k}\sigma}a_{\mathbf{k}'\sigma} - 2\rho_{\mathbf{k}d\sigma}\rho^{\dagger}_{\mathbf{k}'d-\sigma}]. \end{aligned} \quad (7.117)$$

The second part of this term gives rise to the Kondo exchange interaction. To see how, we note that the product

$$\begin{aligned}\frac{4}{\hbar^2}(\Psi^{\dagger}_{\mathbf{k}'}\mathbf{S}\Psi_{\mathbf{k}})\cdot(\Psi^{\dagger}_{d}\mathbf{S}\Psi_{d}) = &(\Psi^{\dagger}_{\mathbf{k}'}\sigma_z\Psi_{\mathbf{k}})\cdot(\Psi^{\dagger}_{d}\sigma_z\Psi_{d})\\ &+ 2(\Psi^{\dagger}_{\mathbf{k}'}\sigma^{+}\Psi_{\mathbf{k}})(\Psi^{\dagger}_{d}\sigma^{-}\Psi_{d})\\ &+ 2(\Psi^{\dagger}_{\mathbf{k}'}\sigma^{-}\Psi_{\mathbf{k}})(\Psi^{\dagger}_{d}\sigma^{+}\Psi_{d})\\ = &\sum_{\sigma}[a^{\dagger}_{\mathbf{k}'\sigma}a_{\mathbf{k}\sigma}(n_{d\sigma} - n_{d-\sigma}) - 2\rho_{\mathbf{k}'d\sigma}\rho^{\dagger}_{\mathbf{k}d-\sigma}] \end{aligned} \quad (7.118)$$

is precisely of the form of the last term in Eq. (7.117). The resulting contribution to $\tilde{H}$ is

$$H_{\text{exch}} = -\frac{1}{\hbar^2}\sum_{\mathbf{k},\mathbf{k}'}J_{\mathbf{k}\mathbf{k}'}(\Psi^{\dagger}_{\mathbf{k}'}\mathbf{S}\Psi_{\mathbf{k}})\cdot(\Psi^{\dagger}_{d}\mathbf{S}\Psi_{d}), \quad (7.119)$$

where

$$J_{\mathbf{kk}'} = (B_{\mathbf{k}'}V_{\mathbf{k}d} + B^*_{\mathbf{k}}V_{\mathbf{k}'d})$$
$$= V_{\mathbf{k}'d}V_{\mathbf{k}d}\left[\frac{1}{\epsilon_{\mathbf{k}'} - (\epsilon_d + U)} + \frac{1}{\epsilon_{\mathbf{k}} - (\epsilon_d + U)} - \frac{1}{\epsilon_{\mathbf{k}} - \epsilon_d} - \frac{1}{\epsilon_{\mathbf{k}'} - \epsilon_d}\right]. \quad (7.120)$$

This term, which arises from the last term in Eq. (7.117), is the Kondo interaction term describing the spin-spin interaction between a conduction electron and an impurity spin. Note that this result is the form (7.10), deduced from second-order perturbation theory but symmetrized in $\mathbf{k}$ and $\mathbf{k}'$. We see here a particular advantage of the similarity transformation method; it generates correctly the interaction matrix elements when the initial and final states do not have the same energy. By contrast, we can identify the second-order scattering amplitude with the interaction matrix element only when the initial and final states have the same energy, in which case Eqs. (7.10) and (7.120) agree. In the vicinity of the Fermi level, $k, k' \sim k_F$, the spin-exchange amplitude reduces to

$$J_{k_F k_F} \equiv J_o = -2|V_{\mathbf{k}d}|^2 \frac{U}{|\epsilon_d|(|\epsilon_d| - U)} < 0, \quad (7.121)$$

as advertised.

All together we can write $\tilde{H}$ as

$$\tilde{H} = H_0 + \frac{1}{2}[S, H_1]$$
$$= H_0 + H_0' + H_0'' + H_{\mathrm{exch}} + H_{\mathrm{dir}} + H_{\mathrm{ch}}. \quad (7.122)$$

The direct term

$$H_{\mathrm{dir}} = \sum_{\mathbf{k},\mathbf{k}'} \frac{1}{4} J_{\mathbf{kk}'}(\Psi_d^\dagger \Psi_d)(\Psi_{\mathbf{k}'}^\dagger \Psi_{\mathbf{k}}) \quad (7.123)$$

results from the first term in Eq. (7.117). Here

$$W_{\mathbf{kk}'} = \frac{1}{2}(A_{\mathbf{k}'}V_{\mathbf{k}d} + A^*_{\mathbf{k}}V_{\mathbf{k}'d})$$
$$= \frac{1}{2}V_{\mathbf{k}'d}V^*_{\mathbf{k}d}\left[\frac{1}{\epsilon_{\mathbf{k}'} - \epsilon_d} + \frac{1}{\epsilon_{\mathbf{k}} - \epsilon_d}\right]. \quad (7.124)$$

The energy denominators occurring in $W_{\mathbf{kk}'}$ involve only the excitation process involving only the lowest state on the impurity, as shown in Fig. (7.2b), whereas $J_{\mathbf{kk}'}$ includes both processes in Fig. (7.2). Because $J_{\mathbf{kk}'}$ and $W_{\mathbf{k}'k}$ result from successive excitation and de-excitation processes, the impurity remains singly occupied in the process they describe.

The term

$$H_0' = -\sum_{\mathbf{k},\mathbf{k}'\sigma}\left(W_{\mathbf{kk}'} + \frac{1}{2}J_{\mathbf{kk}'}n_{d-\sigma}\right)n_{d\sigma}, \tag{7.125}$$

which emerges from the first term in Eq. (7.116), essentially renormalizes the coefficients in H_0. Similarly, the term

$$H_0'' = \sum_{\mathbf{k},\mathbf{k}'} W_{\mathbf{kk}'}\Psi_{\mathbf{k}}^\dagger\Psi_{\mathbf{k}'}, \tag{7.126}$$

which arises from the first term in Eq. (7.116) and the second term in Eq. (7.117), represents a renormalization of the potential felt by single electrons. Both H_0' and H_0'' are unimportant for understanding the Kondo problem. The final term

$$H_{\text{ch}} = -\frac{1}{2}\sum_{\mathbf{k},\mathbf{k}'\sigma}\left(B_{\mathbf{k}}V_{\mathbf{k}'d}\,\rho_{\mathbf{k}\sigma}\rho_{\mathbf{k}'-\sigma} + h.c.\right), \tag{7.127}$$

which arises from the third term in Eq. (7.116), changes the occupancy of the d-impurity by two and thus is also not important for the Kondo problem. The two important terms in the interaction are the spin-exchange process and the direct impurity-electron scattering term.

Let us isolate the terms that correspond to single occupancy on the impurity. We note first that, since H_{ch} eliminates both electrons on the d-impurity, it cannot connect to the one-electron states in the Hilbert space; we drop this term. In addition, in the one-electron subspace, $\Psi_d^\dagger\Psi_d = 1$. As a consequence, H_{dir} is a one-electron term, as are H_0' and H_0''. In this subspace, H_{exch} is the only important term. To second order in $V_{\mathbf{k}d}$, the Anderson model yields the Kondo model with an antiferromagnetic exchange coupling. It is the antiferromagnetic nature of this interaction that leads to condensation into a singlet state at the d-impurity.